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A BDF2 Energy-Stable Scheme for a General Tensor-Based Model of Liquid Crystals

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Abstract. Following the scalar auxiliary variable strategy, a linear semi-discrete scheme in time for the hydrodynamic **Q**-tensor model of liquid crystal polymers is developed. It is shown that the scheme is unconditionally energy stable and uniquely solvable. Numerical simulations show the decreasing energy and the second-order convergence.

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Key words: **Q**-tensor model, unconditional energy stability, linear second order BDF2 scheme.

1. Introduction

Liquid crystals represent an intermediate state of matter between crystalline solids and isotropic fluids. Nematic liquid crystals usually have molecular orientational order but not a positional order. The most popular mathematical model for the flow of low molecular weight nematic liquid crystals is the Ericksen-Leslie model [10], where the orientation of molecules is expressed by a unit vector $\mathbf{d} \in \mathscr{S}^2$. The distortional elasticity is described by the Oseen-Frank energy but in this case, only uniaxial liquid crystals can be modeled. If the orientational symmetry is broken, the Ericksen-Leslie theory fails to capture the asymmetrical feature of the system. Moreover, if defects emerge, the director model is singular and $\mathbf{d}$ cannot be determined. In order to model liquid crystal droplets, Diegel *et al.* [3] coupled the Ericksen's model for nematic liquid crystals and the Cahn-Hilliard interfacial energy equation.

An alternative method to describe the orientation of nematic liquid crystal systems consists in using a Q-tensor — i.e. a second-order tensor of trace zero. The reflective symmetry of the system and biaxiality are naturally built-in into tensor-based theories and defects can also be captured. Furthermore, the director model can be derived from **Q**-tensor theory for weak flows and weak elastic limits [20]. Therefore, the **Q**-tensor based hydrodynamic model is commonly used in nematic liquid crystal flows [1, 5, 6, 18–20].

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In this work, we describe the average orientation of nematic liquid crystals with $\mathbf{Q}$. Set

$$\Lambda := \left\{\mathbf{Q} \in \mathbf{R}^{3\times 3}, \mathrm{tr}\,(\mathbf{Q}) = 0, \mathbf{Q} = \mathbf{Q}^T\right\}$$

and consider the general Landau-De Gennes free energy functional

$$\mathbf{E}(\mathbf{Q}) = \int_\Omega \left(\frac{K}{2}|\nabla \mathbf{Q}|^2 + F_B(\mathbf{Q})\right) d\mathbf{x}, \tag{1.1}$$

where the first term in the integral is the elastic energy, K a material-dependent elastic constant, $F_B(\mathbf{Q})$ the bulk free energy density,

$$F_B(\mathbf{Q}) := \frac{\alpha}{2}\mathrm{tr}\,(\mathbf{Q}^2) + \frac{\beta}{3}\mathrm{tr}\,(\mathbf{Q}^3) + \frac{\gamma}{4}\mathrm{tr}^2(\mathbf{Q}^2)$$

and α, β and $\gamma > 0$ are material-dependent and temperature-dependent constants — cf. [7].

According to [1, 20, 23], the non-dimensional governing equations of nematic liquid crystal flows with hydrodynamics have the form

$$\begin{aligned} &\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \eta\nabla^2\mathbf{u} + \nabla\cdot\sigma(\mathbf{Q},\mathbf{G}) - \mathbf{G}\nabla\mathbf{Q}, \\ &\nabla\cdot\mathbf{u} = 0, \\ &\mathbf{Q}_t + \mathbf{u}\cdot\nabla\mathbf{Q} - S(\nabla\mathbf{u},\mathbf{Q}) = M_1\mathbf{G}, \end{aligned} \tag{1.2}$$

where

$$\begin{aligned} &S(\nabla\mathbf{u},\mathbf{Q}) = W\cdot\mathbf{Q} - \mathbf{Q}\cdot W + a(\mathbf{Q}\cdot D + D\cdot\mathbf{Q}) + \frac{2a}{3}\left(D - \frac{\nabla\cdot\mathbf{u}I}{3}\right) - 2a(D:\mathbf{Q})\left(\mathbf{Q} + \frac{I}{3}\right), \\ &\sigma(\mathbf{Q},\mathbf{G}) = (\mathbf{Q}\cdot\mathbf{G} - \mathbf{G}\cdot\mathbf{Q}) - a(\mathbf{G}\cdot\mathbf{Q} + \mathbf{Q}\cdot\mathbf{G}) - \frac{2a}{3}\mathbf{G} + 2a(\mathbf{Q}:\mathbf{G})\left(\mathbf{Q} + \frac{I}{3}\right), \\ &\mathbf{G} = -\frac{\delta\mathbf{E}(\mathbf{Q})}{\delta\mathbf{Q}} = K\nabla^2\mathbf{Q} - \left[\alpha\mathbf{Q} + \beta\left(\mathbf{Q}^2 - \frac{\mathrm{tr}\,(\mathbf{Q}^2)}{3}\mathbf{I}\right) + \gamma\mathrm{tr}\,(\mathbf{Q}^2)\mathbf{Q}\right], \end{aligned} \tag{1.3}$$

and $D = (\nabla\mathbf{u} + \nabla\mathbf{u}^T)/2$ and $W = \nabla\mathbf{u} - \nabla\mathbf{u}^T/2$ are, respectively, the rate of strain and vorticity tensors. Moreover, the first two terms in $\mathbf{S}(\nabla\mathbf{u},\mathbf{Q})$ and the material derivative of $\mathbf{Q}$ define the Gordon-Schowalter derivative, $\mathbf{G}$ is the molecular field, $\sigma(\mathbf{Q},\mathbf{G})$ the elastic stress tensor, and $a \in [-1,1]$ a geometric parameter of the nematic liquid crystal molecule — cf. [20]. We also impose the initial condition

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{Q}(\mathbf{x},0) = \mathbf{Q}_0(\mathbf{x}),$$

and use one of the following boundary conditions:

1. $\mathbf{u}$ and $\mathbf{Q}$ are periodic on $\partial\Omega$.
2. $\mathbf{u}|_{\partial\Omega} = 0$, $\mathbf{Q}|_{\partial\Omega} = \mathbf{Q}^0$ or $\partial_n\mathbf{Q}|_{\partial\Omega} = 0$.