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A stable scheme and its convergence analysis for a 2D dynamic Q-tensor model of nematic liquid crystals

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We propose an unconditionally stable numerical scheme for a 2D dynamic Q-tensor model of nematic liquid crystals. This dynamic Q-tensor model is an L^2-gradient flow generated by the liquid crystal free energy that contains a cubic term, which is physically relevant but makes the free energy unbounded from below, and for this reason, has been avoided in other numerical studies. The unboundedness of the energy brings significant difficulty in analyzing the model and designing numerical schemes. By using a stabilizing technique, we construct an unconditionally stable scheme, and establish its unique solvability and convergence. Our convergence analysis also leads to, as a byproduct, the well-posedness of the original PDE system for the 2D Q-tensor model. Several numerical examples are presented to validate and demonstrate the effectiveness of the scheme.

Keywords: Q-tensor; nematic liquid crystals; stability; convergence; well-posedness; Fourier spectral method.

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1. Introduction

Liquid crystals are intermediate states of matter between the commonly observed solid and liquid that have no or partial positional order but do exhibit an orientational order. The nematic phase is the simplest among all liquid crystal phases whose rod-like molecules have no translational order but possess a certain degree of long-range orientational order. The Landau–de Gennes theory[9] is a continuum theory to describe the nematic liquid crystals. In this framework, it is widely accepted that the local orientation and the degree of order for the liquid crystal molecules are characterized by a symmetric, traceless $d \times d$ tensor called the Q-tensor in $\mathbb{R}^d$ $(d = 2, 3)$.[2,25] The Q-tensor vanishes in the isotropic phase, and hence serves as an order parameter. The Q-tensor order parameter may exhibit two different phases, namely the uniaxial phase and the biaxial phase. In the former phase, Q has uniaxial symmetry and the symmetry axis is defined by a unit vector $\mathbf{n}$ called the director. In the latter biaxial phase, the structure of Q is more complicated. There exists a vast literature on the mathematical study of the Landau–de Gennes theory, see Refs. 3, 4, 11, 21–24, 27, 28 and the references therein.

The equilibrium states are physically observable configurations which correspond to either global or local minimizers of the free energy subject to certain imposed boundary conditions. Let us consider a nematic liquid crystal filling a smooth, bounded domain $\Omega \subset \mathbb{R}^d$, and for the sake of simplicity, we suppose that the material is spatially homogeneous and the temperature is constant. Historically, the first step toward the understanding of its free energy was attributed to Refs. 26 and 13 where the free energy density functional, namely the Oseen–Frank energy density, is expressed in terms of the director $\mathbf{n} \in \mathbb{S}^{d-1}$ (unit sphere in $\mathbb{R}^d$) with elastic constants $K_1, \ldots, K_4$:

$$W_{\mathrm{OF}} = \frac{K_1}{2}(\nabla\cdot\mathbf{n})^2 + \frac{K_2}{2}|\mathbf{n}\times(\nabla\times\mathbf{n})|^2 + \frac{K_3}{2}|\mathbf{n}\cdot(\nabla\times\mathbf{n})|^2 + \frac{K_2+K_4}{2}[\mathrm{tr}(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2]. \tag{1.1}$$

Here $K_1, \ldots, K_3$ measure 13 the resistance of three basic distortions, called splay, twist and bend, respectively, and the last term in (1.1) is related to the twisted splay distortion, which is a null Lagrange term but is kept in most literature because this term does contribute to the total free energy for some types of boundary value problems.[16] The Oseen–Frank formulation is generally consistent with experiments except near the nematic-smectic[a] phase transition.[10] In order to generalize the Oseen–Frank description close to the clearing point, de Gennes[9] proposed a Ginzburg–Landau-type expansion of the free energy in terms of the tensor parameter Q and its spatial derivatives. The Landau–de Gennes free energy functional

[a]The smectic phase forms well-defined layers that can slide over one another in a manner similar to that of soap. In the smectic phase, molecules have positional ordering in a layered structure, see Ref. 9 for further discussions.

is derived as a nonlinear integral functional of the Q-tensor and its spatial derivatives[2]:

$$\mathcal{E}[Q] = \int_\Omega \mathcal{F}(Q(x))dx, \tag{1.2}$$

where Q is in the Q-tensor space (cf. Refs. 2, 25 and 4) defined by

$$\mathcal{S}^{(d)} \stackrel{\text{def}}{=} \left\{ M \in \mathbb{R}^{d\times d} \,\middle|\, \sum_{i=1}^{d} M^{ii} = 0,\ M^{ij} = M^{ji} \in \mathbb{R},\ \forall\, i,\ j = 1, \ldots, d \right\}.$$

The free energy density functional $\mathcal{F}$ consists of the elastic part $\mathcal{F}_{\text{el}}$ that depends on the gradient of Q, and the bulk part $\mathcal{F}_{\text{bulk}}$ that depends on Q only,[18] i.e.

$$\mathcal{F}(Q) = \mathcal{F}_{\text{el}} + \mathcal{F}_{\text{bulk}}. \tag{1.3}$$

The bulk-free energy density $\mathcal{F}_{\text{bulk}}$ is typically a truncated expansion in the scalar invariants of the tensor Q. In the simplest setting one may take

$$\mathcal{F}_{\text{bulk}} \stackrel{\text{def}}{=} \frac{a}{2}\text{tr}(Q^2) + \frac{b}{3}\text{tr}(Q^3) + \frac{c}{4}\text{tr}^2(Q^2), \tag{1.4}$$

where a, b, c are assumed to be bulk material constants. This bulk term (1.4) embodies the ordering/disordering effects, which drive the nematic-isotropic phase transition. It depends only on the eigenvalues of Q. Meaningful simulations can be performed using an expansion truncated at the fourth order, to which we have to use in order to have a potential with multiple stable local minima.[11]

On the other hand, the elastic-free energy density $\mathcal{F}_{\text{el}}$ gives the strain energy density due to spatial variations in the tensor order parameter. Its simplest form which is invariant under rigid rotations and material symmetry is as follows[2,25]:

$$\mathcal{F}_{\text{el}} \stackrel{\text{def}}{=} L_1|\nabla Q|^2 + L_2\partial_j Q^{ik}\partial_k Q^{ij} + L_3\partial_j Q^{ij}\partial_k Q^{ik} + L_4 Q^{lk}\partial_k Q^{ij}\partial_l Q^{ij}. \tag{1.5}$$

Here and after we use the Einstein summation convention over repeated indices. The material elastic constants L_k $(k = 1, 2, 3, 4)$ are assumed to be non-dimensional. It is worth pointing out that $\mathcal{F}_{\text{el}}$ in (1.5) consists of three independent terms with constants L_1, L_2, L_3 that are quadratic in the first partial derivatives of the components of Q, plus an unusual cubic term with constant L_4. As mentioned in Refs. 18 and 21, the retention of this L_4 cubic term is due to the consideration that it gives a complete reduction of $\mathcal{F}[Q]$ to the classical Oseen–Frank energy density W_{OF}. This is done by formally taking $Q(x) = s_+(\mathbf{n}(x)\otimes\mathbf{n}(x) - \frac{1}{d}\mathbb{I})$, where $s_+ \in \mathbb{R}^+$ and substituting it in (1.1). It is shown in Refs. 18 and 21 that if $L_4 = 0$, then $K_1 \equiv K_3$ during the reduction, which clearly contradicts with experiments. On the other hand, this L_4-term causes the Landau–de Gennes free energy to be unbounded from below.[3]

In order to remedy the aforementioned deficiency in the static configurations, one way is to replace the bulk potential part defined in (1.5) with a singular type potential[3]; alternatively, a dynamic case is later proposed in Ref. 18 to keep the more common bulk potential in (1.5). More specifically, the authors in Ref. 18 study the following L^2-gradient flow in $\mathbb{R}^2$ corresponding to the energy functional $\mathcal{E}[Q]$ where Q takes values in $\mathcal{S}^{(2)}$:

$$\frac{\partial Q^{ij}}{\partial t} = -\left(\frac{\delta \mathcal{E}}{\delta Q}\right)^{ij} + \lambda \delta^{ij} + \mu^{ij} - \mu^{ji}, \quad 1 \leq i,\ j \leq 2. \tag{1.6}$$

In (1.6), λ is the Lagrange multiplier corresponding to the tracelessness constraint and $\mu = (\mu^{ij})_{2\times 2}$ is the Lagrange multiplier corresponding to the matrix symmetry constraint, and $\frac{\delta \mathcal{E}}{\delta Q}$ denotes the variational derivative of $\mathcal{E}$ with respect to Q. In addition, hereafter we always impose the coercivity condition[18] (see also Ref. 11 for its counterpart in 3D):

$$L_1 + L_2 > 0, \quad L_1 + L_3 > 0, \tag{1.7}$$

and

$$c > 0. \tag{1.8}$$

From the modeling point of view, (1.7) is imposed to guarantee that the summation of the first three quadratic terms concerning L_1, L_2, L_3 in $\mathcal{F}_{\mathrm{el}}$ is positive definite, while (1.8) is to ensure $\mathcal{F}_{\mathrm{bulk}}$ is bounded from below. Moreover, as noted in Refs. 7 and 18, the term $\frac{b}{3}\mathrm{tr}(Q^3)$ can be ignored from (1.4) since $\mathrm{tr}(Q^3) = 0$ for any $Q \in \mathcal{S}^{(2)}$.

After expansion, the evolution equation (1.6) reads (see Appendix A in Ref. 18 for details):

$$\begin{aligned}\partial_t Q^{ij} = {} & \zeta \Delta Q^{ij} + L_4 \left\{ 2\partial_k \left(Q^{lk} \partial_l Q^{ij}\right) - \partial_i Q^{kl} \partial_j Q^{kl} + \frac{|\nabla Q|^2 \delta^{ij}}{2} \right\} \\ & - [a + c\,\mathrm{tr}(Q^2)] Q^{ij},\end{aligned} \tag{1.9}$$

for $1 \leq i, j \leq 2$, with initial and boundary conditions given by

$$Q(x,0) = Q^0(x), \quad \text{and} \quad Q(x,t)|_{\partial\Omega} = \tilde{Q}(x), \quad Q^0|_{\partial\Omega} = \tilde{Q}. \tag{1.10}$$

Note that

$$\zeta \stackrel{\text{def}}{=} 2L_1 + L_2 + L_3 > 0 \tag{1.11}$$

under the coercivity condition (1.7).

Since the free energy $\mathcal{E}[Q]$ is unbounded from below when $L_4 \neq 0$, generally one may not expect a global existence result to the problem (1.9)–(1.10) without involving a smallness assumption of $Q(\cdot,t)$. To be more precise, this gradient flow gives us the following energy dissipative law for smooth solutions $Q(\cdot,t)$ that satisfies

$$\frac{d}{dt}\mathcal{E}[Q] = -\int_\Omega \left| \frac{\delta \mathcal{E}}{\delta Q} - \lambda \mathbf{I}_2 + \mu - \mu^T \right|^2 dx,$$

which immediately produces the integral equality

$$\mathcal{E}[Q(\cdot,t)] + \int_0^t \int_\Omega \left| \frac{\delta \mathcal{E}}{\delta Q} - \lambda \mathbf{I}_2 + \mu - \mu^T \right|^2 dx\, ds = \mathcal{E}[Q(\cdot,0)], \quad \forall\, t > 0. \tag{1.12}$$

Here $\mathbf{I}_2$ stands for the 2×2 identity matrix. However, we cannot get any *a priori* control of $\|Q(\cdot,t)\|_{H^1(\Omega)}$ from (1.12) because of the unboundedness of $\mathcal{E}[Q]$.

Fortunately, the mathematical structure of (1.9) is exploited thoroughly in Ref. 18 so that for any smooth solutions to the evolution problem, the smallness of $\|Q_0\|_{L^\infty(\Omega)}$ will be preserved as time evolves. Based on this property plus the coercivity condition (1.7), the authors in Ref. 18 obtain the necessary *a priori* bounds from the energy equality (1.12), which paves the way to obtain the global existence result.

Along the numerical front, there exists only a few studies on the Q-tensor model. For the stationary case with $L_4 = 0$, there have been several studies on phase transitions,[19] density variations,[30] singularities[5,17] and liquid crystal alignments.[8] For the dynamic Q-tensor model with $L_4 = 0$, a spectral method was used in Ref. 32 to study the instability of nanorod dispersions; an adaptive moving mesh method was proposed in Ref. 20; a stable finite element discretization was introduced in Ref. 5 for the gradient flow dynamics with constant orientational order parameter. However, to the best of our knowledge, there has been no study concerning simulation or numerical analysis for the Q-tensor model in the general case with $L_4 \neq 0$. Note that this unusual cubic term ($L_4 \neq 0$) corresponds to the compatibility between the Q-tensor model and the Oseen–Frank model for liquid crystals.[18,21]

In this paper we construct an unconditionally stable numerical scheme for the full dynamic Q-tensor model (1.9)–(1.10). Since the system admits an energy law (1.12),[33] it is desirable to design an energetically stable scheme to approximate the Q-tensor model (1.9)–(1.10). On the other hand, the energy stability (or the energy boundedness) does not imply well-posedness of the evolution problem because the nonzero term $L_4 \neq 0$, unless the L^∞-norm of the solution is kept small. Inspired by this observation, we need to show, in addition to energy stability, that L^∞-norm of the solutions can be kept small, in order to prove the well-posedness of the nonlinear system at each time step. This is much more challenging than establishing the energy stability.

