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Some properties on the Q-Tensor system

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Abstract. We study the coupled Navier-Stokes and Q-Tensor system (analyzed in cf. [8] in the whole $\mathbb{R}^3$) in a bounded three-dimensional domain for several boundary conditions, rewriting the system in a way that properties as symmetry and null-trace for the tensor Q can be proved. We show some analytical results such as: the existence of global in time weak solution, a maximum principle for the Q-tensor, local in time strong solution (which is global assuming an additional regularity criterion for the velocity in the space-periodic boundary condition case), global in time strong solution imposing dominant viscosity (for the space-periodic or homogeneous Neumann boundary condition cases) and regularity criteria for uniqueness of weak solutions.

Keywords: Q-Tensor, Navier-Stokes equations, symmetry, weak solution, strong solution, uniqueness.

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§1. The model of Q-Tensor and main results

1.1. The model

Liquid crystals can be seen as an intermediate phase of matter between crystalline solids and isotropic fluids. Nematic liquid crystals (N) consist of molecules with rod-like shape whose center of mass is isotropically distributed and whose direction is almost constant on average over small regions. Several (N) are described through the velocity and pressure $(\boldsymbol{u}, p)$ and the director vector $\boldsymbol{d}$ (cf. [3]). However, the optic of the liquid crystals can be uniaxial (points have one single refractive index), biaxial (points have two indices of refraction) or isotropic (orientation of molecules is equally distributed in all directions). Only uniaxial liquid crystals can be described by the $(\boldsymbol{u}, p, \boldsymbol{d})$-systems. Isotropic regions within the liquid crystal material are also called "defect patterns".

The Q-Tensor model proposes a new formulation in order to describe the three types of optic for (N). The director vector field $\boldsymbol{d} \in \mathbb{R}^3$ is replaced by the tensor $Q \in \mathbb{R}^{3\times3}$, which is related to the second moment of a probability measure that describes the orientation of the molecules . Concretely (cf. [3]), Q is based on a probability measure $\mu(\boldsymbol{x}, \cdot) : \mathcal{L}(\mathbb{S}^2) \to [0, 1]$ for $\boldsymbol{x} \in \Omega$ that describe the orientation of the molecules, being $\mathcal{L}(\mathbb{S}^2)$ the family of Lebesgue measure sets on the unit sphere. In such a way, $\mu(\boldsymbol{x}, A)$ is the probability that the molecules with centre of mass in a very small neighborhood of the point $\boldsymbol{x} \in \Omega$ are pointing in a direction contained an $A \subset \mathbb{S}^2$. This probability must satisfy $\mu(\boldsymbol{x}, A) = \mu(\boldsymbol{x}, -A)$ in order to reproduce the "head-to-tail" symmetry. As a consequence the first moment of the probability measure vanishes, $\langle p\rangle = \int_{\mathbb{S}^2} p_i \, d\mu(p) = 0$, and the information on μ comes from the tensor of the second moment $M(\mu)_{ij} = \int_{\mathbb{S}^2} p_i \, p_j \, d\mu(p)$, $i, j = 1, 2, 3$. Is is easy to see that $M(\mu) = M(\mu)^t$ and $tr(M) = 1$. If the orientation of the molecules is equally distributed, then the distribution is isotropic and $\mu = \mu_0$, $d\mu_0(p) = \frac{1}{4\pi} \, dA$ and $M(\mu_0) = \frac{1}{3} \, Id$. The de Gennes order-parameter tensor Q measures the deviation of the second moment tensor from its isotropic value and is defined as:

$$Q = M(\mu) - M(\mu_0) = \int_{\mathbb{S}^2} \left(p \otimes p - \frac{1}{3} \, Id \right) d\mu(p) \tag{1.1}$$

Between the properties that definition (1.1) implies we have that Q is symmetric and traceless. These properties are assumed for the solution of the model studied by Paicu and Zarnescu in [8] (a more complete model is studied in [7]). However, they cannot be deduced from the model. Here, we revise the writing of the Q-tensor model maintaining the essential terms given in [8] but rewriting some of them appropriately to obtain the symmetry and traceless properties.

We shall study the following model (QT) for the unknowns $(\boldsymbol{u}, Q, p) : (0,T) \times \Omega \to \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times \mathbb{R}$, where the velocity and the pressure $(\boldsymbol{u}, p)$ verify:

$$\left\{ \begin{array}{rl} D_t \boldsymbol{u} - \nu \Delta \boldsymbol{u} + \nabla p = \nabla \cdot \tau(Q) + \nabla \cdot \sigma(H, Q) & \text{in } \Omega \times (0,T) \\ \nabla \cdot \boldsymbol{u} = 0 & \text{in } \Omega \times (0,T) \end{array} \right. \tag{1.2}$$

being $D_t = \partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u}$ the material derivative, $\nu > 0$ is the viscosity coefficient and the tensors $\tau = \tau(Q)$ and $\sigma = \sigma(H, Q)$ are defined by

$$\left\{ \begin{array}{rcl} \tau_{ij}(Q) & = & -\varepsilon \left(\partial_j Q : \partial_i Q \right) = -\varepsilon \, \partial_j Q_{kl} \, \partial_i Q_{kl}, \ \varepsilon > 0 \quad \text{(symmetric tensor)} \\ \sigma(H, Q) & = & H \, Q - Q \, H \quad \text{(antisymmetric tensor if } Q \text{ and } H \text{ are symmetric)} \end{array} \right.$$

with $H = H(Q) = -\varepsilon \, \Delta Q + f(Q)$ for

$$f(Q) = a \, Q - \frac{b}{3} \left(Q^2 + Q Q^t + Q^t Q \right) + c \, |Q|^2 \, Q \quad \text{with } c > 0, \, a, b \in \mathbb{R},$$

where we denote by $Q : Q = |Q|^2$ the matricial euclidean norm. The tensor is governed by the system:

$$D_t Q - S(\nabla \boldsymbol{u}, Q) = -\gamma \, H(Q) \quad \text{in } \Omega \times (0,T) \tag{1.3}$$

where $S(\nabla \boldsymbol{u}, Q) = \nabla \boldsymbol{u} \, Q^t - Q^t \, \nabla \boldsymbol{u}$ (called the stretching term), $\gamma > 0$ is a material-dependent elastic constant. The tensor H is the variational derivative in $L^2(\Omega)$ of a free energy functional $\mathcal{E}(Q)$, i.e.

$$H = \frac{\delta \mathcal{E}(Q)}{\delta Q}, \qquad \mathcal{E}(Q) = \frac{\varepsilon}{2} |\nabla Q|^2 + F(Q)$$

where function $F(Q)$ is defined as

$$F(Q) = \frac{a}{2} \, |Q|^2 - \frac{b}{3} \, (Q^2 : Q) + \frac{c}{4} \, |Q|^4 \tag{1.4}$$

Note that $F(Q)$ is not a convex function (excepting the case $a > 0$ and $b = 0$) but its more nonlinear part $\frac{c}{4}|Q|^4$ is convex and $F(Q) \to +\infty$ as $|Q| \to +\infty$.

