



Nonstationary models for liquid crystals: A fresh mathematical perspective

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ABSTRACT

In this article, we discuss nonstationary models for inhomogeneous liquid crystals driven out of equilibrium by flow. Emphasis is put on those models which are used in the mathematics as well as in the physics literature, the overall goal being to illustrate the mathematical progress on these models to date. Our discussion includes the Doi–Hess model for the orientational distribution function, the Q -tensor model and the Ericksen–Leslie model which focuses on the director dynamics. We survey particularly the mathematical issues (such as existence of solutions) and linkages between these models. Moreover, we introduce the new concept of relative energies measuring the distance between solutions of equation systems with nonconvex energy functionals and discuss possible applications of this concept for future studies.

1. Introduction

Since their discovery in the 1890s by Reinitzer [1] and Lehmann [2] (see also Heinz [3] and Virchow [4] for earlier descriptions), liquid crystals continue to be one of the most intriguing and fascinating classes of condensed matter, which nowadays have a plethora of applications in optics, photonics, and in material science (for a review, see Ref. [5]).

Typical liquid crystals consist of rod-like (“prolate”) or disk-shaped (“oblate”) organic molecules or colloidal particles. The name “liquid crystal” already suggests their intermediate role between two more conventional states of matter. These are, on the one hand, fully isotropic liquids, which lack of any (positional or orientational) long-range ordering and form the common case for most high-temperature atomic and molecular fluids. On the other hand, crystals, which represent the typical low-temperature state of many materials, are characterized by three-dimensional positional (and possibly orientational) order. Between these cases, liquid crystals are characterized by long-range orientational ordering of the axes of the anisotropic particles without (or with only partial) ordering of the positions of the center of mass. As a result, liquid crystals can *flow*. More generally, liquid crystals respond easily to external thermal, mechanical, or optical perturbations and are therefore typical representatives of *soft* condensed matter systems. The unique structural and dynamical material properties of liquid crystals continues to attract an interdisciplinary community of physicists, chemists, material scientists, and even (applied) mathematicians. This interest is recently also triggered by the important role of liquid-crystal physics in the fields of biophysics (e.g., for the structure of the cytoskeleton or the movement between actin and myosin, see Ahmadi et al. [6]),

in active matter Ref. [7,8] and in astrophysics (emergence of topological defects). Many of these contexts involve physical situations outside thermal equilibrium, where the material properties generally depend on time. The purpose of the present article is to summarize modeling approaches for such *nonstationary* (out-of-equilibrium) liquid crystals from both, a mathematical and a physical perspective.

Clearly, the presence of orientational degrees of freedom makes the theoretical description of liquid crystals more complex than that of ordinary (atomic) fluids. This holds for microscopic (“bottom-up”) approaches such as classical density functional theory (see Ref. [9,10]), but also for coarse-grained approaches such as phase-field crystal modeling (see Ref. [11]) and for mesoscopic (continuum) approaches involving appropriate order parameter fields (see Ref. [12]) or even macroscopic variables, such as a stress tensor (see Section 4). Such mesoscopic approaches have become particularly popular for the description of liquid crystals under *flow*, a situation of major relevance for many applications (see Ref. [13]). Mathematically, continuum approaches for nonstationary liquid crystals involve typically nonlinear coupled (partial) differential equations. While physicists just tend to solve these equations numerically and explore the emerging physical behavior, there are many open problems from the mathematical (and numerical) side concerning, e.g., the existence and uniqueness of solutions. From the physical side, this poses the danger of overseeing important dynamical features, while from the mathematical side, there is a certain risk to concentrate on too simplistic (or even nonphysical) models.

It is in this spirit that we here aim at giving an overview over some of the most relevant nonstationary models that have been considered in *both*, the physics and the mathematics literature, and to elucidate

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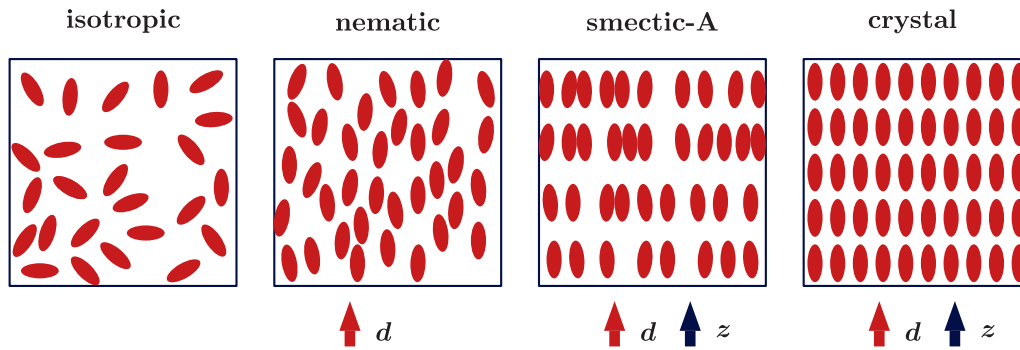


Fig. 1. Schematic illustrating the molecular structure in the most common phases of liquid crystals. The director is denoted by \mathbf{d} and the layer normal by \mathbf{z} .