The novelty of this paper is two-fold. Firstly, we propose a stable scheme for the dynamical Q-tensor model (1.9)–(1.10) and rigorously prove its unique solvability and convergence. Secondly, as a byproduct, we provide a different and simplified approach compared to the one used in Ref. 18 to prove the existence of global weak solutions (see Remark 2.4 about the difference between two approaches for detail).

The rest of the paper is organized as follows. In Sec. 2, we present our semi-discrete numerical scheme for (1.9)–(1.10) and establish its unique solvability and convergence. As a byproduct, we obtain the well-posedness of (1.9)–(1.10). We show some numerical tests in Sec. 3, and demonstrate the accuracy and efficiency of our proposed scheme. Finally, some conclusions are drawn in Sec. 4.

We provide below some notations and definitions to be used in the rest of the paper.

We denote $\Omega \subset \mathbb{R}^2$ a smooth and bounded domain. For matrices $A, B \in \mathbb{R}^{2\times 2}$, we define the Fröbenius product between A and B by

$$A : B \stackrel{\text{def}}{=} \operatorname{tr}(A^t B).$$

For $Q \in \mathbb{R}^{2\times 2}$, we use $|Q|$ to denote its Frobenius norm, i.e.

$$|Q| \stackrel{\text{def}}{=} \sqrt{\operatorname{tr}(Q^t Q)} = \sqrt{\sum_{1\le i,j\le 2} Q^{ij} Q^{ij}}.$$

Besides, we define the matrix-valued L^p $(1 \le p \le \infty)$ space by

$$L^p(\Omega \to \mathbb{R}^{2\times 2}) \stackrel{\text{def}}{=} \{Q : \Omega \to \mathbb{R}^{2\times 2}, |Q| \in L^p(\Omega, \mathbb{R})\}.$$

Further, for any smooth scalar function $u : \Omega \to \mathbb{R}$, we define the following Hölder norms and semi-norms:

$$[u]_{C^\alpha(\bar\Omega)} \stackrel{\text{def}}{=} \sup_{x\ne y\in\Omega} \frac{|u(x)-u(y)|}{|x-y|^\alpha}, \qquad 0<\alpha\le 1.$$

$$[u]_{C^{1+\alpha}(\bar\Omega)} \stackrel{\text{def}}{=} \max_{1\le i\le 2} [\partial_i u]_{C^\alpha(\bar\Omega)}, \qquad [u]_{C^{2+\alpha}} \stackrel{\text{def}}{=} \max_{1\le i,j\le 2} [\partial_i\partial_j u]_{C^\alpha(\bar\Omega)}, \quad 0<\alpha\le 1.$$

$$\|u\|_{C^0(\bar\Omega)} \stackrel{\text{def}}{=} \sup_{x\in\Omega} |u(x)|,$$

$$\|u\|_{C^\alpha(\bar\Omega)} \stackrel{\text{def}}{=} \|u\|_{C^0(\Omega)} + [u]_{C^\alpha(\bar\Omega)}, \qquad 0<\alpha\le 1.$$

$$\|u\|_{C^{1+\alpha}(\bar\Omega)} \stackrel{\text{def}}{=} \|u\|_{C^1(\bar\Omega)} + [u]_{C^{1+\alpha}(\bar\Omega)}, \qquad 0<\alpha\le 1.$$

$$\|u\|_{C^{2+\alpha}(\bar\Omega)} \stackrel{\text{def}}{=} \|u\|_{C^2(\bar\Omega)} + [u]_{C^{2+\alpha}(\bar\Omega)}, \qquad 0<\alpha< 1.$$

For a tensor-valued function $Q : \Omega \to \mathbb{R}^{2\times 2}$, the corresponding norms are defined to be the maximum of each component, for instance, $[Q]_{C^\alpha(\bar\Omega)} \stackrel{\text{def}}{=} \max_{1\le i,j\le 2} [Q^{ij}]_{C^\alpha(\bar\Omega)}$; and the corresponding Hölder space by

$$C^\alpha(\bar\Omega \to \mathbb{R}^{2\times 2}) \stackrel{\text{def}}{=} \left\{Q : \Omega \to \mathbb{R}^{2\times 2}, \max_{1\le i,j\le 2} [Q^{ij}]_\alpha \in C^\alpha(\bar\Omega)\right\}.$$

Without ambiguity, $L^p(\Omega \to \mathbb{R}^{2\times 2})$ will often be abbreviated as $L^p(\Omega)$ $(1\le p\le\infty)$, and $C^{k+\alpha}(\bar\Omega \to \mathbb{R}^{2\times 2})$ as $C^{k+\alpha}(\bar\Omega)$ $(0\le\alpha<1,\ k\in\mathbb{Z}^+)$. For the sake of simplicity, we at times use $\|\cdot\|_{L^p}$ to denote $\|\cdot\|_{L^p(\Omega)}$, and $\|\cdot\|_{C^{k+\alpha}}$ to denote $\|\cdot\|_{C^{k+\alpha}(\bar\Omega)}$, respectively. We denote the partial derivative with respect to x_k of the ij component of Q, by $\partial_k Q^{ij}$.

2. Time Discretization and Its Analysis

Let $\tilde{Q} \in C^{2+\alpha}(\bar{\Omega})$. We start with $Q^0 \in C^{2+\alpha}(\bar{\Omega})$, and for $n = 0, 1, 2, \ldots,$ and $\Delta t > 0$, find Q^{n+1} from the following stabilized discretizations for (1.9)–(1.10):

$$\begin{aligned}\frac{Q^{ij,n+1} - Q^{ij,n}}{\Delta t} &\\ &= \zeta\Delta Q^{ij,n+1} - aQ^{ij,n+1} - c|Q^{n+1}|^2 Q^{ij,n+1} - L(Q^{ij,n+1} - Q^{ij,n})|\nabla Q^{n+1}|^2 \\ &\quad + L_4\left\{2\partial_k(Q^{lk,n}\partial_l Q^{ij,n+1}) - \partial_i Q^{kl,n+1}\partial_j Q^{kl,n+1} + \frac{|\nabla Q^{n+1}|^2}{2}\delta^{ij}\right\}, \end{aligned} \tag{2.1}$$

$$Q^{n+1}|_{\partial\Omega} = \tilde{Q}; \quad 1 \le i,\ j \le 2. \tag{2.2}$$

Several remarks are in order:

- The above scheme is essentially a backward Euler scheme with an additional stabilizing term $-L(Q^{ij,n+1} - Q^{ij,n})|\nabla Q^{n+1}|^2$ which plays an essential role in our analysis below. The stabilizing constant $L > 0$ is to be determined later (cf. (2.4)).
- It is easy to see that (2.1) is a first-order accurate approximation to (1.9).
- (2.1) can be simplified by taking into account of the traceless and symmetry properties of the Q-tensor function (cf. (3.1)), but we consider the current form (2.1) for generality.

Our main result regarding the convergence of (2.1)–(2.2) is stated in Theorem 2.2. Before proving the convergence, we are going to establish the unique solvability first, since the scheme (2.1)–(2.2) is highly nonlinear and its solvability is non-trivial.

2.1. A priori *estimates and well-posedness of* (2.1)–(2.2)

We start with some *a priori* estimates for the time-discrete problem (2.1)–(2.2).

Lemma 2.1. *Let* $Q^n \in C^{2+\alpha}(\bar{\Omega})$, *and assume*

$$\max\{\|Q^n\|_{L^\infty(\Omega)}, \|\tilde{Q}\|_{L^\infty(\partial\Omega)}\} \le \frac{\zeta}{(1+\sqrt{6})|L_4|}, \tag{2.3}$$

and that the stabilized constant L *satisfies*

$$L \ge \frac{(\sqrt{6}+1)|L_4|^2}{\zeta}, \tag{2.4}$$

where ζ *is defined in* (1.11). *Then, if* $Q^{n+1} \in C^{2+\alpha}(\bar{\Omega})$ *is a classical solution of* (2.1)–(2.2), *it holds*

$$\|Q^{n+1}\|_{L^\infty(\Omega)} \le \max\left\{\|Q^n\|_{L^\infty(\Omega)}, \sqrt{\frac{a^-}{c}}\right\}, \tag{2.5}$$

where $a^- = \max\{0, -a\}$.

Proof. Denoting

$$\rho^n = |Q^n|^2, \quad \rho^{n+1} = |Q^{n+1}|^2 \tag{2.6}$$

and multiplying both sides of (2.1) with $2Q^{ij,n+1}$, then summing up for $1 \leq i, j \leq 2$, we get

$$\begin{aligned}
&\frac{|Q^{n+1}|^2 + |Q^{n+1} - Q^n|^2 - |Q^n|^2}{\Delta t} \\
&\quad = \partial_k[(\zeta\delta^{kl} + 2L_4 Q^{lk,n})\partial_l \rho^{n+1}] - (4L_4 Q^{lk,n} + 2\zeta\delta^{kl})\partial_k Q^{ij,n+1}\partial_l Q^{ij,n+1} \\
&\qquad - 2L_4 Q^{ij,n+1}\partial_i Q^{kl,n+1}\partial_j Q^{kl,n+1} + L_4 \mathrm{tr}(Q^{n+1})|\nabla Q^{n+1}|^2 \\
&\quad - (a + c|Q^{n+1}|^2)|Q^{n+1}|^2 - 2L[|Q^{n+1}|^2 - \mathrm{tr}((Q^n)^t Q^{n+1})]|\nabla Q^{n+1}|^2.
\end{aligned} \tag{2.7}$$

Let us assume $\rho^{n+1}(\cdot)$ take its maximum value at some point $x_0 \in \Omega$. Evaluating Eq. (2.1) at x_0, then we have:

Case 1. If $|Q^{n+1}|(x_0) \leq \sqrt{\frac{a^-}{c}}$, then the proof is complete.

Case 2. Otherwise, we can assume $\sqrt{\rho^{n+1}(x_0)} > \sqrt{\rho^n(x_0)}$, because $\sqrt{\rho^{n+1}(x_0)} \leq \sqrt{\rho^n(x_0)}$ will yield the conclusion (2.5) directly. First, for any matrix $Q \in \mathbb{R}^{2\times 2}$ and row vector $b = (b^1, b^2)$, using Cauchy–Schwarz inequality, we have

$$\begin{aligned}
|Q^{ij}b^i b^j| &\leq \frac{1}{2}((2|Q^{11}| + |Q^{12}| + |Q^{21}|)|b^1|^2 + (|Q^{12}| + |Q^{21}| + 2|Q^{22}|)|b^2|^2) \\
&\leq \frac{\sqrt{6}}{2}|Q|(|b^1|^2 + |b^2|^2).
\end{aligned}$$

As a consequence, it holds

$$-(4L_4 Q^{lk,n} + 2\zeta\delta^{kl})\partial_k Q^{ij,n+1}\partial_l Q^{ij,n+1} \leq -(2\zeta - 2\sqrt{6}|L_4|\sqrt{\rho^n})|\nabla Q^{n+1}|^2. \tag{2.8}$$

Besides, using Cauchy–Schwarz repeatedly we get

$$\begin{aligned}
&-2L_4 Q^{ij,n+1}\partial_i Q^{kl,n+1}\partial_j Q^{kl,n+1} + L_4\,\mathrm{tr}(Q^{n+1})|\nabla Q^{n+1}|^2 \\
&\quad = -2L_4(Q^{12,n+1} + Q^{21,n+1})\partial_1 Q^{kl,n+1}\partial_2 Q^{kl,n+1} \\
&\qquad - L_4(Q^{11,n+1} - Q^{22,n+1})\partial_1 Q^{kl,n+1}\partial_1 Q^{kl,n+1} \\
&\qquad + L_4(Q^{11,n+1} - Q^{22,n+1})\partial_2 Q^{kl,n+1}\partial_2 Q^{kl,n+1} \\
&\quad \leq |L_4|(|Q^{11,n+1}| + |Q^{12,n+1}| + |Q^{21,n+1}| + |Q^{22,n+1}|)|\nabla Q^{n+1}|^2 \\
&\quad \leq 2|L_4||Q^{n+1}||\nabla Q^{n+1}|^2.
\end{aligned} \tag{2.9}$$