Finally, we are going to close the system with the following initial and boundary conditions over $\Gamma = \partial\Omega$:

$$\boldsymbol{u}|_{t=0} = \boldsymbol{u}_0, \quad Q|_{t=0} = Q_0 \quad \text{in } \Omega, \tag{1.5}$$

$$\boldsymbol{u}|_\Gamma = \boldsymbol{0} \quad \text{and} \quad \partial_{\boldsymbol{n}} Q|_\Gamma = 0 \quad \text{or} \quad Q|_\Gamma = Q_\Gamma \quad \text{or } (\boldsymbol{u}, Q) \text{ space-periodic} \quad \text{in } (0, T). \tag{1.6}$$

In the present work we want to study several questions related to the existence, uniqueness and regularity for the Q-tensor. In the next subsection, the main results will be stated. The proofs will be sketched in the following sections: In Section 2, we will obtain an energy law and prove the existence of weak solution (Theorem 1). A maximum principle will be obtained in Subsection 2.3 (proof of Lemma 2). In Section 3, the proofs of Theorem 3 and Theorem 4 will be sketched. A weak/strong uniqueness is proved in Section 4 (Theorem 5). A modification of (1.2)-(1.3) implying traceless and symmetry for Q will be deduced in Subsections 5.1 and 5.2. The existence of solution, regularity and uniqueness for the modified model is quickly analyzed in Subsection 5.3.

1.2. The main results

The precise results on existence, regularity and uniqueness of solution for (1.2)-(1.3) can be seen below:

Theorem 1 (**Weak solution).** *Assuming* $(\boldsymbol{u}_0, Q_0) \in \boldsymbol{L}^2(\Omega) \times \boldsymbol{H}^1(\Omega)$ *with* $\nabla \cdot \boldsymbol{u}_0 = 0$ *and* $\boldsymbol{u}_0 \cdot \boldsymbol{n}|_\Gamma = 0$. *Then, there exists a weak solution* $(\boldsymbol{u}, Q)$ *of the system (1.2)-(1.3)-(1.5)-(1.6) in the sense of Definition 1 (see Subsection 2.1).*

The maximum principle will play an important role in most of the following results.

Lemma 2 (**Maximum principle).** *For a given real positive number* α *big enough and depending on the coefficients* (a, b, c) *of the function* $f(Q)$ *such that* $\alpha^2 \geq \frac{b^2}{c^2} - \frac{2a}{c}$, *a function* $\boldsymbol{u} \in L^2(0, T; \mathbf{V}) \cap L^\infty(0, T; \boldsymbol{H})$ *(*$0 < T \leq +\infty$*) and* $Q_0 \in \boldsymbol{H}^1(\Omega)$ *. Let* Q *be any solution for the* Q*-problem, i.e.* $Q \in L^\infty(0, T; \boldsymbol{H}^1(\Omega)) \cap L^2(0, T; \boldsymbol{H}^2(\Omega))$ *satisfying (1.3). If* $|Q_0| \leq \alpha$ *a. e. in* Ω *(and* $Q|_\Gamma = Q_\Gamma$ *with* $|Q_\Gamma| \leq \alpha$ *a. e. on* Γ *in the Dirichlet boundary case), then,* $|Q(\boldsymbol{x}, t)| \leq \alpha$ *a.e. in* $\Omega \times (0, T)$.

Next two results are related to strong solution for the system (i. e. weak solution with the additional regularity (3.1), see Section 3 below). The first one is only possible in the space-periodic case because in the Dirichlet and Neumann cases some boundary integral terms do not vanish and cannot be controlled with strong norms.

Theorem 3 (**Regularity criteria in velocity for space-periodic boundary conditions).** *Assuming* $(\boldsymbol{u}_0, Q_0) \in \boldsymbol{H}^1(\Omega) \times \boldsymbol{H}^2(\Omega)$ *with* $\nabla \cdot \boldsymbol{u}_0 = 0$ *and space-periodic boundary conditions for* $(\boldsymbol{u}, Q)$. *Let* $(\boldsymbol{u}, Q)$ *be a weak solution of the Q-Tensor system (1.2)-(1.3) in* $(0, T)$ *and* $\nabla \boldsymbol{u}$ *has the additional regularity* $\nabla \boldsymbol{u} \in L^2(0, T; \boldsymbol{L}^3(\Omega))$. *Then,* $(\boldsymbol{u}, Q)$ *is the unique strong solution of the system in* $(0, T)$. *On the other hand, without assuming the additional regularity, one has the local in time strong regularity.*

Theorem 4 (Global in time strong solution with big viscosity). *Assuming* $(\boldsymbol{u}_0, Q_0) \in \boldsymbol{H}_0^1(\Omega) \times \boldsymbol{H}^2(\Omega)$ *with* $\nabla \cdot \boldsymbol{u}_0 = 0$ *and homogeneous Neumann for Q or space-periodic boundary conditions for* $(\boldsymbol{u}, Q)$*. Let* $(\boldsymbol{u}, Q)$ *be a weak solution of the Q-Tensor system (1.2)-(1.3) in* $(0, T)$*. Imposing* $\nu > 0$ *a big enough viscosity for (1.2), then,* $(\boldsymbol{u}, Q)$ *is the unique strong solution of the system in* $(0, T)$*.*

Remark 1. The Dirichlet boundary condition case for $(\boldsymbol{u}, Q)$ is treated in [5].