their challenges. These challenges become particularly apparent when treating *inhomogeneous* systems under flow: here one is faced not only with the impact of the flow field on the structure of the liquid crystal, but also *vice versa* with the structure-induced modification on the flow. For a recent review focusing on homogeneous situations alone, see Ref. [13]. For inhomogeneous systems, there are excellent reviews from the physics community describing, e.g., defects (see Refs. [14,15]), phase transitions (see Ref. [16]), and rheology properties (see Ref. [17]) in accordance with experimentally observed behavior. We also like to mention recent reviews on the multiscale approach for liquid crystals (see Ref. [18]) and on bifurcation analysis (see Ref. [19]). Some approaches are even nondeterministic, giving rise to spontaneous defect nucleation and bifurcations (see Refs. [20,21]). A detailed description and comparison of all these physical models is beyond the scope of the article at hand (see Refs. [22,23] for such an overview). Instead, we concentrate on three approaches, which were also in the focus of mathematical studies in recent years: The Doi–Hess theory providing a kinetic approach, the Q-tensor theory for order parameter dynamics, and the Ericksen–Leslie theory.

We concentrate on theories targeting the *nematic* state of liquid crystals. Indeed, depending on the degree of order one distinguishes different mesophases, the two simplest ones of which are illustrated in the left part of Fig. 1. The isotropic state is characterized by translational and orientational disorder. Upon increasing the concentration (lyotropic liquid crystal) or lowering temperature (thermotropic liquid crystal) the system then enters the nematic state, see, e.g., Palffy-Muhoray [5]. Within the equilibrium nematic state, the rod-like molecules are randomly distributed in space but tend to align along a common direction, characterized by the so-called director \mathbf{d} . The resulting system is much more permeable for light sent along the direction of the vector \mathbf{d} than perpendicular to it. This is the fundamental principle underlying all liquid-crystals displays (LCDs). We note that in nonequilibrium, (induced, e.g., by flow) the symmetry of the originally nematic phase can break down in the sense that the orientational order becomes inhomogeneous or biaxial.

In equilibrium smectic phases, the orientational alignment is supplemented by long-range one-dimensional translational order, leading to layers of aligned particles. The corresponding material density exhibits periodic peaks in one direction (see vector \mathbf{z} in Fig. 1). Both, nematic and smectic phases have relevance in material science, such as, e.g., for liquid crystal elastomers which deform as a reaction to thermal, chemical or optical excitement (see Ref. [5]). It is clear, however, that the one-dimensional translational order in the smectic phase poses additional challenges for the theoretical description. We thus focus on systems which are nematic in equilibrium.

The remainder of this article is structured as follows. We start by shortly reviewing the Doi model (Section 2), which provides a “kinetic” equation for the dynamical evolution of the orientational distribution function of the system. We then proceed to the Q-tensor (Section 3) and, as a special case (valid for uniaxial nematics), the Ericksen–Leslie model

(Section 4), both of which focus on the dynamics of an order parameter. For all of these models, we consider both homogeneous and inhomogeneous situations, and we discuss their advantages and drawbacks from the mathematical and physical point of view. Special emphasis is put on the existence of generalized solutions of the governing equations. In Section 5, we then comment on cross-linkages between the three models. In Section 6, we then introduce a new piece of mathematical analysis for nonstationary models of liquid crystals. Specifically, we introduce the concept of relative energies to measure the distance of possible solutions. We prove an inequality showing the continuous dependence of the relative energy on the difference of the initial values. By this we provide a new comparing tool for experimental or computational results or the evolution of a time series of a nematic liquid crystal, since the relative energy serves as a natural measure for the distance between different configurations of liquid crystals.

The article closes with a brief outlook in Section 7.

Notation. For two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$, we denote by $\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^T \mathbf{b}$ the Euclidean inner product, by $\mathbf{a} \times \mathbf{b}$ the vector or outer product, and by $\mathbf{a} \otimes \mathbf{b} = \mathbf{a} \mathbf{b}^T$ the dyadic product. The identity in $\mathbb{R}^{3 \times 3}$ is denoted by I . For $A, B \in \mathbb{R}^{3 \times 3}$, let $A : B = \sum_{i,j=1}^3 A_{ij} B_{ij}$ be the Frobenius inner product. For a vector field \mathbf{v} , we denote by $(\nabla \mathbf{v})_{\text{sym}} = \frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$ the symmetric and by $(\nabla \mathbf{v})_{\text{skw}} = \frac{1}{2}(\nabla \mathbf{v} - (\nabla \mathbf{v})^T)$ the skew-symmetric part of its gradient $\nabla \mathbf{v}$. With $\nabla \times$ we denote the curl operator. By Ω we denote a bounded domain with sufficiently smooth boundary.