Since $\rho^{n+1}(\cdot)$ attains its maximal value at x_0, we have $\partial_l \rho^{n+1}(x_0) = 0$ and the Hessian matrix of ρ^{n+1} at x_0 is semi-negative definite, which implies that

$|\partial_{12}\rho^{n+1}(x_0)| = |\partial_{21}\rho^{n+1}(x_0)| \le \frac{1}{2}(|\partial_{11}\rho^{n+1}(x_0)|+|\partial_{22}\rho^{n+1}(x_0)|)$, $\partial_{11}\rho^{n+1}(x_0) \le 0$, $\partial_{22}\rho^{n+1}(x_0) \le 0$. Cauchy inequality implies that

$$\begin{aligned}
&|Q^{lk,n}(x_0)\partial_{kl}\rho^{n+1}(x_0)| \\
&\quad\le (|Q^{12,n}(x_0)| + |Q^{21,n}(x_0)|)\frac{1}{2}(|\partial_{11}\rho^{n+1}(x_0)| + |\partial_{22}\rho^{n+1}(x_0)|) \\
&\qquad + |Q^{11,n}(x_0)|\,|\partial_{11}\rho^{n+1}(x_0)| + |Q^{22,n}(x_0)|\,|\partial_{22}\rho^{n+1}(x_0)| \\
&\quad\le \sqrt{\sum_{l,k=1,2}|Q^{lk,n}(x_0)|^2}\left(\sum_{l=1,2}|\partial_{ll}\rho^{n+1}(x_0)|^2 + \frac{1}{2}\left(\sum_{l=1,2}|\partial_{ll}\rho^{n+1}(x_0)|\right)^2\right)^{\frac{1}{2}} \\
&\quad\le \frac{\sqrt{6}}{2}|Q^n(x_0)|(-\partial_{11}\rho^{n+1}(x_0) - \partial_{22}\rho^{n+1}(x_0)).
\end{aligned}$$

Therefore, from (2.3), we get

$$\begin{aligned}
&\partial_k[(\zeta\delta^{kl} + 2L_4Q^{lk,n})\partial_l\rho^{n+1}](x_0) \\
&\quad= (\zeta\delta^{kl} + 2L_4Q^{lk,n}(x_0))\partial_k\partial_l\rho^{n+1}(x_0) \\
&\quad\le (\zeta - \sqrt{6}|L_4|\|Q^n\|_{L^\infty})(\partial_{11}\rho^{n+1}(x_0) + \partial_{22}\rho^{n+1}(x_0)) \\
&\quad\le 0.
\end{aligned} \tag{2.10}$$

Using (2.10), (2.8), (2.9) and the assumption (1.8), we see that (2.7) is reduced to

$$\begin{aligned}
&\frac{\rho^{n+1}(x_0) - \rho^n(x_0)}{\Delta t} \\
&\quad\le -(2\zeta - 2\sqrt{6}|L_4|\sqrt{\rho^n})|\nabla Q^{n+1}|^2 + 2|L_4|\sqrt{\rho^{n+1}}|\nabla Q^{n+1}|^2 \\
&\qquad - c\left(\rho^{n+1} - \frac{a^-}{c}\right)\rho^{n+1} - 2L(\rho^{n+1} - \sqrt{\rho^n}\sqrt{\rho^{n+1}})|\nabla Q^{n+1}|^2 \\
&\quad\le -[2\zeta - 2\sqrt{6}|L_4|\sqrt{\rho^n} + 2L\rho^{n+1} - (2|L_4| + 2L\sqrt{\rho^n})\sqrt{\rho^{n+1}}]|\nabla Q^{n+1}|^2. \\
&\quad= -[2\zeta - 2\sqrt{6}|L_4|\sqrt{\rho^n} + g(\sqrt{\rho^{n+1}})]|\nabla Q^{n+1}|^2,
\end{aligned} \tag{2.11}$$

where the quadratic function $g(s) = 2Ls^2 - (2|L_4| + 2L\sqrt{\rho^n})s$ in (2.11) is monotonically increasing in the interval $I_{\rho^n} = \left[\frac{|L_4|}{2L} + \frac{1}{2}\sqrt{\rho^n}, \infty\right)$, and attains its minimum at $\frac{|L_4|}{2L} + \frac{1}{2}\sqrt{\rho^n}$.

If $\sqrt{\rho^n(x_0)} \ge \frac{|L_4|}{L}$, then $\sqrt{\rho^{n+1}(x_0)} > \sqrt{\rho^n(x_0)} \ge \frac{|L_4|}{2L} + \frac{1}{2}\sqrt{\rho^n(x_0)}$, and $g(\sqrt{\rho^{n+1}}) \ge g(\sqrt{\rho^n}) = -2|L_4|\sqrt{\rho^n}$. Based on (2.3), it is easy to check from Eq. (2.11) that for the case $\sqrt{\rho^n(x_0)} \ge \frac{|L_4|}{L}$,

$$\frac{\rho^{n+1}(x_0) - \rho^n(x_0)}{\Delta t} \le -[2\zeta - 2\sqrt{6}|L_4|\sqrt{\rho^n(x_0)} - 2|L_4|\sqrt{\rho^n(x_0)}]|\nabla Q^{n+1}(x_0)|^2 \le 0,$$

which yields $|Q^{n+1}|(x_0) \le \|Q^n\|_{L^\infty(\Omega)}$, and so (2.5) holds.

On the other hand, if $\sqrt{\rho^n(x_0)} < \frac{|L_4|}{L}$, we use the global minimum of the quadratic function $g(\cdot)$ to get $g(\sqrt{\rho^{n+1}}) \geq -\frac{L}{2}\big(\frac{L_4}{L} + \sqrt{\rho^n}\big)^2$. Similarly as above, we derive from Eq. (2.11) that, for L satisfying (2.4), it holds

$$\begin{aligned}
&\frac{\rho^{n+1}(x_0) - \rho^n(x_0)}{\Delta t} \\
&\quad \leq -\left[2\zeta - 2\sqrt{6}|L_4|\sqrt{\rho^n(x_0)} - \frac{L}{2}\left(\frac{|L_4|}{L} + \sqrt{\rho^n(x_0)}\right)^2\right] |\nabla Q^{n+1}(x_0)|^2 \\
&\quad \leq -\left[2\zeta - 2\sqrt{6}|L_4|\frac{\zeta}{(1+\sqrt{6})|L_4|} - \frac{L}{2}\left(\frac{|L_4|}{L} + \frac{|L_4|}{L}\right)^2\right] |\nabla Q^{n+1}(x_0)|^2 \\
&\quad \leq -\left[2\frac{\zeta}{(1+\sqrt{6})} - \frac{2|L_4|^2}{L}\right] |\nabla Q^{n+1}(x_0)|^2 \\
&\quad \leq 0,
\end{aligned}$$

which immediately implies (2.5).

Combining all the arguments above, the proof is complete. □

Remark 2.1. It is easy to check from the proof of Lemma 2.1 that (2.5) is still valid if the right-hand side of (2.3) is replaced by any sufficiently small constant $\eta > 0$, and L satisfies (2.4).

Note that in the above Lemma 2.1 we proved that for classical solutions, the L^∞-norm at the $(n+1)$th step will remain to be small, provided that the L^∞-norm at the nth step is assumed to be small (small boundary data and $\frac{a^-}{c}$ as well). It is also worth mentioning that the smallness assumption of $\frac{a^-}{c}$ makes sense for the usual choices of the double well potential. However, we have not yet proved the existence of such classical solutions to (2.1)–(2.2). To this end, we shall apply the Leray–Schauder theory for the existence of classical solutions. For the reader's convenience, first we recall below the Leray–Schauder fixed point theorem.[14]

Theorem 2.1. (Leray–Schauder fixed point theorem) *Let $\mathcal{B}$ be a Banach space and $\mathcal{T} : \mathcal{B} \times [0,1] \to \mathcal{B}$ a compact map such that*:

(1) $\mathcal{T}(x, 0) = 0$, $\forall\, x \in \mathcal{B}$,
(2) *there exists a constant $M > 0$ such that for each pair $(x, \sigma) \in \mathcal{B} \times [0,1]$ which satisfies $x = \mathcal{T}(x, \sigma)$, we have*

$$\|x\| < M. \tag{2.12}$$

Then the map $\mathcal{T}_1 : \mathcal{B} \to \mathcal{B}$ given by $\mathcal{T}_1 y = \mathcal{T}(y, 1)$, $y \in \mathcal{B}$ has a fixed point.

By virtue of Theorem 2.1, we have

Proposition 2.1. *Let $Q^n \in C^{2+\alpha}(\bar{\Omega} \to \mathbb{R}^{2\times 2})$. Suppose $\|Q^n\|_{C^0(\bar{\Omega})}$, $\|\tilde{Q}\|_{C^0(\partial\Omega)}$ and $\frac{a^-}{c}$ are sufficiently small and L satisfies (2.4). Then there exists a classical* *solution* $Q^{n+1} \in C^{2+\alpha}(\bar{\Omega} \to \mathbb{R}^{2\times 2})$ *to the system* (2.1)–(2.2). *Furthermore*, (2.5) *is also satisfied.*

Proof. To utilize Theorem 2.1, we define

$$\mathcal{B} = C^{1+\alpha}(\bar{\Omega} \to \mathbb{R}^{2\times 2}),$$

and a map

$$\mathcal{T} : \mathcal{B} \times [0,1] \to \mathcal{B}.$$

Here $w \overset{\text{def}}{=} \mathcal{T}(u,\theta) \in C^{2+\alpha}(\bar{\Omega} \to \mathbb{R}^{2\times 2}) \subset \mathcal{B}$ with $u \in \mathcal{B}$, $\theta \in [0,1]$ solves the equation

$$\begin{aligned} &\theta \left\{ \zeta \Delta w^{ij} + 2L_4 \partial_k (Q^{lk,n} \partial_l w^{ij}) - L_4 \partial_i u^{kl} \partial_j u^{kl} + \frac{L_4}{2} |\nabla u|^2 \delta^{ij} - (a + c|u|^2) u^{ij} \right.\\ &\qquad \left. - L(u^{ij} - Q^{ij,n}) |\nabla u|^2 - \frac{u^{ij} - Q^{ij,n}}{\Delta t} \right\} + (1-\theta)\Delta w^{ij} = 0, \quad 1 \le i, \ j \le 2, \\ &w|_{\partial\Omega} = \theta \tilde{Q}. \end{aligned}$$

We proceed to prove that all conditions in Theorem 2.1 are satisfied. To begin with, it is easy to see that $\mathcal{T}(u, 0) = 0$, $\forall\, u \in \mathcal{B}$. Next we assume $(u,\sigma) \in \mathcal{B} \times [0,1]$ satisfies $u = \mathcal{T}(u,\sigma)$, that is,

$$\begin{aligned} &\partial_k \{[(\sigma\zeta + 1 - \sigma)\delta^{kl} + 2\sigma L_4 Q^{lk,n}] \partial_l u^{ij}\} \\ &\qquad = \sigma \left\{ L_4 \partial_i u^{kl} \partial_j u^{kl} - \frac{L_4}{2} |\nabla u|^2 \delta^{ij} + (a + c|u|^2) u^{ij} + L(u^{ij} - Q^{ij,n}) |\nabla u|^2 \right. \\ &\qquad\qquad \left. + \frac{u^{ij} - Q^{ij,n}}{\Delta t} \right\} \\ &\qquad \doteq \sigma f^{ij}, \quad 1 \le i, \ j \le 2, \end{aligned} \tag{2.13}$$

$$u|_{\partial\Omega} = \sigma \tilde{Q}. \tag{2.14}$$

Then, following the same procedure in Lemma 2.1, one may conclude

$$\|u\|_{C^0} \le \max\left\{ \|Q^n\|_{C^0}, \sqrt{\frac{a^-}{c}} \right\}, \tag{2.15}$$

provided that $\|Q^n\|_{C^0}$, $\|\tilde{Q}\|_{C^0(\partial\Omega)}$ and $\frac{a^-}{c}$ are sufficiently small. As a consequence, using the classical Schauder estimate (see Theorem 6.6 in Ref. 14), interpolation inequality and Young's inequality, one can derive from (2.13)–(2.14) that for sufficiently small $\|Q^n\|_{C^0}$, we have

$$\begin{aligned} \|u\|_{C^{2+\alpha}} &\le C\|u\|_{C^0} + C\|\tilde{Q}\|_{C^{2+\alpha}} + C\|\sigma f\|_{C^\alpha} \\ &\le C\|Q^n\|_{C^0} + C + C\|f\|_{C^\alpha} \\ &\le C + C\||\nabla u|^2\|_{C^\alpha} + C\|au + c|u|^2 u\|_{C^\alpha} + C\|u|\nabla u|^2\|_{C^\alpha} \\ &\quad + C\|Q^n|\nabla u|^2\|_{C^\alpha} + C(\|u\|_{C^\alpha} + \|Q^n\|_{C^\alpha}) \end{aligned}$$