Next uniqueness result improves the regularity criteria appearing in [10] (for the nematic liquid crystal model with stretching terms), and moreover it does not use the maximum principle in the proof.

Theorem 5 (Regularity criteria for uniqueness). *Assuming* $(\boldsymbol{u}_0, Q_0) \in \boldsymbol{L}^2(\Omega) \times \boldsymbol{H}^1(\Omega)$ *with* $\nabla \cdot \boldsymbol{u}_0 = 0$ *and* $\boldsymbol{u}_0 \cdot \boldsymbol{n}|_\Gamma = 0$*. Let* $(\boldsymbol{u}, Q)$ *be a weak solution of the Q-Tensor system (1.2)-(1.3)-(1.5)-(1.6) in* $(0, T)$ *such that* $\nabla \boldsymbol{u}$ *has the additional regularity* $\nabla \boldsymbol{u} \in L^2(0, T; \boldsymbol{L}^3(\Omega))$ *and* ΔQ *has the additional regularity* $\Delta Q \in L^4(0, T; \boldsymbol{L}^2(\Omega))$*. Then, this solution coincides in* $(0, T)$ *with any weak solution associated to the same data.*

§2. Existence of weak solution

2.1. Variational formulation

Taking into account that $\partial_i F(Q) = F'(Q) : \partial_i Q = f(Q) : \partial_i Q$, the symmetric tensor can be rewritten as:

$$
\begin{aligned}
(\nabla \cdot \tau)_i &= -\varepsilon\, \partial_j \Big(\partial_j Q : \partial_i Q\Big) = -\varepsilon\, \Delta Q : \partial_i Q - \varepsilon \partial_j Q : \partial^2_{ij} Q \\
&= H(Q) : \partial_i Q - \partial_i \Big(F(Q) + \frac{\varepsilon}{2} |\nabla Q|^2\Big),
\end{aligned}
\tag{2.1}
$$

where $|\nabla Q|^2 = \partial_j Q : \partial_j Q$. Then, testing (1.2) by $(\bar{\boldsymbol{u}}, \bar{p})$, we arrive at the following variational formulation of (1.2):

$$
\left\{
\begin{aligned}
&(D_t \boldsymbol{u}, \bar{\boldsymbol{u}}) + \nu(\nabla \boldsymbol{u}, \nabla \bar{\boldsymbol{u}}) - (q, \nabla \cdot \bar{\boldsymbol{u}}) - ((\bar{\boldsymbol{u}} \cdot \nabla) Q, H) + (\sigma(H, Q), \nabla \bar{\boldsymbol{u}}) = 0, \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall \bar{\boldsymbol{u}} \text{ with } \bar{\boldsymbol{u}}|_{\partial\Omega} = \boldsymbol{0} \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (\nabla \cdot \boldsymbol{u}, \bar{p}) = 0, \qquad \forall \bar{p}
\end{aligned}
\right.
\tag{2.2}
$$

where $q = p + F(Q) + \dfrac{\varepsilon}{2} |\nabla Q|^2$ is a new solenoidal function (including the pressure).

In which follows, it will be of great help the following Lemma:

Lemma 6. *For any A, B, C* $\in \mathcal{M}(\mathbb{R}^{n \times n})$*, the following identity holds:*

$$
AB : C = B : A^t C \quad \text{and} \quad A : BC = AC^t : B. \tag{2.3}
$$

Using Lemma 6, we obtain that $S(\nabla \boldsymbol{u}, Q) : \bar{H} = \sigma(\bar{H}, Q) : \nabla \boldsymbol{u}$. Indeed,

$$
S(\nabla \boldsymbol{u}, Q) : \bar{H} \;=\; (\nabla \boldsymbol{u}\, Q^t - Q^t\, \nabla \boldsymbol{u}) : \bar{H} = \nabla \boldsymbol{u} : \bar{H} Q - \nabla \boldsymbol{u} : Q \bar{H} = \nabla \boldsymbol{u} : \sigma(\bar{H}, Q)
$$

Therefore, testing (1.3) by $\bar{H}$ and $-\varepsilon\,\Delta Q + f(Q) = H$ by $\bar{Q}$, we arrive at the following variational formulation of (1.3):

$$\left\{ \begin{array}{rcl} (\partial_t Q, \bar{H}) + (\boldsymbol{u}\cdot\nabla Q, \bar{H}) - (\nabla \boldsymbol{u}, \sigma(\bar{H}, Q)) + \gamma\,(H, \bar{H}) & = & 0 \\ \varepsilon\,(\nabla Q, \nabla \bar{Q}) + (f(Q), \bar{Q}) - (H, \bar{Q}) & = & 0 \end{array} \right. \tag{2.4}$$

Definition 1 (Weak solution)**.** Considering the initial data $(\boldsymbol{u}_0, Q_0) \in \boldsymbol{L}^2(\Omega) \times \boldsymbol{H}^1(\Omega)$ with $\nabla\cdot\boldsymbol{u}_0 = 0$ and $\boldsymbol{u}_0\cdot\boldsymbol{n}|_{\partial\Omega} = 0$, we say that $(\boldsymbol{u}, Q)$ is a weak solution of the system (1.2)-(1.3) if:

$$\begin{array}{rcl} \boldsymbol{u} & \in & L^\infty(0,T;\boldsymbol{L}^2(\Omega)) \cap L^2(0;T;\boldsymbol{H}^1(\Omega)) \\ Q & \in & L^\infty(0,T;\boldsymbol{H}^1(\Omega)) \cap L^2(0;T;\boldsymbol{H}^2(\Omega)) \end{array}$$

and satisfies (2.2) and (2.4).