2. The Doi model

From a microscopic point of view, the liquid-crystalline systems can be considered as an ensemble of (rigid or flexible) rods or disks which perform thermal motion and interact pairwise via repulsive (“steric”) and, possibly, additional attractive (e.g., van-der Waals) forces. These pairwise forces can then be supplemented by coupling to a flow field or other external perturbations. Within the Doi model (see Refs. [24,25]), which is sometimes also referred to as Doi–Hess model (see Beris and Edwards [26, p. 463]) due to the parallel work of Hess (see Refs. [27] and [12]), the fluctuating ensemble of rods is described by a (nonnegative) probability distribution function $f = f(\mathbf{x}, \mathbf{n}, t)$ where f is the probability density that at time t a molecule at point \mathbf{x} is aligned in direction \mathbf{n} . The latter is an element of the unit sphere \mathbb{S}^2 in \mathbb{R}^3 such that $|\mathbf{n}| = 1$. Here and henceforth we assume the particles themselves to have uniaxial symmetry, such that one vector is fully sufficient to describe their orientation.

The key element of the Doi–Hess approach is a Fokker–Planck equation for the probability density $f = f(\mathbf{x}, \mathbf{n}, t)$ describing its temporal (or spatio-temporal) evolution. Mathematically, these are (partial) differential equations of first order in time. Note that the first-order nature implies that the motion of the molecules is assumed to be “overdamped”, a situation which typically occurs if the rods are suspended in a

viscous solvent. Due to this assumption one often rather refers to a Smoluchowski (see Ref. [28]) than a Fokker–Planck equation.

Before discussing these dynamical equations, we first briefly state two important properties of f : First, f is normalized such that

$$\int_{\mathbb{S}^2} f(\mathbf{x}, \mathbf{n}, t) d\mathbf{n} = 1 \quad (1)$$

for all $\mathbf{x} \in \Omega$ and all $t \geq 0$, where $\Omega \subset \mathbb{R}^3$ denotes the spatial domain occupied by the liquid crystal. For a fully isotropic and homogeneous fluid, where the directions and positions are uniformly distributed and f is just a constant, (Eq. (1)) immediately implies that $f = 1/(4\pi)$.

A second important property of the distribution function f concerns its symmetry: Because of the head-to-tail symmetry characterizing many (nonpolar) rod-like molecules, one typically cannot distinguish between the directions \mathbf{n} and $-\mathbf{n}$. It would thus be convenient to consider the manifold $\mathbb{R}P^2$, the real projective plane in \mathbb{R}^3 , instead of \mathbb{S}^2 . Since this manifold is, however, nonorientable, one rather endows the function f with the symmetry assumption

$$f(\mathbf{x}, \mathbf{n}, t) = f(\mathbf{x}, -\mathbf{n}, t) \quad (2)$$

for all $(\mathbf{x}, \mathbf{n}, t) \in \Omega \times \mathbb{S}^2 \times [0, \infty)$.

2.1. Homogeneous systems: Doi–Onsager model

In the absence of any spatial structure, that is, for a spatially homogeneous system, the probability density f reduces to a function of the orientation (and time) such that $f = f(\mathbf{n}, t)$. In this case, the Doi model is often referred to as the Doi–Onsager model (see, e.g., Zhang and Zhang [29]).

The main orientational phenomenon for a homogeneous liquid-crystalline system in *thermal equilibrium* is the phase transition between the isotropic state (where $f = 1/(4\pi)$) and the nematic state, where f is a nontrivial function of the orientation (yet stationary in time). In his pioneering work of 1949, Onsager [30] proposed the first statistical-physical theory of the equilibrium isotropic-nematic transition in a system of rods with purely repulsive interactions. Within this theory, the transition results from a competition between the “excluded volume” interactions (originating from the mutual repulsion of the rods) and the orientational entropy. We will come back to some elements of the Onsager theory later in this section.

Here we proceed by first stating, in a quite general form, the governing equation describing the temporal evolution of the probability density f (often called “kinetic” equation) in the homogeneous case. In writing this equation, we allow for an orientation-dependent potential $V = V(\mathbf{n}, f(\mathbf{n}, t))$ affecting the orientation of the rods, and for a flow velocity field \mathbf{v} such that $\nabla \mathbf{v}$ is constant. The governing equation then reads

$$\frac{\partial f(\mathbf{n}, t)}{\partial t} = \frac{1}{\text{De}} \mathcal{R} \cdot \left(\mathcal{R} f(\mathbf{n}, t) + f(\mathbf{n}, t) \mathcal{R} V(\mathbf{n}, f(\mathbf{n}, t)) \right) - \mathcal{R} \cdot \left(\mathbf{n} \times \nabla \mathbf{v} f(\mathbf{n}, t) \right). \quad (3)$$

Here, \mathcal{R} is a rotational differential operator to be specified below, and the nonnegative dimensionless constant De is the so-called Deborah number, which quantifies the ratio between the rotational Brownian motion of the molecules and the motion due to convection (note that (Eq. 3) is already in dimensionless form, see Yu and Zhang [31] for the scaling arguments).