$$
\begin{aligned}
&\le C + C\|u\|_{C^\alpha} + C\||\nabla u|^2\|_{C^\alpha} + C\|u|\nabla u|^2\|_{C^\alpha} + C\|Q^n|\nabla u|^2\|_{C^\alpha}\\
&\le C + C\|u\|_{C^0}^{\frac{2}{2+\alpha}}\|u\|_{C^{2+\alpha}}^{\frac{\alpha}{2+\alpha}} + C\||\nabla u|\|_{C^0}\||\nabla u|\|_{C^\alpha}\\
&\quad + C(\|u\|_{C^0} + \|Q^n\|_{C^0})\||\nabla u|^2\|_{C^\alpha} + C\big(\|u\|_{C^\alpha} + \|Q^n\|_{C^\alpha}\big)\||\nabla u|^2\|_{C^0}\\
&\le C + C\|u\|_{C^0}^{\frac{2}{2+\alpha}}\|u\|_{C^{2+\alpha}}^{\frac{\alpha}{2+\alpha}} + C\|u\|_{C^0}\|u\|_{C^{2+\alpha}}\\
&\quad + C(\|u\|_{C^0} + \|Q^n\|_{C^0})\|u\|_{C^0}\|u\|_{C^{2+\alpha}} + C\|u\|_{C^0}^2\|u\|_{C^{2+\alpha}}\\
&\quad + C\|Q^n\|_{C^0}^{\frac{2}{2+\alpha}}\|Q^n\|_{C^{2+\alpha}}^{\frac{\alpha}{2+\alpha}}\|u\|_{C^0}^{\frac{2+2\alpha}{2+\alpha}}\|u\|_{C^{2+\alpha}}^{\frac{2}{2+\alpha}}\\
&\le C + \frac{1}{2}\|u\|_{C^{2+\alpha}}. \qquad (2.16)
\end{aligned}
$$

In the above $C > 0$ is a generic constant that may depend on Ω, Δt, $\|Q_0\|_{C^0}$, $\|\tilde{Q}\|_{C^{2+\alpha}}$, $\|Q^n\|_{C^{2+\alpha}}$ and coefficients of the system. Therefore (2.12) is valid. In addition, it is easy to check that $\mathcal{T}$ is a compact map due to the compact embedding $C^{2+\alpha}(\bar{\Omega}) \hookrightarrow C^{1+\alpha}(\bar{\Omega})$. Thus all conditions in Theorem 2.1 are satisfied and in conclusion $\mathcal{T}_1 y = \mathcal{T}(y, 1)$ has a fixed point, which is equivalent to say that the system (2.1)–(2.2) admits a classical solution $Q^{n+1} \in C^{2+\alpha}(\bar{\Omega})$. $\square$

For classical solutions whose existence was proved in Proposition 2.1 above, we proceed to establish some useful uniform estimates. Before that, we recall several well-known results that involves Gagliardo–Nirenberg inequalities and elliptic PDE theory.

Lemma 2.2. *There exists a positive constant $C = C(\Omega)$, such that for any $f \in H^2(\Omega)$ and $g \in H^{\frac{3}{2}}(\partial\Omega)$, with $f|_{\partial\Omega} = g$, it holds*:

$$
\begin{aligned}
\|f\|_{L^\infty(\Omega)} &\le C\|f\|^{\frac{1}{2}}\left(\|\Delta f\|^{\frac{1}{2}} + \|f\|^{\frac{1}{2}} + \|g\|^{\frac{1}{2}}_{H^{\frac{3}{2}}}\right),\\
\|D^2 f\| &\le C\left(\|\Delta f\| + \|f\| + \|g\|_{H^{\frac{3}{2}}(\partial\Omega)}\right).
\end{aligned} \qquad (2.17)
$$

For any $f \in H^2(\Omega)$, the following interpolation inequality holds

$$
\|\nabla f\|_{L^4}^2 \le C\|f\|_{L^\infty}\left(\|\Delta f\|_{L^2} + \|f\| + \|g\|_{H^{\frac{3}{2}}}\right). \qquad (2.18)
$$

And further for $f \in H_0^1(\Omega)$, the following Ladyzhenskaya inequality is valid:

$$
\|f\|_{L^4(\Omega)}^2 \le C\|\nabla f\|\|f\|. \qquad (2.19)
$$

Remark 2.2. The proofs of (2.17) follow from Theorems 5.2, 5.8 in Ref. 1 together with Theorem 6.3.2.4 in Ref. 12. The estimate (2.18) is a consequence of Ref. 6 combined with the elliptic regularity result previously mentioned.

Proposition 2.2. *The classical solutions established in Proposition* 2.1 *satisfy the following uniform bounds*:

$$\|\nabla Q^{n+1}\|^2_{L^2(\Omega)} \le CT + C\|\Delta Q^0\|^2_{L^2(\Omega)}\Delta t + \|\nabla Q^0\|^2_{L^2(\Omega)}, \quad \forall\, 0 \le n < \left[\frac{T}{\Delta t}\right], \tag{2.20}$$

$$\sum_{n=1}^{\left[\frac{T}{\Delta t}\right]} \|\Delta Q^n\|^2_{L^2(\Omega)}\Delta t \le CT + \|\nabla Q^0\|^2_{L^2(\Omega)} + \|\Delta Q^0\|^2_{L^2(\Omega)}\Delta t, \tag{2.21}$$

provided that there exists a sufficiently small (*but computable*) *constant* $\varepsilon > 0$ *such that*

$$\max\left\{\|Q^0\|_{L^\infty(\Omega)}, \|\tilde{Q}\|_{L^\infty(\partial\Omega)}, \sqrt{\frac{a^-}{c}}\right\} \le \varepsilon. \tag{2.22}$$

Here $C > 0$ *is a constant that only depends on* ζ, ε, Ω, a, c *and* L_4, *but independent of* n *or* Δt.

Proof. Multiplying Eq. (2.1) with $-\Delta Q^{ij,n+1}$ and integrating over Ω, we find

$$\begin{aligned}
&\frac{1}{2\Delta t}\int_\Omega |\nabla Q^{n+1}|^2 + |\nabla Q^{n+1} - \nabla Q^n|^2 - |\nabla Q^n|^2\, dx \\
&\quad = -\zeta\int_\Omega |\Delta Q^{n+1}|^2\, dx + a\int_\Omega Q^{ij,n+1}\Delta Q^{ij,n+1} dx \\
&\qquad + c\int_\Omega |Q^{n+1}|^2 Q^{ij,n+1}\Delta Q^{ij,n+1} dx \\
&\qquad + L\int_\Omega |\nabla Q^{n+1}|^2 (Q^{ij,n+1} - Q^{ij,n})\Delta Q^{ij,n+1} dx \\
&\qquad - 2L_4\int_\Omega Q^{lk,n}\partial_{kl}Q^{ij,n+1}\Delta Q^{ij,n+1} dx - L_4\int_\Omega \Big\{2\partial_k Q^{lk,n}\partial_l Q^{ij,n+1} \\
&\qquad - \partial_i Q^{kl,n+1}\partial_j Q^{kl,n+1} + \frac{|\nabla Q^{n+1}|^2}{2}\delta^{ij}\Big\}\Delta Q^{ij,n+1} dx \\
&\quad = -\zeta\int_\Omega |\Delta Q^{n+1}|^2\, dx + I_1 + \cdots + I_5.
\end{aligned} \tag{2.23}$$

We estimate below the terms I_1 through I_5 individually. To begin with, it follows from (2.5) and (2.22) that

$$\|Q^{n+1}\|_{L^\infty(\Omega)} \le \varepsilon. \tag{2.24}$$

Using Young's inequality and (2.24), we obtain

$$I_1 + I_2 \le \frac{\zeta}{8}\|\Delta Q^{n+1}\|^2 + C(\|Q^{n+1}\|^2_{L^2} + \|Q^{n+1}\|^6_{L^6})$$

$$\le \frac{\zeta}{8}\|\Delta Q^{n+1}\|^2 + C\big(\varepsilon^2+\varepsilon^6\big)|\Omega|$$
$$\le \frac{\zeta}{8}\|\Delta Q^{n+1}\|^2 + C. \tag{2.25}$$

By (2.24) and Lemma 2.2, we get

$$\begin{aligned}I_3 &\le L\|\nabla Q^{n+1}\|_{L^4}^2(\|Q^{n+1}\|_{L^\infty}+\|Q^n\|_{L^\infty})\|\Delta Q^{n+1}\|_{L^2}\\ &\le C(\|Q^{n+1}\|_{L^\infty}+\|Q^n\|_{L^\infty})\|Q^{n+1}\|_{L^\infty}\Big(\|\Delta Q^{n+1}\|_{L^2}+\|Q^{n+1}\|_{L^2}+\|\tilde{Q}\|_{H^{\frac{3}{2}}(\partial\Omega)}\Big)\\ &\quad\times\|\Delta Q^{n+1}\|_{L^2}\\ &\le C\varepsilon^2\Big(\|\Delta Q^{n+1}\|_{L^2}+\|Q^{n+1}\|_{L^2}+\|\tilde{Q}\|_{H^{\frac{3}{2}}(\partial\Omega)}\Big)\|\Delta Q^{n+1}\|_{L^2}\\ &\le \frac{\zeta}{8}\|\Delta Q^{n+1}\|^2 + C,\end{aligned} \tag{2.26}$$

and

$$\begin{aligned}I_4 &\le 2|L_4|\|Q^n\|_{L^\infty}\|\nabla^2 Q^{n+1}\|_{L^2}\|\Delta Q^{n+1}\|_{L^2}\\ &\le C\|Q^n\|_{L^\infty}\Big(\|\Delta Q^{n+1}\|_{L^2}+\|Q^{n+1}\|_{L^2}+\|\tilde{Q}\|_{H^{\frac{3}{2}}(\partial\Omega)}\Big)\|\Delta Q^{n+1}\|_{L^2}\\ &\le \frac{\zeta}{8}\|\Delta Q^{n+1}\|^2 + C.\end{aligned} \tag{2.27}$$

Similarly as in the estimate of I_3, we can obtain

$$\begin{aligned}I_5 &\le 2|L_4|\|\nabla Q^n\|_{L^4}\|\nabla Q^{n+1}\|_{L^4}\|\Delta Q^{n+1}\|_{L^2} + 2|L_4|\|\nabla Q^{n+1}\|_{L^4}^2\|\Delta Q^{n+1}\|_{L^2}\\ &\le \frac{\zeta}{4}\|\Delta Q^n\|^2+\frac{\zeta}{8}\|\Delta Q^{n+1}\|^2 + C.\end{aligned} \tag{2.28}$$

Combining the above we conclude that $\forall\, 0 \le n < \big[\frac{T}{\Delta t}\big]$, it holds

$$\begin{aligned}&\|\nabla Q^{n+1}\|_{L^2}^2+\|\nabla Q^{n+1}-\nabla Q^n\|_{L^2}^2-\|\nabla Q^n\|_{L^2}^2\\ &\quad\le -\zeta\|\Delta Q^{n+1}\|_{L^2}^2\Delta t+\frac{\zeta}{2}\|\Delta Q^n\|_{L^2}^2\Delta t + C\Delta t.\end{aligned} \tag{2.29}$$

As a consequence, summing up the above estimate (2.29) for n from 0 to $\big[\frac{T}{\Delta t}\big]-1$ leads to (2.20) and (2.21). □

Based on the uniform estimates (2.20) and (2.21) established in Proposition 2.2, we can further obtain the uniqueness result concerning the classical solutions of the system (2.1)–(2.2).