2.2. Energy law

For a rigorous justification of the existence of a weak solution see [4]. Considering space-periodic, homogeneous Neumann or stationary non-homogeneous Dirichlet boundary conditions, we can obtain:

$$\begin{array}{rcl} (\partial_t Q, H) & = & (\partial_t Q, -\varepsilon\Delta Q + f(Q)) = \varepsilon(\nabla(\partial_t Q), \nabla Q) + (\partial_t Q, F'(Q)) \\ & = & \dfrac{d}{dt}\left(\dfrac{\varepsilon}{2}\,\|\nabla Q\|^2_{L^2(\Omega} + \displaystyle\int_\Omega F(Q)\,d\boldsymbol{x}\right) = \dfrac{d}{dt}\displaystyle\int_\Omega \mathcal{E}(Q)\,d\boldsymbol{x}. \end{array}$$

Thus, taking $(\bar{\boldsymbol{u}}, \bar{p}) = (\boldsymbol{u}, p)$ in (2.2) and $(\bar{H}, \bar{Q}) = (H, \partial_t Q)$ in (2.4), the following “energy equality" holds:

$$\frac{d}{dt}\left(\frac{1}{2}\|\boldsymbol{u}\|^2_{L^2(\Omega)} + \int_\Omega \mathcal{E}(Q)\,d\boldsymbol{x}\right) + \nu\|\nabla\boldsymbol{u}\|^2_{L^2(\Omega)} + \gamma\|H\|^2_{L^2(\Omega)} \quad = \quad 0. \tag{2.5}$$

The obtaining of regularity bounds for $(\boldsymbol{u}, Q)$ cannot be directly obtained because of $\int_\Omega \mathcal{E}(Q)\,d\boldsymbol{x}$ is not a positive term due to $F(Q)$. But, we can define $F_\mu(Q) = F(Q) + \mu$ with $\mu = \mu(a, b, c)$ big enough (see [4]) in such a way that:

$$F_\mu(Q) \geq \frac{c}{8}\,|Q|^4 \geq 0 \tag{2.6}$$

Therefore, replacing $\mathcal{E}(Q)$ by $\mathcal{E}_\mu(Q) = \dfrac{1}{2}|\nabla Q|^2 + F_\mu(Q) \geq 0$ in (2.5), we can obtain some estimates until infinite time. Indeed, assuming finite total energy of initial data, i.e.

$$\int_\Omega \mathcal{E}_\mu(Q_0)\,d\boldsymbol{x} + \frac{1}{2}\|\boldsymbol{u}_0\|^2_{L^2(\Omega)} < +\infty,$$

(the boundeness of Ω, $|\Omega| < +\infty$, is here essential due to $\displaystyle\int_\Omega F_\mu(Q_0)\,d\boldsymbol{x} = \int_\Omega F(Q_0)\,d\boldsymbol{x} + \mu|\Omega|$), then the following estimates hold:

$$\left\{\begin{array}{rcl} \boldsymbol{u} & \in & L^\infty(0,+\infty;\boldsymbol{L}^2(\Omega)) \cap L^2(0,+\infty;\mathbf{H}^1(\Omega)), \\ \nabla Q & \in & L^\infty(0,+\infty;\boldsymbol{L}^2(\Omega)) \\ H & \in & L^2(0,+\infty;\boldsymbol{L}^2(\Omega)) \\ F_\mu(Q) & \in & L^\infty(0,+\infty;L^1(\Omega)) \end{array}\right. \tag{2.7}$$

In particular, from (2.6) and (2.7), we deduce:

$$Q \in L^\infty(0,+\infty;\boldsymbol{L}^4(\Omega)), \quad Q \in L^\infty(0,+\infty;\boldsymbol{H}^1(\Omega)) \hookrightarrow L^\infty(0,+\infty;\boldsymbol{L}^6(\Omega)) \tag{2.8}$$

In order to finish the deduction of regularity for ΔQ, we remark that $H(Q) = -\varepsilon\Delta Q + f(Q)$ and:

$$|f(Q)| \quad \le \quad C(a,b,c)\left(|Q| + |Q|^2 + |Q|^3\right)$$

which together with (2.8):

$$f(Q) \in L^\infty(0,+\infty;\boldsymbol{L}^2(\Omega)) \quad \Rightarrow \quad \Delta Q \in L^\infty(0+\infty;\boldsymbol{L}^2(\Omega)) + L^2(0,+\infty;\boldsymbol{L}^2(\Omega)).$$

Thus, for any finite time $T > 0$, we have that:

$$Q \in L^2(0,T;\boldsymbol{H}^2(\Omega)) \quad \forall T > 0.$$

Remark 2. The regularity for $\partial_t Q$ can be obtained taking into account the regularity for the remaining terms appearing in the model (1.3). Concretely, we can get:

$$\partial_t Q \in L^{4/3}(0,T;\boldsymbol{L}^2(\Omega)) \tag{2.9}$$

Remark 3. Finally, in the case of time-dependent nonhomogeneous Dirichlet boundary conditions for Q, we need to lift the boundary data. Using the following "elliptic" lifting function

$$-\Delta\widetilde{Q}(t) = \mathbf{0} \quad \text{in } \Omega, \quad \widetilde{Q}(t) = Q_\Gamma(t) \quad \text{on } \Gamma$$

instead of (2.5) a modified energy equality holds for $\widehat{Q} = Q - \widetilde{Q}$, where some terms depending on $\partial_t\widetilde{Q}$ appear on the right hand side of (2.5).

2.3. A maximum principle

Considering the inner product of the Q-system by Q and taking into account that the stretching terms vanish, we can obtain:

$$\partial_t\left(|Q|^2-\alpha^2\right) + \boldsymbol{u}\cdot\nabla\left(|Q|^2-\alpha^2\right) - \gamma\,\varepsilon\,\Delta\left(|Q|^2-\alpha^2\right) + 2\,\gamma\, f(Q) : Q \le 0 \quad \text{in } \Omega\times(0,+\infty) \tag{2.10}$$

Testing (2.10) by $\psi(Q) := (|Q|^2-\alpha^2)_+$ and integrating in Ω, we obtain:

$$\frac{d}{dt}\|\psi(Q)\|^2_{L^2(\Omega)} + \gamma\,\varepsilon\|\nabla\psi(Q)\|^2_{L^2(\Omega)} - \gamma\,\varepsilon\int_\Gamma \partial_{\boldsymbol{n}}\psi(Q)\,\psi(Q)\,d\sigma + 2\gamma\int_\Omega (f(Q):Q)\,\psi(Q)\,d\boldsymbol{x} \le 0 \tag{2.11}$$

because the boundary term $-\gamma\,\varepsilon \int_\Gamma \partial_{\boldsymbol{n}}\psi(Q)\,\psi(Q)\,d\sigma$ vanishes. Note that in the case of Dirichlet boundary condition $Q|_\Gamma = Q_\Gamma$ one has $\psi(Q)|_\Gamma = \mathbf{0}$ (because $|Q_\Gamma| \le \alpha$) and the case of Neumann boundary condition $\partial_{\boldsymbol{n}}Q|_\Gamma = 0$ one has $\partial_{\boldsymbol{n}}\psi(Q)|_\Gamma = 0$. Therefore, in both cases the boundary integral term of (2.11) vanishes. An easy treatment of the potential term $f(Q)$ leads to:

$$\|\psi(Q(t))\|^2_{L^2(\Omega)} \le \|\psi(Q_0)\|^2_{L^2(\Omega)} = \|\left(|Q_0|^2 - \alpha^2\right)_+\|^2_{L^2(\Omega)} = 0,$$

hence the Maximum's Principle $\|Q(t)\|_{L^\infty} \le \alpha$ in $(0,+\infty)$ is deduced.