The first term on the right-hand side of (Eq. (3)), $\text{De}^{-1} \mathcal{R} \cdot \mathcal{R} f$, describes the rotational diffusion of the rods due to rotational Brownian motion. The operator \mathcal{R} depends on \mathbf{n} and is defined as

$$\mathcal{R} = \mathbf{n} \times \frac{\partial}{\partial \mathbf{n}}, \quad (4)$$

it can be seen as the gradient with respect to \mathbf{n} restricted to the sphere. The composition $\mathcal{R} \cdot \mathcal{R}$ then represents the Laplace–Beltrami operator on

the sphere \mathbb{S}^2 (see also Zhang and Zhang [29]). With $|\mathbf{n}| = 1$, we find

$$\begin{aligned} \mathcal{R} \cdot \mathcal{R} f &= \sum_{j=1}^3 \left(1 - n_j^2 \right) \frac{\partial^2 f}{\partial n_j^2} - \sum_{i,j=1,i \neq j}^3 n_i n_j \frac{\partial^2 f}{\partial n_i \partial n_j} - 2 \sum_{j=1}^3 n_j \frac{\partial f}{\partial n_j} \\ &= \Delta_{\mathbf{n}} f - (\mathbf{n} \otimes \mathbf{n}) : \nabla_{\mathbf{n}}^2 f - 2 \mathbf{n} \cdot \frac{\partial f}{\partial \mathbf{n}}, \end{aligned} \quad (5)$$

where $\Delta_{\mathbf{n}}$ is the Laplacian and $\nabla_{\mathbf{n}}^2$ is the Hessian with respect to \mathbf{n} . In spherical coordinates we have $\mathbf{n} = [\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta]^T$ with $\phi \in [0, 2\pi)$ and $\theta \in [0, \pi)$. The diffusion term then becomes

$$\mathcal{R} \cdot \mathcal{R} f = \frac{1}{\sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial \theta^2} + \cot \theta \frac{\partial f}{\partial \theta}. \quad (6)$$

We now consider the second term on the right-hand side of (Eq. (3)) which involves the potential V describing effects of alignment. This potential is, in general, a function of the direction \mathbf{n} and the probability density f , i.e., $V = V(\mathbf{n}, f(\mathbf{n}, t))$. Many different choices of V have been suggested in the literature. Here we follow Kuzuu and Doi [24] who write the potential as a sum of two parts, $V = V_{MI} + V_H$, where V_{MI} models pair interactions on a mean-field level, and V_H accounts for the interaction of each rod with an external magnetic field (if present).

The latter term is a single-particle contribution and thus depends only on \mathbf{n} . It can be written as (see also Ref. [32, Section 3.2.1]),

$$V_H(\mathbf{n}) = -\frac{1}{2} (\chi_{\parallel} - \chi_{\perp}) (\mathbf{n} \cdot \mathbf{H})^2, \quad (7)$$

where \mathbf{H} is the externally controlled magnetic field and χ_{\parallel} and χ_{\perp} are the (magnetic) susceptibilities parallel to the molecular axis \mathbf{n} and perpendicular to \mathbf{n} , respectively.

The mean-field potential V_{MI} describes the (effective) interaction of the particles and is given by

$$V_{MI}(\mathbf{n}, f) = \int_{\mathbb{S}^2} \beta(\mathbf{n}, \hat{\mathbf{n}}) f(\hat{\mathbf{n}}, t) d\hat{\mathbf{n}}, \quad (8)$$

where the integral kernel $\beta = \beta(\mathbf{n}, \hat{\mathbf{n}})$ describes the interaction of two molecules pointing in the directions \mathbf{n} and $\hat{\mathbf{n}}$. Again, different choices of β can be found in the literature. In the original Onsager model [30], the kernel β is given by

$$\beta(\mathbf{n}, \hat{\mathbf{n}}) = \alpha |\mathbf{n} \times \hat{\mathbf{n}}| \quad (9)$$

with a positive constant α . The latter represents the coupling strength (see Refs. [24,32]) and depends on quantities characterizing the microscopic configuration. Another kernel function that is often studied is due to Maier and Saupe (see Ref. [33]),

$$\beta(\mathbf{n}, \hat{\mathbf{n}}) \sim -(\mathbf{n} \cdot \hat{\mathbf{n}})^2 = |\mathbf{n} \times \hat{\mathbf{n}}|^2 - 1. \quad (10)$$

This expression can be considered as an approximation of the cross product (for small angle) in the corresponding Onsager term (9). A third example is the “dipole-like” potential given by

$$\beta(\mathbf{n}, \hat{\mathbf{n}}) \sim -\mathbf{n} \cdot \hat{\mathbf{n}}. \quad (11)$$

We stress that, from a physical perspective, (Eq. (11)) corresponds to a mean-field version of the full dipole-dipole potential, which involves an additional dependency on the connecting vector between the particles (see Ref. [34]). Still, (Eq. (11)) reflects one key feature of the interaction between molecules are possessing a dipole moment (see Fatkullin and Slastikov [35]): That is, the interaction potential changes its sign if the direction of one of the molecules is reversed. This is in contrast to the Maier–Saupe and Onsager potential.