Proposition 2.3. *Let $Q^n \in C^{2+\alpha}(\bar{\Omega})$. Suppose $P^{n+1}, Q^{n+1} \in C^{2+\alpha}(\bar{\Omega})$ are two classical solutions to the problem* (2.1)–(2.2) *that satisfy* (2.24). *If ε in Proposition* 2.2 *is chosen to be suitably small* (*but independent of n or Δt*), *then*

$$P^{n+1} \equiv Q^{n+1}.$$

Proof. Let $\bar{R}^{n+1} = Q^{n+1} - P^{n+1}$. We have

$$\begin{aligned}
&\frac{\bar{R}^{ij,n+1}}{\Delta t}\\
&\quad = \zeta\Delta\bar{R}^{ij,n+1} - a\bar{R}^{ij,n+1} - c(|Q^{n+1}|^2 Q^{ij,n+1} - |P^{n+1}|^2 P^{ij,n+1})\\
&\qquad - L(Q^{ij,n+1}|\nabla Q^{n+1}|^2 - P^{ij,n+1}|\nabla P^{n+1}|^2) + LQ^{ij,n}(|\nabla Q^{n+1}|^2 - |\nabla P^{n+1}|^2)\\
&\qquad + 2L_4\partial_k(Q^{lk,n}\partial_l\bar{R}^{ij,n+1}) - L_4(\partial_i Q^{lk,n+1}\partial_j Q^{lk,n+1} - \partial_i P^{lk,n+1}\partial_j P^{lk,n+1})\\
&\qquad + \frac{L_4}{2}(|\nabla Q^{n+1}|^2 - |\nabla P^{n+1}|^2)\delta^{ij}, \qquad (2.30)\\
&\bar{R}^{n+1}|_{\partial\Omega} = 0. \qquad (2.31)
\end{aligned}$$

Multiplying Eq. (2.30) with $\bar{R}^{n+1}$, integrating over Ω and using the boundary condition (2.31), we obtain

$$\begin{aligned}
\frac{\|\bar{R}^{n+1}\|_{L^2}^2}{\Delta t} &= -\zeta\|\nabla\bar{R}^{n+1}\|_{L^2}^2 - a\|\bar{R}^{n+1}\|_{L^2}^2\\
&\quad - c\int_\Omega (|Q^{n+1}|^2 Q^{ij,n+1} - |P^{n+1}|^2 P^{ij,n+1})\bar{R}^{ij,n+1}dx\\
&\quad - L\int_\Omega (|\nabla Q^{n+1}|^2 Q^{ij,n+1} - |\nabla P^{n+1}|^2 P^{ij,n+1})\bar{R}^{ij,n+1}dx\\
&\quad + L\int_\Omega (|\nabla Q^{n+1}|^2 - |\nabla P^{n+1}|^2)Q^{ij,n}\bar{R}^{ij,n+1}dx\\
&\quad - 2L_4\int_\Omega Q^{lk,n}\partial_l\bar{R}^{ij,n+1}\partial_k\bar{R}^{ij,n+1}dx\\
&\quad - L_4\int_\Omega (\partial_i Q^{lk,n+1}\partial_j Q^{lk,n+1} - \partial_i P^{lk,n+1}\partial_j P^{lk,n+1})\bar{R}^{ij,n+1}dx\\
&\quad + \frac{L_4}{2}\int_\Omega (|\nabla Q^{n+1}|^2 - |\nabla P^{n+1}|^2)\mathrm{tr}(\bar{R}^{n+1})dx\\
&= -\zeta\|\nabla\bar{R}^{n+1}\|_{L^2}^2 + I_1 + \cdots + I_7. \qquad (2.32)
\end{aligned}$$

Note that both P^{n+1} and Q^{n+1} satisfy (2.20)–(2.21) and (2.24). Hence

$$\begin{aligned}
I_1 + I_2 &\le -a\|\bar{R}^{n+1}\|_{L^2}^2 + c\|\bar{R}^{n+1}\|_{L^2}^2(\|Q^{n+1}\|_{L^\infty}^2\\
&\qquad + \|Q^{n+1}\|_{L^\infty}\|P^{n+1}\|_{L^\infty} + \|P^{n+1}\|_{L^\infty}^2)\\
&\le c\left(3\varepsilon^2 - \frac{a}{c}\right)\|\bar{R}^{n+1}\|_{L^2}^2\\
&\le 4c\varepsilon^2\|\bar{R}^{n+1}\|_{L^2}^2,
\end{aligned}$$

where we used (2.22) to derive the last inequality.

Using (2.5), (2.24) and Lemma 2.2, we have

$$\begin{aligned}
I_3 &\le L[\|P^{n+1}\|_{L^\infty}(\|\nabla Q^{n+1}\|_{L^4}+\|\nabla P^{n+1}\|_{L^4})\times\|\nabla\bar R^{n+1}\|_{L^2}\|\bar R^{n+1}\|_{L^4}\\
&\quad+\|\bar R^{n+1}\|_{L^4}^2\|\nabla Q^{n+1}\|_{L^4}^2]\\
&\le CL\|\bar R^{n+1}\|_{L^2}\|\nabla\bar R^{n+1}\|_{L^2}\|Q^{n+1}\|_{L^\infty}\left(\|\Delta Q^{n+1}\|_{L^2}+\|Q^{n+1}\|_{L^2}+\|\tilde Q\|_{H^{\frac32}(\partial\Omega)}\right)\\
&\quad+CL\|P^{n+1}\|_{L^\infty}\|\bar R^{n+1}\|_{L^2}^{\frac12}\|\nabla\bar R^{n+1}\|_{L^2}^{\frac32}\left[\left(\|\Delta Q^{n+1}\|_{L^2}+\|Q^{n+1}\|_{L^2}+\|\tilde Q\|_{H^{\frac32}(\partial\Omega)}\right)^{\frac12}\right.\\
&\quad\left.\times\|Q^{n+1}\|_{L^\infty}^{\frac12}+\|P^{n+1}\|_{L^\infty}^{\frac12}\left(\|\Delta P^{n+1}\|_{L^2}+\|P^{n+1}\|_{L^2}+\|\tilde Q\|_{H^{\frac32}(\partial\Omega)}\right)^{\frac12}\right]\\
&\le CL\|\bar R^{n+1}\|_{L^2}\|\nabla\bar R^{n+1}\|_{L^2}\|Q^0\|_{L^\infty}(\|\Delta Q^{n+1}\|_{L^2}+1)\\
&\quad+CL\|\bar R^{n+1}\|_{L^2}^{\frac12}\|\nabla\bar R^{n+1}\|_{L^2}^{\frac32}\|Q^0\|_{L^\infty}^{\frac32}(\|\Delta Q^{n+1}\|_{L^2}+\|\Delta P^{n+1}\|_{L^2}+1)^{\frac12}\\
&\le C\varepsilon\|\bar R^{n+1}\|_{L^2}\|\nabla\bar R^{n+1}\|_{L^2}(\|\Delta Q^{n+1}\|_{L^2}+1)\\
&\quad+C\varepsilon^{\frac32}\|\bar R^{n+1}\|_{L^2}^{\frac12}\|\nabla\bar R^{n+1}\|_{L^2}^{\frac32}(\|\Delta Q^{n+1}\|_{L^2}+\|\Delta P^{n+1}\|_{L^2}+1)^{\frac12}\\
&\le\frac{\zeta}{8}\|\nabla\bar R^{n+1}\|_{L^2}^2+C\varepsilon(\|\Delta Q^{n+1}\|_{L^2}^2+\|\Delta P^{n+1}\|_{L^2}^2+1)\|\bar R^{n+1}\|_{L^2}^2.
\end{aligned}$$

Similarly,

$$\begin{aligned}
I_4 &\le L\|\nabla\bar R^{n+1}\|_{L^2}\|\bar R^{n+1}\|_{L^4}(\|\nabla Q^{n+1}\|_{L^4}+\|\nabla P^{n+1}\|_{L^4})\|Q^n\|_{L^\infty}\\
&\le\frac{\zeta}{8}\|\nabla\bar R^{n+1}\|_{L^2}^2+C\varepsilon\big(\|\Delta Q^{n+1}\|_{L^2}^2+\|\Delta P^{n+1}\|_{L^2}^2+1\big)\|\bar R^{n+1}\|_{L^2}^2.
\end{aligned}$$

We derive from (2.5) that

$$I_5\le 2|L_4|\|Q^n\|_{L^\infty}\|\nabla\bar R^{n+1}\|_{L^2}^2\le 2|L_4|\varepsilon\|\nabla\bar R^{n+1}\|_{L^2}^2\le\frac{\zeta}{8}\|\nabla\bar R^{n+1}\|_{L^2}^2.$$

We can control I_6 and I_7 in a manner similar for I_3, namely:

$$\begin{aligned}
I_6+I_7 &\le 2|L_4|\|\nabla\bar R^{n+1}\|_{L^2}\|\bar R^{n+1}\|_{L^4}(\|\nabla Q^{n+1}\|_{L^4}+\|\nabla P^{n+1}\|_{L^4})\\
&\le\frac{\zeta}{8}\|\nabla\bar R^{n+1}\|_{L^2}^2+C\varepsilon(\|\Delta Q^{n+1}\|_{L^2}^2+\|\Delta P^{n+1}\|_{L^2}^2+1)\|\bar R^{n+1}\|_{L^2}^2.
\end{aligned}$$

After summing up the above inequalities in (2.32), we get

$$\begin{aligned}
\frac{\|\bar R^{n+1}\|_{L^2}^2}{\Delta t} &\le -\frac{\zeta}{2}\|\nabla\bar R^{n+1}\|_{L^2}^2+4c\varepsilon^2\|\bar R^{n+1}\|_{L^2}^2\\
&\quad+C\varepsilon(\|\Delta Q^{n+1}\|_{L^2}^2+\|\Delta P^{n+1}\|_{L^2}^2+1)\|\bar R^{n+1}\|_{L^2}^2. \qquad (2.33)
\end{aligned}$$

Finally, we derive from (2.21) and the above inequality that

$$\|\bar R^{n+1}\|_{L^2}^2\le 4c\varepsilon^2\|\bar R^{n+1}\|_{L^2}^2+C\varepsilon(2CT+C+\Delta t)\|\bar R^{n+1}\|_{L^2}^2\le\frac12\|\bar R^{n+1}\|_{L^2}^2,$$

provided ε is chosen to be sufficiently small. Therefore we conclude

$$\bar{R}^{n+1} \equiv 0. \qquad \square$$

2.2. *Convergence*

Next we shall construct a family of approximate solutions using linear interpolation in time. The above *a priori* estimates for the set of discrete solutions allow us to obtain the existence of a time-continuous limit function which we will show to be a solution of the original PDE system (1.9)–(1.10).

Let us fix the initial data Q^0 and step size $h \stackrel{\text{def}}{=} \Delta t$ and define a piecewise linear interpolation $t \in [0,T) \to Q_h(\cdot,t)$ as

$$Q_h(x,t) = Q^n(x) + \frac{Q^{n+1}(x) - Q^n(x)}{h}(t - nh), \quad \forall\, x \in \Omega,\ nh \le t < (n+1)h, \tag{2.34}$$

where $0 \le n < \left[\frac{T}{h}\right]$. Based on Eq. (2.1) and the above construction (2.34), we know that Q_h satisfies

$$\begin{aligned} \partial_t Q_h^{ij}(t,x) &= \zeta \Delta Q_h^{ij}(x,nh) - aQ_h^{ij}(x,nh) - c|Q_h(x,nh)|^2 Q_h^{ij}(x,nh) \\ &\quad - L[Q_h^{ij}(nh,x) - Q_h^{ij}(nh-h,x)]|\nabla Q_h(nh,x)|^2 \\ &\quad + L_4 \Bigg\{ 2\partial_k [Q_h^{lk}(nh-h,x)\partial_l Q_h^{ij}(x,nh)] - \partial_i Q_h^{kl}(x,nh)\partial_j Q_h^{kl}(x,nh) \\ &\quad + \frac{|\nabla Q_h(x,nh)|^2}{2}\delta^{ij} \Bigg\}, \end{aligned} \tag{2.35}$$

$$\forall\, x \in \Omega, \quad (n-1)h \le t < nh,\ \ 1 \le n \le \left[\frac{T}{h}\right]. \tag{2.36}$$

We collect from Proposition 2.2 and Eq. (2.35) the following uniform bounds:

$$\|\nabla Q_h(\cdot,t)\|^2_{L^2(\Omega)} \le CT + C\|\Delta Q^0\|^2_{L^2(\Omega)}\Delta t + \|\nabla Q^0\|^2_{L^2(\Omega)}, \quad \forall\, t \in (0,T), \tag{2.37}$$

$$\int_0^T \|\Delta Q_h(\cdot,t)\|^2_{L^2(\Omega)} dt \le CT + C\|\Delta Q^0\|^2_{L^2(\Omega)}\Delta t + \|\nabla Q^0\|^2_{L^2(\Omega)}, \tag{2.38}$$

$$\int_0^T \|\partial_t Q_h(\cdot,t)\|^2_{L^2(\Omega)} dt \le CT + C. \tag{2.39}$$

In the above $C > 0$ is a generic constant that does not depend on h.

As a consequence, as $h \to 0$, we have from Aubin–Lions lemma (see Ref. 31) that the following results hold.