§3. Strong regularity

In this section, we will see some regularity results about the generic model for the Q-Tensor system without necessarily imposing the restrictions of symmetry and traceless.

We want to prove some results associated to the existence of a strong solution for (1.2)-(1.3), which is already a weak solution in the sense of Definition 1 that also verified the stronger regularity:

$$\boldsymbol{u} \in L^\infty(0,T;\boldsymbol{H}^1_0(\Omega)) \cap L^2(0,T;\boldsymbol{H}^2(\Omega)), \quad Q \in L^\infty(0,T;\boldsymbol{H}^2(\Omega)) \cap L^2(0,T;\boldsymbol{H}^3(\Omega)) \quad (3.1)$$

3.1. Space-periodic or homogeneous Neumann boundary conditions

We multiply (1.2) by $A\boldsymbol{u}$ and (1.3) by $-\Delta H$, obtaining:

$$(\nabla(\partial_t Q), \nabla H) + (\nabla(\boldsymbol{u}\cdot\nabla Q), \nabla H) - (\nabla S(\nabla\boldsymbol{u}, Q), \nabla H) + \gamma\|\nabla H\|^2_{L^2(\Omega)} = 0 \quad (3.2)$$

and

$$\frac{1}{2}\frac{d}{dt}\|\nabla\boldsymbol{u}\|^2_{L^2(\Omega)} + \nu\|A\boldsymbol{u}\|^2_{L^2(\Omega)} + (\boldsymbol{u}\cdot\nabla\boldsymbol{u}, A\boldsymbol{u}) - (A\boldsymbol{u}\cdot\nabla Q, H) + (\sigma(H,Q), \nabla(A\boldsymbol{u})) = 0 \quad (3.3)$$

First, we analyze the terms presenting more difficulties to be treat. One of them is:

$$(\nabla\partial_t Q, \nabla H) = \frac{1}{2\varepsilon}\frac{d}{dt}\|H\|^2_{L^2(\Omega)} - (\partial_t(f(Q)), H) + \varepsilon\int_\Gamma \partial_{\boldsymbol{n}}(\partial_t Q)\,H\,d\sigma \quad (3.4)$$

that needs to impose homogeneous Neumann boundary conditions $\partial_{\boldsymbol{n}}Q|_{\partial\Omega} = \mathbf{0}$ or space-periodic boundary conditions.

Remark 4. In the non-homogeneous Dirichlet boundary case, the boundary term in (3.4) does not vanish because $H|_\Gamma \ne \mathbf{0}$ due to the stretching term in (1.3).

In a second step, we try to control the terms $-(\nabla S(\nabla\boldsymbol{u}, Q), \nabla H) + (\sigma(H,Q), \nabla(A\boldsymbol{u}))$. On the basis that

$$S(\nabla(\Delta\boldsymbol{u}), Q) : H = \sigma(H,Q) : \nabla(\Delta\boldsymbol{u}) \quad (3.5)$$

we would like to apply:

$$-(\nabla S(\nabla\boldsymbol{u}, Q), \nabla H) = (\Delta S(\nabla\boldsymbol{u}, Q), H) - \int_\Gamma \partial_{\boldsymbol{n}} S(\nabla\boldsymbol{u}, Q)\,H\,d\sigma$$

where, since $S(\cdot,\cdot)$ is quadratic,

$$\Delta S(\nabla\boldsymbol{u}, Q) = S(\nabla(\Delta\boldsymbol{u}), Q) + 2S(\nabla(\nabla\boldsymbol{u}), \nabla Q) + S(\nabla\boldsymbol{u}, \Delta Q).$$

3.2. Sketch of the proof of Theorem 3

If the boundary term $-\int_\Gamma \partial_{\boldsymbol{n}} S(\nabla \boldsymbol{u}, Q)\, H\, d\sigma$ disappear (as for the space-periodic boundary conditions), some of the terms will vanish using (3.5) and the fact that for space-periodic boundary conditions $-\Delta \boldsymbol{u} = A\boldsymbol{u}$ holds. The remaining terms will have one of the following forms:

$$J_1 = \int_\Omega |D^2\boldsymbol{u}||\nabla Q||H|\, d\boldsymbol{x}, \quad J_2 = \int_\Omega |\nabla \boldsymbol{u}||\Delta Q||H|\, d\boldsymbol{x}, \quad J_3 = \int_\Omega |\nabla \boldsymbol{u}||\nabla Q||\nabla H|\, d\boldsymbol{x},$$

$$J_4 = \int_\Omega |\boldsymbol{u}||\nabla \boldsymbol{u}||A\boldsymbol{u}|\, d\boldsymbol{x}, \quad J_5 = \int_\Omega |\boldsymbol{u}||\Delta Q||\nabla H|\, d\boldsymbol{x} \quad J_6 = \int_\Omega |\boldsymbol{u}||\nabla Q||\Delta Q|\, d\boldsymbol{x}$$

In summary, if the boundary term

$$-\int_\Gamma \partial_{\boldsymbol{n}} S(\nabla \boldsymbol{u}, Q)\, H\, d\sigma \tag{3.6}$$

vanishes, adequate estimates can be obtained for the J_i-terms, $i = 1, \dots, 6$ (they were also obtained by the authors cf. [2] and by Sun & Liu (cf. [9]). These estimates can be made in two ways: one to obtain local in time strong estimates for $(\boldsymbol{u}, Q)$, and another one to obtain global in time strong estimates for $(\boldsymbol{u}, Q)$ supposing additional regularity hypothesis over $\nabla \boldsymbol{u}$ and ∇Q.