The last term on the right-hand side in Eq. (3) models the impact of an imposed flow profile onto the alignment of the molecules. Note that since f was assumed to be independent of \mathbf{x} (homogeneity), the velocity gradient $\nabla \mathbf{v}$ needs to be constant. Explicitly, the cross product yields

$$\mathbf{n} \times \nabla \mathbf{v} \mathbf{n} = \sum_{j=1}^3 \begin{bmatrix} n_2 \frac{\partial v_3}{\partial x_j} - d_3 \frac{\partial v_2}{\partial x_j} \\ n_3 \frac{\partial v_1}{\partial x_j} - d_1 \frac{\partial v_3}{\partial x_j} \\ n_1 \frac{\partial v_2}{\partial x_j} - d_2 \frac{\partial v_1}{\partial x_j} \end{bmatrix} n_j. \quad (12)$$

Combined with the application of the rotational operator one obtains (with $|\mathbf{n}| = 1$)

$$\begin{aligned} \mathcal{R} \cdot (\mathbf{n} \times \nabla \mathbf{v} \mathbf{n} f) &= \left(\mathbf{n} \times \frac{\partial}{\partial \mathbf{n}} \right) \cdot (\mathbf{n} \times \nabla \mathbf{v} \mathbf{n} f) \\ &= (\mathbf{n} \cdot \mathbf{n}) \left(\frac{\partial}{\partial \mathbf{n}} \cdot \nabla \mathbf{v} \mathbf{n} f \right) - \frac{\partial}{\partial \mathbf{n}} \cdot \mathbf{n} (\mathbf{n} \cdot \nabla \mathbf{v} \mathbf{n} f) \\ &= \frac{\partial}{\partial \mathbf{n}} \cdot \left((|\mathbf{n}|^2 \mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \nabla \mathbf{v} \mathbf{n} f \right) \\ &= (\nabla \cdot \mathbf{v}) f - 3 \mathbf{n} \cdot \nabla \mathbf{v} \mathbf{n} f + (\nabla \mathbf{v} \mathbf{n}) \cdot (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \frac{\partial}{\partial \mathbf{n}} f. \end{aligned} \quad (13)$$

Having discussed the physical interpretation of the different terms in (Eq. 3), we close with some more mathematical remarks. Importantly, the evolution Eq. (3) can be interpreted as the *gradient flow* of a certain (free) energy functional with respect to the Wasserstein metric (see Villani [36]). To be precise, consider the free energy functional

$$F[f] = \int_{\mathbb{S}^2} \left(f(\mathbf{n}) (\ln f(\mathbf{n}) - 1) + \frac{1}{2} V_{MI}(\mathbf{n}, f(\mathbf{n})) f(\mathbf{n}) + V_H(\mathbf{n}) f(\mathbf{n}) \right) d\mathbf{n}, \quad (14)$$

where the notation $F[f]$ indicates the functional dependence of F on the probability density. Performing the variational derivative of F with respect to f one obtains (using the definition of V_{MI} in Eq. (8) and the symmetry of β)

$$\frac{\delta F}{\delta f}[f] = \ln f + V_{MI} + V_H = \ln f + V. \quad (15)$$

Here $\delta F/\delta f$ denotes the variational derivative of F with respect to f (see Ref. [37]). Consider now the first two terms on the right-hand side of (Eq. 3) or, equivalently, the evolution equation in the absence of (or for a constant) velocity field \mathbf{v} . By using the functional derivative given above it is easy to see that

$$\frac{\partial f}{\partial t} = \frac{1}{\text{De}} \mathcal{R} \cdot (\mathcal{R} f + f \mathcal{R} V) = \frac{1}{\text{De}} \mathcal{R} \cdot \left(f \mathcal{R} \left(\frac{\delta F}{\delta f}[f] \right) \right). \quad (16)$$

The first term on the right-hand side of Eq. (3) with the interaction potential V can thus be interpreted as the gradient flow of the free energy functional F (14) with respect to the Wasserstein metric. In other words, the free energy functional is a Lyapunov-type function for Eq. (3).

We note in passing that the first member of (Eq. 16) is also referred to as Smoluchowski equation on the sphere (see Ref. [38]). Global existence of a solution to Eq. (16) with the Maier-Saupe potential (10) has been shown in Ref. [38] for initial data given by a nonnegative continuous function on \mathbb{S}^2 . Moreover, it has been shown that solutions are nonnegative and normalized. Furthermore, energy estimates and the typical structure of steady-state solutions have been studied. Many other authors have also studied Eq. (16) from the mathematical point of view (for a review, see Zhang and Zhang [29]). In particular, Zhang and Zhang [29] consider the three above-mentioned interaction kernels (9), (10), and (11). Other results concerning the homogeneous case can be found in Refs [35,39,40].

Finally, it is interesting to note that even the full evolution Eq. (3) for homogeneous systems, which involves a coupling to a flow field with spatially constant $\nabla \mathbf{v}$, can be written as gradient flow, as long as $\nabla \mathbf{v}$ is symmetric, i.e., $\nabla \mathbf{v} = (\nabla \mathbf{v})_{\text{sym}}$. This can be achieved by adding to the free energy functional ((14)) the “dissipation” potential

$$W[f] = \frac{1}{2} \int_{\mathbb{S}^2} (\mathbf{n} \cdot (\nabla \mathbf{v})_{\text{sym}} \mathbf{n}) f d\mathbf{n}. \quad (17)$$

A typical case with constant derivative of the velocity field is a system in a planar Couette shear flow. Kuzuu and Doi [24] derived from this model the homogeneous Ericksen–Leslie equation (see Section 4) by taking into account perturbations of the equilibrium state at a small Deborah number, De .