Theorem 2.2. (Main result) *Let $Q^0, \tilde{Q} \in C^{2+\alpha}(\bar{\Omega} \to \mathbb{R}^{2\times 2})$. Suppose $\|Q^0\|_{C^0(\bar{\Omega})}$, $\|\tilde{Q}\|_{C^0(\partial\Omega)}$ and $\frac{a^-}{c}$ are sufficiently small and L satisfies* (2.4)*. Then the numerical scheme* (2.1)–(2.2) *admits unique solutions Q^n for $n \ge 1$, and the piecewise linear* *interpolation* $Q_h(t)$ *of the numerical solution given in* (2.34) *converges to an exact solution of* (1.9)–(1.10), *i.e.*:

$$Q_h(\cdot,t) \to Q(\cdot,t) \quad \textit{strong in } L^2(0,T;H^1(\Omega)),$$
$$Q_h(\cdot,t) \to Q(\cdot,t) \quad \textit{weakly in } L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)),$$

where $Q(\cdot,t)$ *solves*:

$$\begin{aligned} \partial_t Q^{ij} &= \zeta \Delta Q^{ij} - [a + c\,\mathrm{tr}(Q^2)]Q^{ij} \\ &\quad + L_4 \left\{ 2\partial_k(Q^{lk}\partial_l Q^{ij}) - \partial_i Q^{kl}\partial_j Q^{kl} + \frac{|\nabla Q|^2\delta^{ij}}{2} \right\}, \\ Q|_{\partial\Omega} &= \tilde{Q}, \quad Q(0,x) = Q^0(x) \end{aligned}$$

in the weak sense defined in Definition 2.1 *below.*

We can also check directly that the limit solution Q always lies in the Q-tensor space $\mathcal{S}^{(2)}$, provided $Q^0, \tilde{Q} \in \mathcal{S}^{(2)}$.

Next, we recall the notion of weak solutions discussed in Ref. 18.

Definition 2.1. For any $T \in (0,+\infty)$, a function Q satisfying

$$Q \in L^\infty(0,T;H^1 \cap L^\infty) \cap L^2(0,T;H^2), \quad \partial_t Q \in L^2(0,T;L^2),$$

and $Q \in S^{(2)}$ a.e. in $\Omega \times (0,T)$, is called a weak solution of the problem (1.9)–(1.10), if it satisfies the initial and boundary conditions (1.10), and we have

$$\begin{aligned} &-\int_{\Omega\times[0,T]} Q : \partial_t R\,dx\,dt \\ &\quad= -2L_1 \int_{\Omega\times[0,T]} \partial_k Q : \partial_k R\,dx\,dt - \int_{\Omega\times[0,T]} \big[a + c\mathrm{tr}(Q^2)\big]Q : R\,dx\,dt \\ &\qquad - 2(L_2+L_3)\int_{\Omega\times[0,T]} \partial_k Q_{ik}\partial_j R_{ij}\,dx\,dt \\ &\qquad + (L_2+L_3)\int_{\Omega\times[0,T]} \partial_k Q_{lk}\partial_l R_{ii}\,dx\,dt \\ &\qquad - 2L_4\int_{\Omega\times[0,T]} Q_{lk}\partial_k Q_{ij}\partial_l R_{ij}\,dx\,dt - L_4\int_{\Omega\times[0,T]} \partial_i Q_{kl}\partial_j Q_{kl} R_{ij}\,dx\,dt \\ &\qquad + \frac{L_4}{2}\int_{\Omega\times[0,T]} |\nabla Q|^2 R_{ii}\,dx\,dt - \int_\Omega Q_0 : R(0)dx. \end{aligned}$$

Here $R \in C_c^\infty([0,T)\times\Omega \to \mathbb{R}^{2\times 2})$ is arbitrary.

Summing up the above, we obtained the well-posedness result for (1.9)–(1.10), which was also established in Refs. 7 and 18 by using completely different approaches.

Corollary 2.1. *Let* $Q^0, \tilde{Q} \in C^{2+\alpha}(\bar{\Omega})$. *For any fixed* $T > 0$, *suppose* $\|Q^0\|_{L^\infty(\Omega)}$, $\|\tilde{Q}\|_{L^\infty(\partial\Omega)}$ *and* $\frac{a^-}{c}$ *are sufficiently small. Then there exists a unique solution* $Q(x,t)$ *to the problem* (1.9)–(1.10), *with the following properties*:

$$Q \in L^\infty(0,T; L^\infty(\Omega) \cap H^1(\Omega)) \cap L^2(0,T; H^2(\Omega)),$$

and $Q(x,t) \in \mathcal{S}^{(2)}\ \forall\,(x,t) \in \Omega \times [0,T]$. *Further,* $\|Q\|_{L^\infty(\Omega)}$ *always stays small during evolution.*

It is worth mentioning that the regularity in Corollary 2.1 can be improved using bootstrap argument so that the weak solution Q is indeed a classical solution.

Next let us recall Lemma 3.2 in Ref. 18 that relates to the continuous dependence on the initial data.

Lemma 2.3. *Let*

$$Q_i \in L^\infty(0,T; L^\infty(\Omega) \cap H^1(\Omega)) \cap L^2(0,T; H^2(\Omega)) \quad (i = 1,2)$$

be two global weak solutions to the problem (1.9)–(1.10) *on* $(0,T)$, *with initial data* $Q_{01}, Q_{02} \in L^\infty(\Omega) \cap H^1(\Omega)$. *Suppose* $\|Q_{0i}\|_{L^\infty(\Omega)}$ $(i = 1,2)$ *are sufficiently small. Then for any* $t \in (0,T)$, *we have*

$$\|(Q_1 - Q_2)(t)\|_{L^2(\Omega)} \le Ce^{Ct}\|Q_{01} - Q_{02}\|_{L^2(\Omega)}, \tag{2.40}$$

where $C > 0$ *is a constant that depends on* Ω, Q_{0i} $(i = 1,2)$, $\tilde{Q}$ *and the coefficients of the system, but not* t.

By virtue of Lemma 2.3, we may relax the regularity assumption on the initial data Q^0, and henceforth we state the existence result as follows:

Corollary 2.2. *Let* $Q^0 \in H^1(\Omega) \cap L^\infty(\Omega)$, $\tilde{Q} \in C^{2+\alpha}(\bar{\Omega})$. *For any fixed* $T > 0$, *suppose* $\|Q^0\|_{L^\infty(\Omega)}$, $\|\tilde{Q}\|_{L^\infty(\partial\Omega)}$ *and* $\frac{a^-}{c}$ *are sufficiently small. Then there exists a unique global weak solution* $Q(x,t)$ *to the problem* (1.9)–(1.10) *that satisfies*:

$$Q \in L^\infty(0,T; L^\infty(\Omega) \cap H^1(\Omega)) \cap L^2(0,T; H^2(\Omega)),$$

$$Q(x,t) \in \mathcal{S}^{(2)}, \quad \forall\,(x,t) \in \Omega \times [0,T].$$

Further, the smallness of the L^∞*-norm of* Q *is preserved during evolution.*

Proof. For $Q^0 \in L^\infty(\Omega) \cap H^1(\Omega)$, let us use the standard mollifier to establish $Q^{\varepsilon,0} \in C^{2+\alpha}$ $(\varepsilon \to 0)$ with $Q^{\varepsilon,0} \to Q^0$ in $H^1(\Omega)$, and $\|Q^{\varepsilon,0}\|_{L^\infty} \le \|Q^0\|_{L^\infty}$. Then $Q^\varepsilon(t)$ is the corresponding solution with initial data $Q^{\varepsilon,0}$. As $Q^\varepsilon \in L(0,T; L^\infty \cap H^1) \cap L^2(0,T; H^2)$ and such bounds depend on the $L^\infty \cap H^1$ bound of Q^0 only, Q^ε is a Cauchy sequence in $L^\infty(0,T; L^2(\Omega))$. Hence we define $Q(x,t) = \lim_{\varepsilon\to 0} Q^\varepsilon(x,t)$

that solves the equation weakly. Then we may proceed as before and the proof is complete. □

Remark 2.3. It is pointed out in Corollary 2.2 that the initial data Q^0 of the evolution problem (1.9)–(1.10) can be relaxed from $C^{2+\alpha}$ to $H^1 \cap L^\infty$. Regarding the boundary data $\tilde{Q}$, however, it seems that we cannot relax its regularity because of the Schauder estimates used in Proposition 2.1. On the other hand, one may easily find that it suffices to assume $\tilde{Q} \in C^0(\partial\Omega)$ to perform the maximum principle argument in Lemma 2.1.

Remark 2.4. This part can be considered as an ongoing work after the PDE analysis in Ref. 18. First of all, concerning the preservation of smallness of $\|Q_0\|_{L^\infty(\Omega)}$, the proof (see Proposition 2.1 in Ref. 18) is based on a time-continuity argument that heavily relies on the structure of the PDE system (1.9). However, it is no longer valid once we perform the time discretization to the PDE system. To this end we need to add a stabilizing term and such arguments are achieved in an alternative way shown in Lemma 2.1. Secondly, to prove the existence of solutions, in Ref. 18 a quite lengthy and complicated three-level approximation scheme combining singular potential and Galerkin method is proposed; while here in Proposition 2.1 we use Leray–Schauder existence theory to obtain the existence of regular solutions to the discrete-in-time scheme (2.1)–(2.2) for each fixed n and Δt first, then we establish uniform energy estimates for each Q^n and next study the convergence from the discrete-in-time problem to the PDE problem as the time step $\Delta t \to 0$.

3. Numerical Experiments

We have shown in the previous section that the proposed numerical scheme preserves the symmetric and traceless properties of the tensor Q^n ($n \geq 1$), provided the initial state Q^0 and boundary value are in the Q-tensor space $\mathcal{S}^{(2)}$. By parametrizing Q as

$$Q(\cdot,t) = \begin{pmatrix} p(\cdot,t) & q(\cdot,t) \\ q(\cdot,t) & -p(\cdot,t) \end{pmatrix}, \quad Q(\cdot,0) = Q^0 = \begin{pmatrix} p^0 & q^0 \\ q^0 & -p^0 \end{pmatrix}, \tag{3.1}$$

the numerical scheme (2.1)–(2.2) can be rewritten as:

$$\begin{aligned} \frac{p^{n+1}-p^n}{\Delta t} &= -ap^{n+1} - 2c(|p^{n+1}|^2 + |q^{n+1}|^2)p^{n+1} - 2L(p^{n+1}-p^n) \\ &\quad \times (|\nabla p^{n+1}|^2 + |\nabla q^{n+1}|^2) + 2L_4(p^n\partial_{xx}p^{n+1} - p^n\partial_{yy}p^{n+1} \\ &\quad + 2q^n\partial_{xy}p^{n+1} + \partial_x p^n \partial_x p^{n+1} - \partial_y p^n \partial_y p^{n+1}) \\ &\quad + L_4(2\partial_x q^n \partial_y p^{n+1} + 2\partial_y q^n \partial_x p^{n+1} + |\partial_y p^{n+1}|^2 + |\partial_y q^{n+1}|^2 \\ &\quad - |\partial_x p^{n+1}|^2 - |\partial_x q^{n+1}|^2) + \zeta\Delta p^{n+1}, \end{aligned}$$

$$\begin{aligned}\frac{q^{n+1}-q^n}{\Delta t} &= -aq^{n+1} - 2c(|p^{n+1}|^2 + |q^{n+1}|^2)q^{n+1} \\ &\quad - 2L(q^{n+1}-q^n)(|\nabla p^{n+1}|^2 + |\nabla q^{n+1}|^2) \\ &\quad + 2L_4(p^n\partial_{xx}q^{n+1} - p^n\partial_{yy}q^{n+1} + 2q^n\partial_{xy}q^{n+1} + \partial_x p^n\partial_x q^{n+1} \\ &\quad - \partial_y p^n\partial_y q^{n+1}) + 2L_4(\partial_x q^n\partial_y q^{n+1} + \partial_y q^n\partial_x q^{n+1} - \partial_x p^{n+1}\partial_y p^{n+1} \\ &\quad - \partial_x q^{n+1}\partial_y q^{n+1}) + \zeta\Delta q^{n+1}. \end{aligned} \tag{3.2}$$

We now describe briefly our numerical approach. For simplicity of implementation, we consider the periodic boundary conditions and use the Fourier spectral method[15] for the space variable. Thus at each time step, we have a coupled nonlinear system for the Fourier approximation of (p^{n+1}, q^{n+1}), which will be solved by using the Newton iteration method. In detail, we start with $(p^{(0)}, q^{(0)}) = (p^n, q^n)$, and update the Newton iteration $(p^{(k)}, q^{(k)})$ for $k \geq 1$ as:

$$p^{(k)} = p^{(k-1)} + \tilde{p}^{(k)}, \quad q^{(k)} = q^{(k-1)} + \tilde{q}^{(k)},$$

till the convergence criteria is satisfied. At each Newton iteration, we need to solve a coupled linearized system for $(\tilde{p}^{(k)}, \tilde{q}^{(k)})$ $(k \geq 1)$:

$$\begin{aligned} \frac{\tilde{p}^{(k)}}{\Delta t} &= \zeta\Delta\tilde{p}^{(k)} - a\tilde{p}^{(k)} + \text{other terms}, \\ \frac{\tilde{q}^{(k)}}{\Delta t} &= \zeta\Delta\tilde{q}^{(k)} - a\tilde{q}^{(k)} + \text{other terms}. \end{aligned} \tag{3.3}$$

These linearized systems always have non-constant coefficients that make a direct solution by Fourier spectral method difficult and expensive. Therefore, we solve them by using the preconditioned BiCGSTAB method with a preconditioner coming from a suitable linear system with constant coefficients, for which the Fourier spectral method reduces to a diagonal system. In our computations, the preconditioner is $(\frac{1}{\Delta t} - \zeta\Delta + a)^{-1}$, which will be applied to both sides of (3.3). The Newton iteration procedure will be terminated once the residue of the preconditioned linear system becomes smaller than a prescribed threshold, e.g. 10^{-12}. Hence, the cost of each BiCGSTAB iteration is simply a matrix-vector product which can be done in $O(N^2 \log N)$ (N being the number of modes in each direction) operations with a pseudo-spectral matrix-free approach using FFT.[15,29]

We now present some numerical results obtained by using the above approach.