In fact, calling $y(t) = \|H(t)\|^2_{L^2(\Omega)} + \|\nabla \boldsymbol{u}(t)\|^2_{L^2(\Omega)}$ and $Y(t) = \gamma \|\nabla H(t)\|^2_{L^2(\Omega)} + \nu \|A\boldsymbol{u}(t)\|^2_{L^2(\Omega)}$, we obtain (see cf. [4, 5],):

- looking for a local in time strong solution, an estimate of kind:

$$y'(t) + Y(t) \le C\left(y(t)^3 + y(t) + 1\right) \tag{3.7}$$

- looking for a global in time strong solution, assuming additional regularity hypothesis, we get:

$$y'(t) + Y(t) \le a(t)\, y(t) + b(t) \tag{3.8}$$

  for $a \in L^1(0,T)$ a function described in terms of the additional regularity hypothesis:

$$\nabla \boldsymbol{u} \in L^2(0,T; \boldsymbol{L}^3(\Omega)) \quad \text{and} \quad \nabla Q \in L^4(0,T; \boldsymbol{L}^6(\Omega)). \tag{3.9}$$

Remark 5 (**Non-Hilbertian regularity for** ∇Q). We can argue as in the study for the Nematic Liquid Crystal model (without stretching term) with periodic boundary conditions given in [6]. Taking $-\nabla\cdot\left(|\nabla Q|^{p-2}\nabla Q\right)$ as test function in (1.3), splitting $f(Q)$ in two parts:

$$f(Q) = F_c'(Q) + F_e'(Q)$$

and considering space-periodic or homogeneous Neumann boundary conditions, we get:

$$\begin{aligned}
\frac{2}{p}\frac{d}{dt}\|\nabla Q\|^p_{L^p(\Omega)} \quad &+ \quad \gamma\,\varepsilon \int_\Omega |D^2 Q|^2 |\nabla Q|^{p-2}\, d\boldsymbol{x} + \gamma\,\varepsilon\,(p-2)\left(\frac{2}{p}\right)^2 \|\nabla(|\nabla Q|^{p/2})\|^2_{L^2(\Omega)} \\
&+ \quad c\,\gamma \int_\Omega \left[|Q|^2|\nabla Q|^p + 2\,|\nabla Q|^{p-2}\,(Q : \nabla Q)^2\right] d\boldsymbol{x} \\
&\le \quad C_{\gamma,\varepsilon}\left(\|\nabla \boldsymbol{u}\|^{\frac{2q}{2q-3}}_{L^q(\Omega)}\|\nabla Q\|^p_{L^p(\Omega)} + \|\nabla Q\|^p_{L^p(\Omega)}\|\nabla \boldsymbol{u}\|^{\frac{2q}{2q-3}}_{L^q(\Omega)} + \|\nabla \boldsymbol{u}\|^{\frac{q(p-1)}{2q-3}}_{L^q(\Omega)}\right)
\end{aligned}$$

where an explicit study for the boundary terms appearing shows that they can also vanish for homogeneous Neumann boundary conditions. Since $\frac{q(p-1)}{2q-3} \le \frac{2q}{2q-3}$ if and only if $p \le 3$, only assuming the additional regularity hypothesis for $\nabla \boldsymbol{u}$ of (3.9) in particular we obtain non-Hilbertian regularity for ∇Q when $p = 3$, that is,

$$\nabla Q \in L^\infty(0, T; \boldsymbol{L}^3(\Omega)) \cap L^3(0, T; \mathbf{L}^9(\Omega)).$$

Hence, $\nabla Q \in L^4(0, T; \boldsymbol{L}^6(\Omega))$.

Inequalities (3.7) and (3.8), together with Remark 5 allow to prove Theorem 3.

3.3. Ideas for the proof of Theorem 4

However, the conclusion for the system, supposing homogeneous Neumann boundary conditions for Q cannot be assure because we do not know how to vanish (3.6). An alternative way needs to estimate directly the terms $-(\nabla S(\nabla \boldsymbol{u}, Q), \nabla H) - (\nabla \cdot \sigma(H, Q), A\boldsymbol{u})$. This time, instead of obtaining terms of type J_1 and J_2, we obtain terms as follows:

$$J_6 = \int_\Omega |D^2 \boldsymbol{u}||Q||\nabla H| \, d\boldsymbol{x}$$

which can be bounded as:

$$J_6 \quad \le \quad C \, \|A\boldsymbol{u}\|_{L^2(\Omega)} \|Q\|_{L^\infty(\Omega)} \|\nabla H\|_{L^2(\Omega)} \tag{3.10}$$

Observe that in any case we need to impose the following condition in order to guarantee the existence of strong solution for the model:

$$\nu > \frac{2}{\gamma} \|Q\|^2_{L^\infty(\Omega)} \tag{3.11}$$

which can be obtained assuming the viscosity ν is big enough (arriving to the conclusion of Theorem 4). Similar estimates can be also seen in [1] (without stretching terms) and in [10] (with stretching terms) for the nematic model.

§4. Regularity criterion for the uniqueness of the model

In order to obtain a regularity criterion for the uniqueness of the weak solution (in energy norms), we decompose the term $H(Q)$ in the following way:

$$H(Q) = -\varepsilon \Delta Q + F_c'(Q) + F_e'(Q) := H_c(Q) + F_e'(Q) \tag{4.1}$$

with $F_c(Q) = \dfrac{c}{4} |Q|^4$ the convex part of $F(Q)$ and $F_e(Q) = \dfrac{a}{2} |Q|^2 - \dfrac{b}{3} (Q^2 : Q)$ the non-convex part.