2.2. Inhomogeneous Doi model

Inhomogeneous flow situations occur, e.g., as a result of an externally imposed flow field with velocity gradient depending on the spatial variable \mathbf{x} . Another intriguing possibility is a *spontaneous* breaking of the symmetry, resulting in the formation of shear bands (see Ref. [41]).

For inhomogeneous systems, the probability density f depends on \mathbf{x} (as well as on orientation \mathbf{n} and time t), and the dynamical evolution equation (3) is no longer valid. The required modifications of (Eq. 3) concern, first, the incorporation of translational diffusion (and other translational effects, see Ref. [25, Section 8]). To be specific, the governing kinetic equation for f in the inhomogeneous case is given by Ref. [42]

$$\begin{aligned} \frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla) f &= \frac{\epsilon^2}{\text{De}} \nabla \cdot \left((D_{\parallel}^* \mathbf{n} \otimes \mathbf{n} + D_{\perp}^* (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})) (\nabla f + f \nabla V) \right) \\ &+ \frac{1}{\text{De}} \mathcal{R} \cdot (\mathcal{R} f + f \mathcal{R} V) - \mathcal{R} \cdot (\mathbf{n} \times \nabla \mathbf{v} \mathbf{n} f). \end{aligned} \quad (18)$$

In the first term on the right-hand side, the parameter ϵ quantifies the ratio between the lengths of the rods and a characteristic length describing the spatial extension of the flow region. Further, D_{\parallel}^* and D_{\perp}^* are shape dependent, translational diffusion constants characterizing the diffusion parallel and perpendicular to the molecular axis \mathbf{n} , respectively. Typically one has $D_{\parallel}^* > D_{\perp}^*$ (see Ref. [28]), that is, a molecule moves more easily parallel (than perpendicular) to \mathbf{n} , consistent with the naïve perception. Eq. (18) also allows for a spatial dependence of the alignment potential $V = V(\mathbf{x}, \mathbf{n}, f(\mathbf{x}, \mathbf{n}, t))$ (see Section 2.1) where we introduced this quantity for the homogeneous case), which may occur, e.g., through an inhomogeneous magnetic field, or through a spatial dependence of the kernel of the mean-field interaction V_{MI} . Usually one assumes this kernel (now called $\tilde{\beta}$) to be translationally invariant Ref. [43], which implies that $\tilde{\beta}$ depends on $\mathbf{x} - \hat{\mathbf{x}}$ instead of \mathbf{x} and $\hat{\mathbf{x}}$ separately. A typical ansatz reads Ref. [42]

$$\tilde{\beta}(\mathbf{x} - \hat{\mathbf{x}}, \mathbf{n}, \hat{\mathbf{n}}) := \chi(\mathbf{x} - \hat{\mathbf{x}}) \beta(\mathbf{n}, \hat{\mathbf{n}}), \quad (19)$$

where χ denotes a suitable mollifier¹ modeling the range of interaction of the rods, and the orientation-dependent function β appearing on the right-hand side is given, e.g., by one of the ansatzes (9), (10), or (11). The resulting mean-field potential V_{MI} then becomes

$$V_{MI}(\mathbf{x}, \mathbf{n}, f) = \int_{\Omega} \int_{\mathbb{S}^2} \tilde{\beta}(\mathbf{x} - \hat{\mathbf{x}}, \mathbf{n}, \hat{\mathbf{n}}) f(\hat{\mathbf{x}}, \hat{\mathbf{n}}, t) d\hat{\mathbf{n}} d\hat{\mathbf{x}}. \quad (20)$$

The second main modification (as compared to the kinetic description of homogeneous flow) is that the evolution equation for $f = f(\mathbf{x}, \mathbf{n}, t)$ has to be supplemented by an equation of motion for the velocity field \mathbf{v} . The latter can be derived from the conservation of momentum and the incompressibility condition resulting from the conservation of mass. This results in a Navier–Stokes-like system of equations given by

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla p &= \nabla \cdot \boldsymbol{\sigma} + \mathbf{b}, \\ \nabla \cdot \mathbf{v} &= 0. \end{aligned} \quad (21)$$

Here p denotes the isotropic (scalar) pressure (up to an additive constant), $\boldsymbol{\sigma}$ is the (additional) stress tensor describing frictional effects (see

¹ Consider the compactly supported smooth function $\rho \in C_c^\infty(\mathbb{R}^d)$, defined by $\rho(\mathbf{x}) = \begin{cases} c \exp\left(-\frac{1}{1-|\mathbf{x}|^2}\right) & \text{if } |\mathbf{x}| < 1 \\ 0 & \text{else} \end{cases}$. The constant c is chosen such that $\int_{\mathbb{R}^d} \rho(\mathbf{x}) d\mathbf{x} = 1$.

1. The suitable mollifiers χ are then defined by $\chi(\mathbf{x}) = (1/L^3)\rho(\mathbf{x}/L)$. The constant L describes the interaction radius of the molecules in the material.

below), and \mathbf{b} is a body force per unit mass. Note that we consider an incompressible medium such that the density is constant and for simplicity set to one.