Example 1. (Accuracy test) We set $\Omega = [-2, 2] \times [-2, 2]$ and take the initial data at $x = (x_1, x_2)^T \in \Omega$ to be

$$p^0(x) = \sin(\pi x_1/2)\sin(\pi x_2/2), \quad q^0(x) = \cos(\pi x_1/2)\cos(\pi x_2/2). \tag{3.4}$$

The other parameters are given as:

$$\zeta = 2, \quad a = 0.5, \quad c = 4, \quad L_4 = 0.1. \tag{3.5}$$

Since we do not know the explicit form of the exact solution, we take the "reference" solution $(p(\cdot, t_n), q(\cdot, t_n))$ to be the numerical solution obtained by using the proposed scheme with the stabilizing constant $L = 0.5$, space mesh size $h_e = 1/128$ which well resolves the solution, and a small time step $\tau_e = 10^{-5}$.

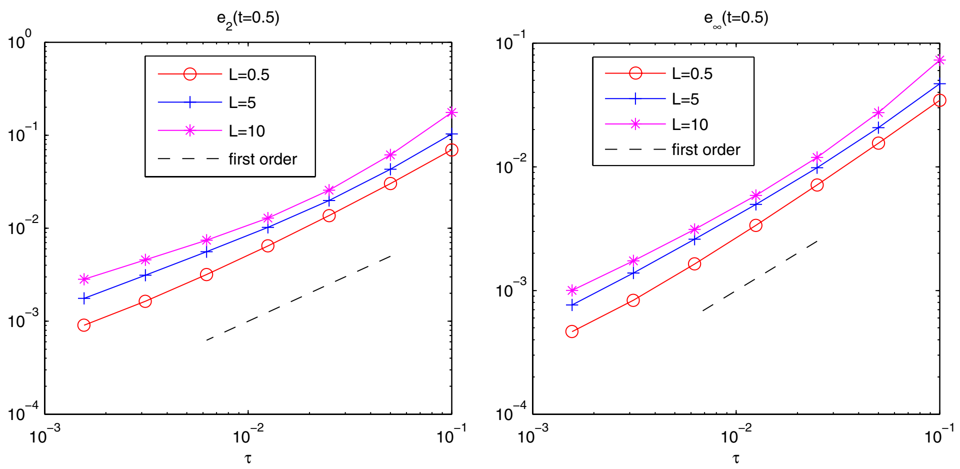
We first look at the the temporal errors. We take the space mesh size $h = 1/32$ such that the spatial errors are negligible. Let (p_τ^n, q_τ^n) be the numerical approximations obtained by our scheme at $t = t_n$ with $h = 1/32$ and time step τ, and we introduce the L^2 and L^∞ error functions as:

$$e_2(t_n) = \sqrt{\|p_\tau^n - p_{\tau_e}^n\|_{L^2}^2 + \|q_\tau^n - q_{\tau_e}^n\|_{L^2}^2},$$

$$e_\infty(t_n) = \|\sqrt{|p_\tau^n - p_{\tau_e}^n|^2 + |q_\tau^n - q_{\tau_e}^n|^2}\|_\infty.$$

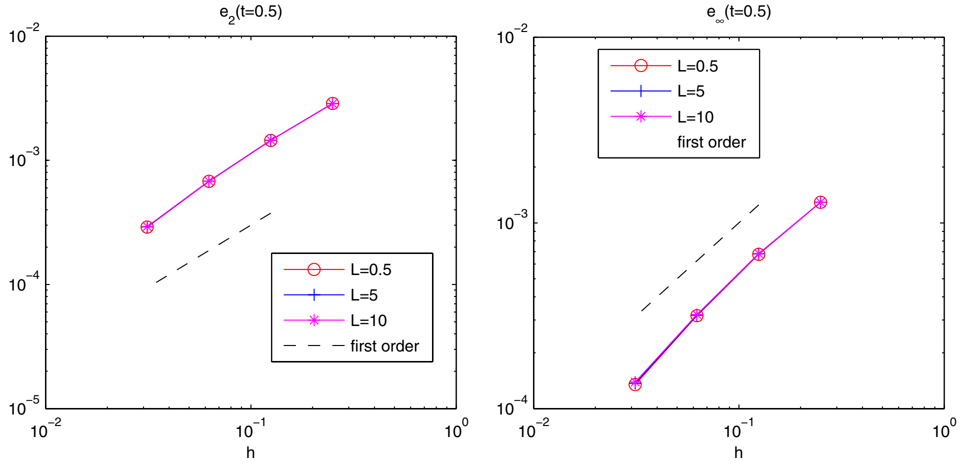
Figure 1 shows the temporal errors for different stabilizing constant L. It is clear that the scheme is first-order accurate in time.

To demonstrate that $h = 1/32$ is sufficient for the temporal convergence order test, we provide spatial error tests in Fig. 2. In Fig. 2, the reference solution is computed with $h_e = 1/128$, $\tau_e = 10^{-5}$ and $L = 0.1$, while the other numerical solutions are computed with $\tau_e = 10^{-5}$, different h and stabilization parameter L. From Fig. 2, we observe that the errors are indistinguishable for different parameters L with a fine time step τ_e, and $h = 1/32$ is sufficient for the temporal convergence order check in Fig. 1. In addition, the accuracy of the reference solution is limited by time step $\tau_e = 10^{-5}$, and spectral accuracy is not observed in Fig. 1.



(a) (b)

Fig. 1. Temporal error $e_2(t = 0.5)$ (a) and $e_\infty(t = 0.5)$ (b) for Example 1. The dashed line segments stand for the first-order convergence.



(a) (b)

Fig. 2. Spatial error e_2 $(t = 0.5)$ (a) and e_∞ $(t = 0.5)$ (b) for Example 1. The dashed line segments stand for the first-order convergence.

Example 2. We choose $\Omega = [-2, 2] \times [-2, 2]$ with periodic boundary conditions and $\zeta = 0.4, a = -2, c = 4, L_4 = 0.08, L = 0.1$. We set the initial state

$$Q^0(x) = s^0(x)\left(\mathbf{n}^0 \otimes \mathbf{n}^0 - \frac{1}{2}\mathbf{I}_2\right), \tag{3.6}$$

with $s^0(x) = 0.2$ and

$$\mathbf{n}^0(x) = \begin{cases} (1,0)^t, & x \in [-1,1] \times [-1,1]; \\ (0,1)^t, & \text{otherwise}; \end{cases} \tag{3.7}$$

being the unit vector in $\mathbb{R}^2$ representing the direction of the liquid crystal at position x.

Example 3. We choose the same parameters as in Example 2 but with the initial state

$$Q^0(x) = s^0(x)\left(\mathbf{n}^0 \otimes \mathbf{n}^0 - \frac{1}{2}\mathbf{I}_2\right), \tag{3.8}$$

with $s^0(x) = 0.2$ and

$$\mathbf{n}^0(x) = \begin{cases} (1,0)^t, & x \in [-1.5,1.5] \times [-1.5,1.5]; \\ (0,1)^t, & \text{otherwise}. \end{cases} \tag{3.9}$$

In the computations for Examples 2 and 3, we choose $\tau = 0.0025$ and $h = 1/32$. The orientation of the liquid crystal is understood through the link between the Q-tensor model and the Oseen–Frank theory, i.e. for $Q = s_+(\mathbf{n} \otimes \mathbf{n} - \mathbf{I}_2/2)$ $(s_+ > 0, \mathbf{n} \in \mathbb{S}^1)$, $\mathbf{n}$ stands for the orientation which is an eigenvector of Q corresponding to the dominant eigenvalue. Figures 3 and 4 show the orientation of the liquid crystal

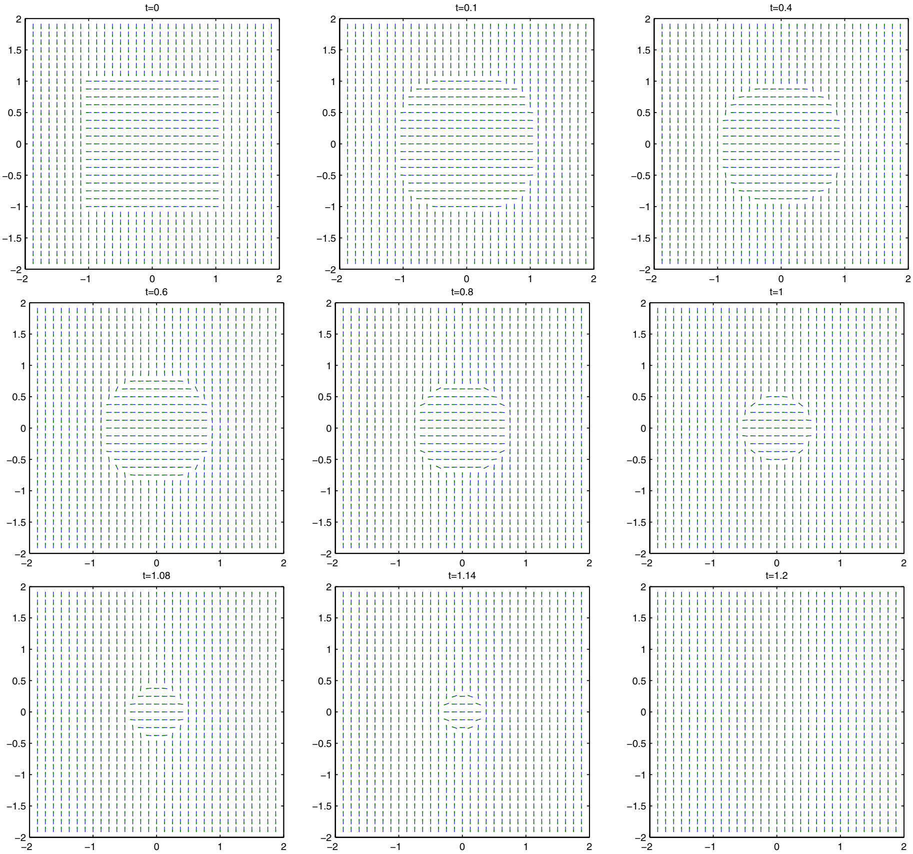


Fig. 3. (Example 2) Orientation of liquid crystal at different time t.

during the time evolution. We observe from Fig. 3 that the final steady states depend on the initial data. For Example 2 (cf. Fig. 3), initially there are more vertical molecules than horizontal molecules. The set with horizontal molecules shrinks with time, and the liquid crystal directions eventually approach to the uniform vertical configuration. On the other hand, for Example 3 (cf. Fig. 4), there are more horizontal molecules than vertical molecules at $t = 0$. The set of horizontal molecules expands toward boundary while its shape oscillates, and the liquid crystal directions eventually approach to the uniform horizontal configuration. We have also checked the numerical results with refined mesh size h and time step τ, and it is confirmed that the dynamics obtained by the chosen parameters are accurate.