Let $(\mathbf{u}_1, q_1, Q_1, H_c(Q_1))$, $(\mathbf{u}_2, q_2, Q_2, H_c(Q_2))$ be two solutions of the problem (1.2)-(1.3) (recall that $(H_c)_i = -\varepsilon \Delta Q_i + F_c'(Q_i)$), and $\mathbf{u} = \mathbf{u}_1 - \mathbf{u}_2$, $q = q_1 - q_2$, $Q = Q_1 - Q_2$, $H_c = H_c(Q_1) - H_c(Q_2)$. Using decomposition for H given in (4.1), taking into account that $H =$

$H(Q_1) - H(Q_2)$ can be decomposed as $H = -\varepsilon\,\Delta Q + F'_c(Q_1) - F'_c(Q_2) + F'_e(Q_1) - F'_e(Q_2) = H_c + F'_e(Q_1) - F'_e(Q_2))$, and (2.1), then $(\mathbf{u}, q, Q, H_c)$ is the solution of the following problem in $\Omega \times (0, T)$:

$$\left\{\begin{array}{rcl} \partial_t \mathbf{u} & - & \nu\Delta\mathbf{u} + \nabla q + \mathbf{u}_1 \cdot \nabla\mathbf{u} - (H_c : \partial_i Q_1)_i - \nabla\cdot\sigma(Q_1, H_c) \\ & = & -\mathbf{u}\cdot\nabla\mathbf{u}_2 + \left((F'_e(Q_1) - F'_e(Q_2) : \partial_i Q_1\right)_i + (H(Q_2) : \partial_i Q)_i \\ & + & \nabla\cdot\sigma(Q_1, F'_e(Q_1) - F'_e(Q_2)) + \nabla\cdot\sigma(Q, H(Q_2)) \\ \nabla\cdot\mathbf{u} & = & 0 \\ \partial_t Q & + & \gamma\, H_c + (\mathbf{u}\cdot\nabla)Q_1 - S(\nabla\mathbf{u}, Q_1) \\ & = & -(\mathbf{u}_2\cdot\nabla)Q - \gamma\,(F'_e(Q_1) - F'_e(Q_2)) + S(\nabla\mathbf{u}_2, Q) \\ -\varepsilon\,\Delta Q & + & F'_c(Q_1) - F'_c(Q_2) = H_c \end{array}\right. \tag{4.2}$$

Taking $(\mathbf{u}, q)$ as test function in $(4.2)_{1-2}$, H_c as test function in $(4.2)_3$ and Q_t as test function in $(4.2)_4$, the following terms cancel (like obtaining the energy law):

$$(\mathbf{u}_1\cdot\nabla\mathbf{u}, \mathbf{u}) = 0, \quad -(H_c : \partial_i Q_1, \mathbf{u}_i) + (\mathbf{u}\cdot\nabla Q_1, H_c) = 0,$$

$$(\sigma(Q_1, H_c), \nabla\mathbf{u}) - (S(\nabla\mathbf{u}, Q_1), H_c) = 0 \tag{4.3}$$

A care treatment of the terms, specially those containing time-derivatives, leads to:

$$\begin{array}{c} \dfrac{1}{2}\dfrac{d}{dt}\left(\|\mathbf{u}\|^2_{L^2(\Omega)} + \varepsilon\,\|Q\|^2_{H^1(\Omega)} + c\,\displaystyle\int_\Omega \left[2\,(R : Q)^2 + |R|^2\,|Q|^2\right]\,d\mathbf{x}\right) \\ +\nu\|\nabla\mathbf{u}\|^2_{L^2(\Omega)} + \gamma\|H_c\|^2_{L^2(\Omega)} \leq C(t)\,\left(\|\mathbf{u}\|^2_{L^2(\Omega)} + \|Q\|^2_{H^1(\Omega)}\right) \end{array} \tag{4.4}$$

with $C \in L^2(0, T)$ having the form:

$$C(t) = C\,\left(\|\nabla\mathbf{u}_2\|^2_{L^3(\Omega)} + \|\mathbf{u}_2\|^2_{L^3(\Omega)} + \|\nabla Q_1\|^2_{L^3(\Omega)} + \|H(Q_2)\|^4_{L^2(\Omega)} + \|R_t\|_{L^{3/2}(\Omega)}\right) \tag{4.5}$$

where $R \in (Q_1, Q_2)$, using the weak regularity of $(\mathbf{u}, Q)$, we need to impose the following additional hypothesis to guarantee that $C(t) \in L^1(0, T)$, which are:

$$\nabla\mathbf{u}_2 \in L^2(0, T; \boldsymbol{L}^3(\Omega)), \quad H(Q_2) \in L^4(0, T; \boldsymbol{L}^2(\Omega)) \tag{4.6}$$

(thanks to (2.9), we have $R_t \in L^{4/3}(0, T; \boldsymbol{L}^2(\Omega))$). Taking into account that:

$$H(Q_2) = -\varepsilon\Delta Q_2 + f(Q_2),$$

the fact that $Q_2 \in L^\infty(0, T; \boldsymbol{H}^1(\Omega))$, the additional regularity $H(Q_2) \in L^4(0, T; \boldsymbol{L}^2(\Omega))$ reduces to:

$$\Delta Q_2 \in L^4(0, T; \boldsymbol{L}^2(\Omega)).$$

§5. How to enforce the symmetry and traceless properties of Q

The traceless and symmetry for the model supposed by Paicu and Zarnescu in [7, 8] and necessary for the description of Q (see Subsection 1.1) need to be inherent to the model. Here, we slightly reformulate equation (1.3) in this way.

5.1. Rewriting H to obtain traceless of Q

We will use a modified expression from H that is written as:

$$\widetilde{H} = H + \alpha(Q)\, I \tag{5.1}$$

that allows to obtain $tr(Q) = 0$ for a certain scalar function $\alpha(Q)$ that we will choose below. Observe that $tr(S(\nabla \boldsymbol{u}, Q)) = 0$, $tr(\partial_t Q) = \partial_t\, tr(Q)$, $tr(\boldsymbol{u} \cdot \nabla Q) = \boldsymbol{u} \cdot \nabla\, tr(Q)$ and

$$tr(H) = -\varepsilon\, \Delta tr(Q) + \left[a + c\, |Q|^2\right] tr(Q) - \frac{b}{3}\left(tr(Q^2) + 2|Q|^2\right).$$

Therefore, taking the trace of equation (1.3) and denoting $\phi = tr(Q)$, the following PDE for ϕ holds:

$$\partial_t \phi + \boldsymbol{u} \cdot \nabla \phi + \gamma \left(-\varepsilon\, \Delta \phi + \left(a + c\, |Q|^2\right) \phi - \frac{b}{3} \left(tr(Q^2) + 2|Q|^2\right)\right) = 0 \tag{5.2}$$