We note that, for highly viscous fluids, the first member of Eq. (21) is often replaced by its limiting form valid for low Reynolds numbers (overdamped limit). In this limit, the entire material derivative, that is, the time derivative and the nonlinear term in the velocity, are set to zero, yielding the so-called stationary Stokes equation.

Irrespective of the choice for the material derivative, the stress tensor σ of a complex fluid like a liquid crystal is commonly written as a sum of an elastic and a viscous part, i.e.,

$$\sigma = \sigma_{\text{elast}} + \sigma_{\text{visc}}, \quad (22)$$

where the viscous part σ_{visc} is given by (see Ref. [25, Section 8.6] for a derivation)

$$\sigma_{\text{visc}} = 2\nu(\nabla\mathbf{v})_{\text{sym}} + \frac{1}{2}\xi_r \int_{\mathbb{S}^2} ((\nabla\mathbf{v})_{\text{sym}} : \mathbf{n} \otimes \mathbf{n}) \mathbf{n} \otimes \mathbf{n} f(\cdot, \mathbf{n}, \cdot) d\mathbf{n}, \quad (23)$$

with ν and ξ_r being the viscosity of the fluid and the rotational friction constant, respectively. The dots in the integral indicate the dependence of f on \mathbf{x} and t , which are also transferred to the tensors σ_{visc} and $(\nabla\mathbf{v})_{\text{sym}}$. The first term on the right-hand side of Eq. (23) describes the isotropic friction; it already occurs in an atomic fluid and thus also appears in the standard Navier–Stokes equation. Note that $2\nabla \cdot (\nabla\mathbf{v})_{\text{sym}} = \Delta\mathbf{v}$ for an incompressible fluid. The second term on the right-hand side of Eq. (23) represents the additional friction due to the motion of the rod-like molecules. Depending on the physical state considered, the viscous stress tensor can still be a function of \mathbf{x} and t .

For the elastic part of the stress tensor, Wang et al. [44] have suggested the expression

$$\sigma_{\text{elast}} = - \int_{\mathbb{S}^2} \left(\mathbf{n} \times \left(\mathcal{R} \frac{\delta F}{\delta f} [f] \right) \right) \otimes \mathbf{n} f(\cdot, \mathbf{n}, \cdot) d\mathbf{n}, \quad (24)$$

and for the body force appearing in Eq. (21)

$$\mathbf{b} = \int_{\mathbb{S}^2} \nabla \frac{\delta F}{\delta f} [f] f(\cdot, \mathbf{n}, \cdot) d\mathbf{n}. \quad (25)$$

The system of equations for the inhomogeneous flowing liquid crystals given by Eqs. (18) and (21) has been studied in a number of mathematically oriented publications. Specifically, Zhang and Zhang [42] have shown local existence as well as global existence for small Deborah number and large viscosity. Numerical simulations for some special cases such as plane Couette and Poiseuille flow have been presented in Ref. [31].

In an earlier study, Doi [45] considered a simplified case of Eq. (18) where the molecular interactions are neglected, i.e., the potential V is assumed to be constant, and the translational diffusion is isotropic (i.e., $D_{\parallel}^* = D_{\perp}^*$). Eq. (18) then reduces to (see also Ref. [46])

$$\frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla) f = - \frac{\partial}{\partial \mathbf{n}} \cdot ((\nabla\mathbf{v}\mathbf{n} - (\mathbf{n} \cdot \nabla\mathbf{v}\mathbf{n})\mathbf{n})f) + D\Delta f + \frac{1}{\text{De}} \mathcal{R} \cdot \mathcal{R} f, \quad (26)$$

where $D = D_{\parallel}^* \varepsilon^2 / \text{De}$. This Eq. (26) represents again an overdamped Fokker–Plank equation (see, e.g., Ref. [47]). If V is assumed to be constant, the elastic part of the stress tensor (24) could be calculated using integration by parts:

$$\begin{aligned} \sigma_{\text{elast}} &= - \int_{\mathbb{S}^2} (\mathbf{n} \times \mathcal{R} f \otimes \mathbf{n}) d\mathbf{n} = - \int_{\mathbb{S}^2} f \frac{\partial}{\partial \mathbf{n}} \cdot (\mathbf{n} \otimes (|\mathbf{n}|^2 I - \mathbf{n} \otimes \mathbf{n})) d\mathbf{n} \\ &= 3 \int_{\mathbb{S}^2} \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I \right) f d\mathbf{n}. \end{aligned} \quad (27)$$

More general expressions for the stress tensors can be found in Refs. [25] and [47]. The definition (27) is very similar to the definition of the Q -tensor in Eq. (31) below. For the body force \mathbf{b} we infer, since f is a probability measure (see Eq. (1)), that

$$\mathbf{b} = \int_{\mathbb{S}^2} \nabla f(\mathbf{x}, \mathbf{n}, t) d\mathbf{n} = \nabla \int_{\mathbb{S}^2} f(\mathbf{x}, \mathbf{n}, t) d\mathbf{n} = 0. \quad (28)$$

for all $\mathbf{x} \in \Omega$ and $t > 0$. Finally, the rotational friction is assumed to vanish (compare to Eq. (23)), i.e., $\xi_r = 0$. As in Ref. [48], one finally ends up with the system consisting of Eq. (26) and the Navier–Stokes-like equation,