Next, we examine the time evolution of L^∞-norm of $|Q|^2$ and bulk energy $\mathcal{F}_{\text{bulk}}$ (1.4), see Fig. 5. We observe that, when the L^∞-bound of the Q-tensor order parameter is sufficiently small, the elliptic part in the equation will force the system approach to a uniform state, and $|Q|^2$ will approach to the minimizer of the bulk energy $\mathcal{F}_{\text{bulk}}$ (1.4), which is constant 0.5. In all our numerical results, the L^∞-norm

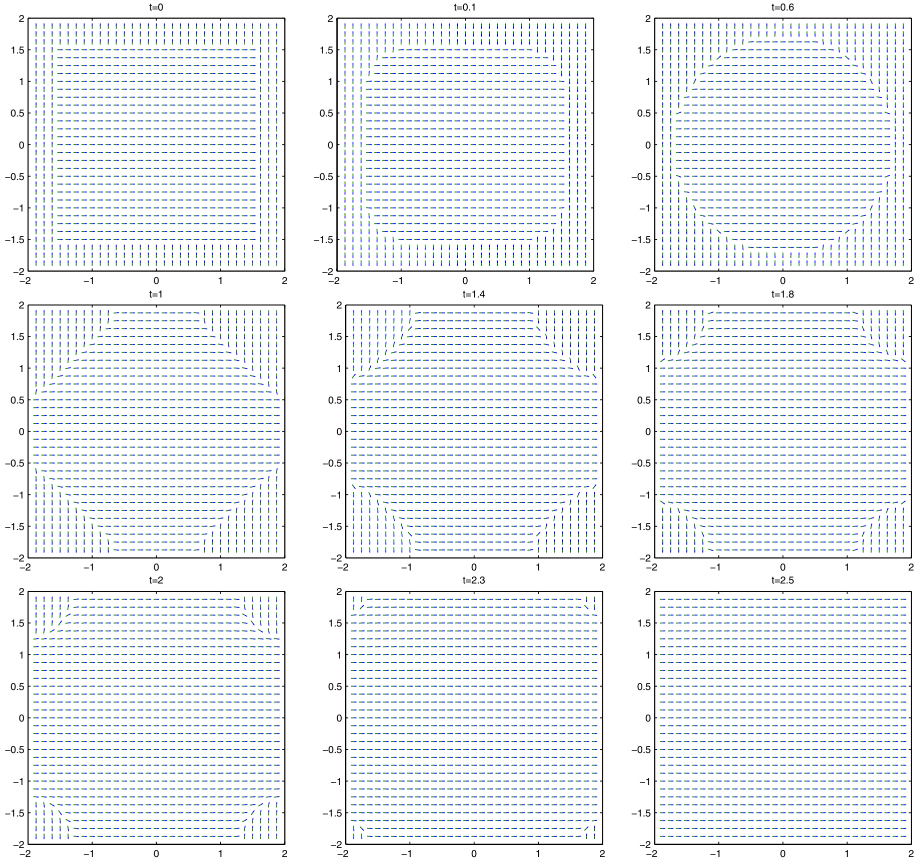


Fig. 4. (Example 3) Orientation of liquid crystal at different time t.

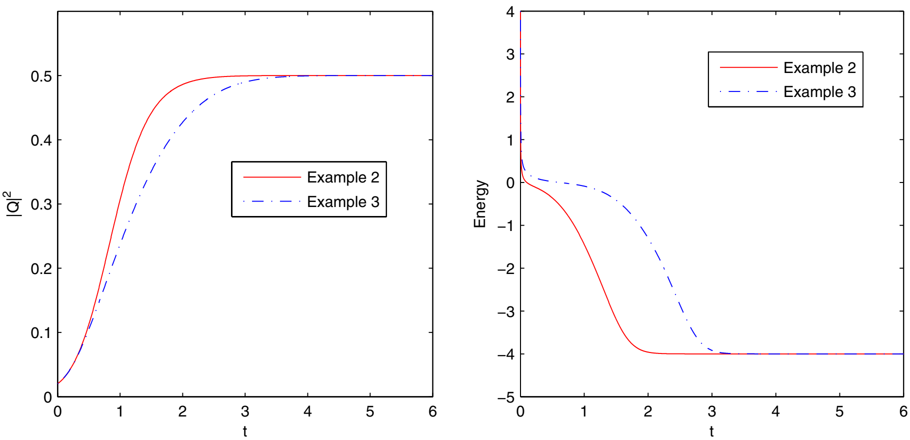


Fig. 5. Evolutions of $|Q|^2$ and the energy for Examples 2 and 3.

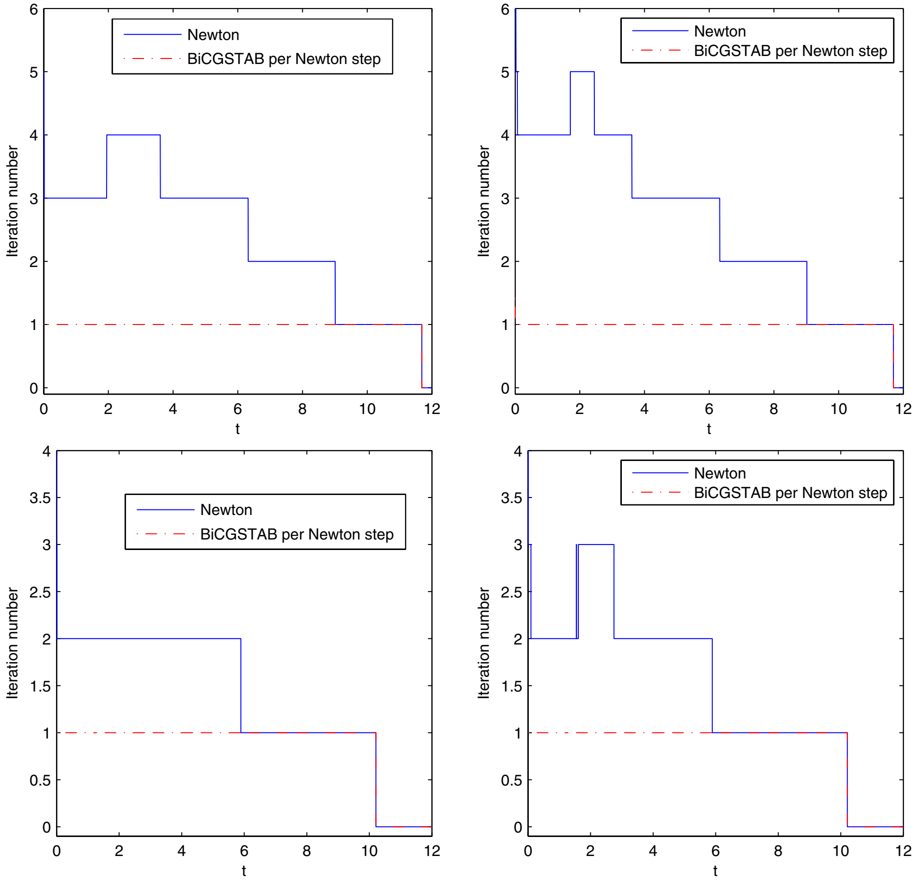


Fig. 6. Numbers of Newton iteration and BiCGSTAB iterations per Newton step at each time step for Example 3 with stabilizing constant $L = 0.1$ (left) and $L = 10$ (right). $\tau = 2.5e-3$, $h = 1/32$ for the top panel; $\tau = 1e-4$ and $h = 1/64$ for the bottom panel. The tolerance of absolute error for Newton iteration is 10^{-12} (measured in maximum norm of the residue) and the tolerance of relative error for BiCGSTAB is 10^{-4} (measured in L^2-norm of the residue).

of the numerical solutions remains to be small for small initial data, as proved in the analysis.

Finally we examine the computational effectiveness of our approach by looking at the convergence of Newton iterations and BiCGSTAB iterations at each time step during the evolution of Example 3. Figure 6 displays the number of Newton iterations and BiCGSTAB iterations per Newton step on average at each time step, with tolerance 10^{-12} (absolute error of the residue) for the Newton iterations and 10^{-4} (relative error) for the BiCGSTAB iterations. We observe that the number of Newton iterations per time step ranges between 1–4, and the BiCGSTAB iterations per Newton step is around one, which indicates that, on average, the BiCGSTAB converges in just one iteration for each linearized system. These results indicate that

Table 1. Computation time of simulations for Example 3 with final time $T = 3$, spatial unknowns $N \times N$, time step τ and stabilization parameter L.

	$(N = 128, \tau = 10^{-3}, L = 0.1)$	$(2N, \tau/2, L)$	$(2N, \tau/2, 100L)$	$(4N, \tau/2, L)$
Time (s)	1064	6345	6422	27771

our numerical approach is very efficient. In Table 1, we list the computation time for different sets of computational parameters, which demonstrates the efficiency of our algorithm. All computations are done with Matlab 2012b 64-bit on a personal laptop with Intel(R) Core(TM) i7-3630QM CPU@2.4GHz, 8G RAM, Windows 7 operating system.

For general Dirichlet boundary conditions (strong anchoring) and Robin-type boundary conditions (weak anchoring), Legendre or Chebyshev spectral methods (or finite difference methods) can be used for spatial discretization, which can handle non-periodic boundary conditions and maintain high accuracy. The discretized system can be solved using the same strategy described in the paper and further numerical studies on the general boundary conditions will be addressed in our future work.

4. Conclusion

In this paper, we proposed an unconditionally stable numerical scheme to solve a 2D Q-tensor model for liquid crystal, and established its unique solvability and convergence rigorously. As a byproduct of our convergence analysis, we also established the well-posedness of the original PDE system for the 2D Q-tensor model, which has been shown previously with completely different approaches.[18] The approach presented here was simpler and avoided complicate approximation schemes used in Ref. 18.

The main difficulty in the analysis came from an unusual cubic L_4-term in the elastic energy, which made the free energy unbounded from below and caused great challenges in both analysis and computation. By adding a stabilized term in our scheme, we were able to show that the L^∞-norm of the numerical solution can be kept small which guaranteed the stability and the well-posedness. Numerical tests showed that the scheme is indeed first-order accurate for a wide range of stabilizing constants, and produces physically consistent numerical simulations.

We only discussed a 2D Q-tensor model in this paper. Extensions to the 3D case, as well as the full dynamical model coupled with Navier–Stokes equations entail significant analytical difficulties, and they will be considered in our future work.

Appendix A

Here, we provide the derivation of (1.9) from the gradient flow (1.6) with Lagrangian multipliers, which can also be found in the Appendix of Ref. 18.

First of all, we can find

$$\left(\frac{\delta \mathcal{E}}{\delta Q}\right)^{ij} = -2L_1\Delta Q^{ij} + aQ^{ij} - bQ^{jk}Q^{ki} + c\mathrm{tr}(Q^2)Q^{ij} - 2(L_2+L_3)\partial_j\partial_k Q^{ik}$$
$$- 2L_4\partial_l Q^{ij}\partial_k Q^{lk} - 2L_4\partial_l\partial_k Q^{ij}Q^{lk} + L_4\partial_i Q^{kl}\partial_j Q^{kl}. \tag{A.1}$$

Using the matrix symmetry constraint $Q^{ij} = Q^{ji}$, we substitute the above equality in (1.6), and get

$$\mu^{ij} - \mu^{ji} = (L_2+L_3)(\partial_i\partial_k Q^{jk} - \partial_j\partial_k Q^{ik}).$$

In the meantime, we compute the trace of Eq. (1.6), and by the traceless constraint $\mathrm{tr}(Q) = 0$ we have

$$\lambda = -\frac{b}{2}\mathrm{tr}(Q^2) - (L_2+L_3)\partial_l\partial_k Q_{lk} + \frac{L_4}{2}|\nabla Q|^2.$$

Substituting λ, μ and $\frac{\delta\mathcal{E}}{\delta Q}$ in (1.6), it gives

$$\frac{\partial Q^{ij}}{\partial t} = 2L_1\Delta Q^{ij} - aQ^{ij} - c\,\mathrm{tr}(Q^2)Q^{ij} + (L_2+L_3)(\partial_j\partial_k Q^{ik} + \partial_i\partial_k Q^{jk})$$
$$- (L_2+L_3)\partial_l\partial_k Q^{lk}\delta^{ij} + 2L_4\partial_l Q^{ij}\partial_k Q^{lk} + 2L_4\partial_l\partial_k Q^{ij}Q^{lk}$$
$$- L_4\partial_i Q^{kl}\partial_j Q^{kl} + \frac{L_4}{2}|\nabla Q|^2\delta^{ij}. \tag{A.2}$$

Note that in (A.2), we use the fact that $\mathrm{tr}(Q^3) = 0$ for $Q \in \mathcal{S}^{(2)}$. Hence, without loss of generality, we assume $b = 0$ in 2D.

Further, since $Q \in \mathcal{S}^{(2)}$, it can be expanded as $Q = \begin{pmatrix} p & q \\ q & -p \end{pmatrix}$. We can collect the terms in (A.2) with factor $L_2 + L_3$ and tedious but straightforward computation shows

$$(L_2+L_3)(\partial_j\partial_k Q^{ik} + \partial_i\partial_k Q^{jk}) - (L_2+L_3)\partial_l\partial_k Q^{lk}\delta^{ij} = (L_2+L_3)\Delta Q^{ij}. \tag{A.3}$$

Inserting (A.3) into (A.2), we derive our main Eq. (1.9).

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