The term with coefficient b (which has no sign) and the term with a (that can be negative if $a < 0$) are the main difficulties in order to get $tr(Q(t)) = 0\ \forall t \in (0, T)$ whenever $tr(Q_0) = 0$ (and $tr(Q_\Gamma) = 0$ when Dirichlet conditions for Q are assumed). Two possibilities can be considered:

$$\alpha_1(Q) = \frac{a}{3}\, tr(Q) + \frac{b}{9}\, tr(Q^2 + QQ^t + Q^t Q). \tag{5.3}$$

$$\alpha_2(Q) = -\frac{tr(f(Q))}{3}\, I \tag{5.4}$$

From (5.2), in both cases one has :

$$\partial_t \phi + \boldsymbol{u} \cdot \nabla \phi - \alpha \Delta \phi \leq 0, \quad \alpha > 0 \tag{5.5}$$

endowed with the same boundary conditions as before. Assuming that $\phi(0) = 0$, therefore $\phi(t) = 0\ \forall t$. Thus, $tr(Q(t)) = 0$ for all $t \geq 0$.

5.2. Rewriting S to obtain symmetry of Q

5.2.1. The new expression for the stretching term $S(\nabla \boldsymbol{u}, Q)$

First, taking the transpose of equation (1.3) we look for the equation verified by Q^t. Thanks to the fact that $|Q|^2 = |Q^t|^2$ it is easy to see that $(f(Q))^t = f(Q^t)$. Then, the term $S(\nabla \boldsymbol{u}, Q)^t$ is splitting in two using that $\nabla \boldsymbol{u} = \boldsymbol{D} + \boldsymbol{W}$, for $\boldsymbol{D} = D(\nabla \boldsymbol{u}) = \frac{1}{2}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^t\right)$ (symmetric part of $\nabla \boldsymbol{u}$) and $\boldsymbol{W} = W(\nabla \boldsymbol{u}) = \frac{1}{2}\left(\nabla \boldsymbol{u} - (\nabla \boldsymbol{u})^t\right)$ (antisymmetric part of $\nabla \boldsymbol{u}$), which leads to:

$$S(\nabla \boldsymbol{u}, Q)^t = -S(\boldsymbol{D}, Q^t) + S(\boldsymbol{W}, Q^t)$$

Thus,

$$S(\nabla \boldsymbol{u}, Q) - S(\nabla \boldsymbol{u}, Q)^t = S(\boldsymbol{D}, Q + Q^t) + S(\boldsymbol{W}, Q - Q^t)$$

and considering the scalar product by $Q - Q^t$ ($Q - Q^t$ is antisymmetric):

$$S(\boldsymbol{D}, Q + Q^t) : (Q - Q^t) \neq 0, \quad S(\mathbf{W}, Q - Q^t) : (Q - Q^t) = 0 \tag{5.6}$$

One way to prove the symmetry of Q could be to consider an adequate system verified by $E = Q - Q^t$ to deduce $E(t) = \mathbf{0}\ \forall t > 0$ if $E_0 = \mathbf{0}$ (and $E|_\Gamma = 0$ in the Dirichlet case). In general,

$$D_t E - S(\boldsymbol{D}, Q + Q^t) - S(\boldsymbol{W}, E) + \gamma(-\varepsilon \Delta E + f(Q) - f(Q^t)) = 0 \tag{5.7}$$

Taking E as test function in (5.7) and using that $S(\boldsymbol{W}, E) : E = 0$, we obtain:

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\|E\|^2_{L^2(\Omega)} - \int_\Omega S(\boldsymbol{D}, Q + Q^t) : E\, d\boldsymbol{x} \\ &\quad + \gamma\left(a\,\|E\|^2_{L^2(\Omega)} + c\int_\Omega |Q|^2\,|E|^2\, d\boldsymbol{x} + \varepsilon \|\nabla E\|^2_{L^2(\Omega)}\right) \\ &\quad \leq \frac{2|b|}{3}\gamma \int_\Omega |Q||E|^2\, d\boldsymbol{x} \end{aligned} \tag{5.8}$$

To avoid the dependence on $\boldsymbol{u}$ in estimate (5.8), we consider the stretching term S does not depend on $\boldsymbol{D}$, replacing $S(\nabla \boldsymbol{u}, Q)$ by $S(\boldsymbol{W}, Q)$ in the differential system for Q. Thus, from (5.8), choosing $E(0) = 0$, that is, assuming symmetric initial data Q_0, we can conclude $Q(t)$ will be symmetric $\forall t > 0$.

5.2.2. *The new expression for the tensor $\sigma(Q, H)$*

Once the term $S(\nabla \boldsymbol{u}, Q)$ has been replaced by $S(\boldsymbol{W}, Q)$, then Q and H are symmetric. Now, we have to modify the tensor $\sigma(H, Q)$ for the energy law to be still valid. First, we decompose both Q and H in their symmetric and antisymmetric parts:

$$Q = D(Q) + W(Q), \quad D(Q) = \frac{Q + Q^t}{2}, \quad W(Q) = \frac{Q - Q^t}{2}$$
$$H = D(H) + W(H), \quad D(H) = \frac{H + H^t}{2}, \quad W(H) = \frac{H - H^t}{2}$$

Remark 6. Observe that the symmetry of Q and H implies $W(Q) = \mathbf{0}$ and $W(H) = \mathbf{0}$.

Thus, using linearity,

$$\sigma(Q, H) \quad = \quad \sigma(D(Q), D(H))$$

which implies the antisymmetric character of the tensor $\sigma(Q, H)$ in such a way that:

$$\sigma : \boldsymbol{D} = 0 \quad \Rightarrow \quad \sigma : \nabla \boldsymbol{u} = \sigma : \boldsymbol{W} = S(\boldsymbol{W}, Q) : H$$

5.3. Consequences of $tr(Q) = 0$ and symmetry of Q over the model

Considering $\alpha(Q)$ given by (5.3) or (5.4) and the stretching term equal to $S(\boldsymbol{W}, Q)$ (the tensor $\sigma(Q, H)$ is now antisymmetric), it is possible to reproduce every result on existence, uniqueness and regularity for the model (1.2)-(1.3) to this new traceless and symmetric model.

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