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Weak solutions for an initial–boundary Q-tensor problem related to liquid crystals

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ABSTRACT

The coupled Navier–Stokes and Q-tensor system is considered in a bounded three-dimensional domain under homogeneous Dirichlet boundary conditions for the velocity $\boldsymbol{u}$ and either nonhomogeneous Dirichlet or homogeneous Neumann boundary conditions for the tensor Q. The corresponding initial-value problem in the whole space $\mathbb{R}^3$ was analyzed in Paicu and Zarnescu (2012).

In this paper, three main results concerning weak solutions will be proved: the existence of global in time weak solutions (bounded up to infinite time), a uniqueness criteria and a maximum principle for Q. Moreover, we identify how to modify the system to deduce symmetry and traceless for Q, for any weak solution. The presence of a stretching term in the Q-system plays a crucial role in all the analysis.

1. The Q-tensor system 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, for instance, rod-like shape whose center of mass is isotropically distributed and whose direction is almost constant on average over small regions. Several models of (N) are described through the velocity and pressure $(\boldsymbol{u}, p)$ and a director vector denoted by $\boldsymbol{d}$ or $\boldsymbol{n}$ (cf. [8,13]).

The optical behavior of liquid crystals can change from one point to the other and can be of different types, namely uniaxial (points having one single refractive index and a unit-vector field $\boldsymbol{n}(\boldsymbol{x}) \in \mathbb{S}^2$ represents the preferred direction of molecular alignment), biaxial (points having two indices of refraction, with more than one preferred direction of molecular

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alignment) or isotropic (points where the orientation of molecules is equally distributed in all directions). The two main continuum theories for nematic liquid crystals (cf. [8,3,6]) are: the Oseen–Frank theory, restricted to uniaxial nematic liquid crystal materials, and the more general Landau–De Gennes theory, which can account the three types of optic for (N): uniaxial, biaxial and isotropic phases.

In the Landau–De Gennes theory, the director vector $\boldsymbol{d}$ appearing in the Oseen–Frank theory is replaced by a symmetric and traceless matrix $Q \in \mathbb{R}^{3\times 3}$, known as the Q-tensor order parameter, which measures the deviation of the second moment tensor from its isotropic value. A nematic liquid crystal is said to be isotropic when $Q = 0$, uniaxial when the Q-tensor has two equal non-zero eigenvalues and can be written in the special form:

$$Q(\boldsymbol{x}) = s\left(\boldsymbol{n}(\boldsymbol{x}) \otimes \boldsymbol{n}(\boldsymbol{x}) - \frac{1}{d}\,\mathbb{I}\right) \quad \text{with } s \in \mathbb{R}\setminus\{0\},\ \boldsymbol{n} \in \mathbb{S}^2$$

and biaxial when Q has three different eigenvalues and can be represented as follows (see Proposition 1 in [14]):

$$Q = s\left(\boldsymbol{n}\otimes\boldsymbol{n} - \frac{1}{d}\,\mathbb{I}\right) + r\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{d}\,\mathbb{I}\right) \quad s, r \in \mathbb{R};\ \boldsymbol{n}, \mathbf{m} \in \mathbb{S}^2.$$

The definition of the Q-tensor is related to the second moment of a probability measure $\mu(\boldsymbol{x}, \cdot) : \mathcal{L}(\mathbb{S}^2) \to [0, 1]$ for each $\boldsymbol{x} \in \Omega$, being $\mathcal{L}(\mathbb{S}^2)$ the family of Lebesgue measurable sets on the unit sphere. For any $A \subset \mathbb{S}^2$, $\mu(\boldsymbol{x}, A)$ is the probability that the molecules with center of mass in a very small neighborhood of the point $\boldsymbol{x} \in \Omega$ are pointing in a direction contained in A. This probability (cf. [21]) must satisfy $\mu(\boldsymbol{x}, A) = \mu(\boldsymbol{x}, -A)$ in order to reproduce the so-called "head-to-tail" symmetry. As a consequence, the first moment of the probability measure vanishes, that is

$$\langle p\rangle(\boldsymbol{x}) = \int_{\mathbb{S}^2} p_i\, d\mu(\boldsymbol{x}, p) = 0.$$

Then, the main information on μ comes from the second moment tensor

$$M(\mu)_{ij} = \int_{\mathbb{S}^2} p_i\, p_j\, d\mu(p), \quad i, j = 1, 2, 3.$$

It is easy to see that $M(\mu) = M(\mu)^t$ and $\mathrm{tr}(M) = 1$. 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 $M(\mu_0) = \frac{1}{3}\,\mathbb{I}$. The deviation of the second moment tensor from its isotropic value is therefore measured as:

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

From (1), Q is symmetric and traceless. These properties are assumed (but not rigorously justified) in the problem studied by Paicu and Zarnescu in [15] and Abels et al. in [1] (and in the more complete problem studied by the same authors in [16,2], respectively). These equations are also described in [9,19] for fluids with constant density.

Now, firstly a generalization of the Q-tensor model given in [15] will be studied, and secondly some terms of this generic model will be rewritten appropriately to assure that any weak solution must be symmetric and traceless.

We are going to start studying a generic Q-tensor model in a smooth and bounded domain $\Omega \subset \mathbb{R}^3$, for the unknowns $(\boldsymbol{u}, p, Q) : (0, T) \times \Omega \to \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}^{3\times 3}$, satisfying the momentum and incompressibility equations

$$\begin{cases} D_t\boldsymbol{u} - \nu\Delta\boldsymbol{u} + \nabla p = \nabla\cdot\tau(Q) + \nabla\cdot\sigma(H, Q) & \text{in } \Omega \times (0, T), \\ \nabla\cdot\boldsymbol{u} = 0 & \text{in } \Omega \times (0, T), \end{cases} \tag{2}$$

and the Q-tensor system:

$$D_t Q - S(\nabla\boldsymbol{u}, Q) = -\gamma\, H(Q) \quad \text{in } \Omega \times (0, T). \tag{3}$$

Here, $D_t = \partial_t + (\boldsymbol{u}\cdot\nabla)$ denotes the material time derivative, $\nu > 0$ is the viscosity coefficient and $\gamma > 0$ is a material-dependent elastic constant.

In (3), $S(\nabla\boldsymbol{u}, Q) = \nabla\boldsymbol{u}\, Q^t - Q^t\, \nabla\boldsymbol{u}$ is the so-called stretching term.

In (2) the tensors $\tau = \tau(Q)$ and $\sigma = \sigma(H, Q) \in \mathbb{R}^{3\times 3}$ are defined by

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