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla p &= \nu \Delta \mathbf{v} + \nabla \cdot \sigma_{\text{elast}}, \\ \nabla \cdot \mathbf{v} &= 0, \end{aligned} \quad (29)$$

where σ_{elast} is given in Eq. (27). Otto and Tazavaras [46] have been able to show existence of strong solutions to the initial and boundary value problem for Eq. (29) in the limit of large viscosity ν , where the Navier–Stokes-like equation reduces to the (stationary) Stokes equation with an additional stress tensor. Bae and Trivisa [48] have proved global existence of weak solutions to Eqs. (26) and (29) and extended this result also to compressible fluid flow (see Bae and Trivisa [49]). For more general stress tensors σ , certain regularity results are derived in Ref. [47,50].

3. Q-tensor theory

3.1. The Q-tensor and corresponding free energy functionals

So far we have focused on the dynamics of the entire space- and orientation dependent probability density, $f = f(\mathbf{x}, \mathbf{n}, t)$. A common simplification, pioneered by Nobel price laureate Pierre G. de Gennes (see de Gennes [32]), consists in studying rather the dynamical evolution of the lowest-order moment of f . For a liquid crystalline comprised of *nonpolar* particles, the lowest (nonvanishing) moment is the so-called Q -tensor, a second-rank tensorial quantity which provides a complete description of the orientational state of the system. The dynamics is then referred to as Q -tensor dynamics.

At this point it seems worth to state the major *physical* argument why one should generally use a second-rank order parameter tensor to describe the orientational structure and dynamics rather than just the average orientation, which would correspond to the nematic director. The latter is a vectorial quantity and thus seems, at least on first sight, easier to handle (indeed, the dynamics of the nematic director within the so-called Ericksen–Leslie theory will be discussed in Section 4). However, reducing the system’s dynamics to that of the director implicitly assumes that the orientational order is *uniaxial*. This assumption can break down in the presence of topological defects within the nematic phase (see Refs. [51,52]), but also as a result of strong shear flow (see Refs. [53]) inducing complex states of orientational motion.

To introduce Q , we recall (see Section 2) that f is a normalized, positive definite probability density on the sphere which is invariant against reversal of the molecular orientation \mathbf{n} . Thus, the first moment is zero, that is

$$\int_{\mathbb{S}^2} \mathbf{n} f(\mathbf{x}, \mathbf{n}, t) d\mathbf{n} = 0 \quad \text{for all } \mathbf{x} \in \Omega, t \geq 0. \quad (30)$$

The second moment Q -tensor then is given as (see, e.g., de Gennes [32, Section 2.1])

$$Q(\mathbf{x}, t) := \int_{\mathbb{S}^2} \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I \right) f(\mathbf{x}, \mathbf{n}, t) d\mathbf{n}. \quad (31)$$

It is obvious that Q is symmetric and thus possesses a complete system of orthonormal eigenvectors \mathbf{e}_i with real eigenvalues λ_i ($i = 1, 2, 3$). Therefore, Q can be represented by the spectral decomposition (see Ref. [54]),

$$Q = \lambda_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + \lambda_2 \mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \otimes \mathbf{e}_3. \quad (32)$$

Since the eigenvectors \mathbf{e}_i are unit vectors and since f is a probability density, the eigenvalues are bounded (see Ref. [55]) according to

$$-\frac{1}{3} \leq \lambda_i = \mathbf{e}_i \cdot Q \mathbf{e}_i = \int_{\mathbb{S}^2} (\mathbf{e}_i \cdot \mathbf{n})^2 f(\mathbf{x}, \mathbf{n}, t) d\mathbf{n} - \frac{1}{3} \leq \frac{2}{3}. \quad (33)$$

This condition is often called physical condition (see Ref. [55]). Further, because of $|\mathbf{n}| = 1$, the tensor Q is always traceless such that

$$\text{tr}Q = \lambda_1 + \lambda_2 + \lambda_3 = 0. \tag{34}$$

An analysis of the eigenvalues yields information about the ordering state of the system. Specifically, Q allows to distinguish between three different states: isotropic, uniaxial or biaxial. In the isotropic phase, $f = 1/(4\pi)$. A short calculation then shows that the tensor Q is zero since $\int_{\mathbb{S}^2} \mathbf{n} \otimes \mathbf{n} d\mathbf{n} = (4\pi/3)I$, and so are the eigenvalues λ_i . Uniaxial nematic phases are characterized by a spectrum where two of the eigenvalues of Q coincide, whereas the third one is different. Finally, biaxial states are characterized by three different eigenvalues (see Mottram and Newton [56]).

We briefly mention an alternative way to decompose the Q -tensor (see Ref. [54]), which requires only two eigenvectors but two additional scalar order parameters. This form is given by

$$Q = s\left(e_1 \otimes e_1 - \frac{1}{3}I\right) + r\left(e_2 \otimes e_2 - \frac{1}{3}I\right). \tag{35}$$

The parameters s and r are related to the eigenvalues in Eq. (32) via

$$s = \lambda_1 - \lambda_3 = 2\lambda_1 + \lambda_2, \quad r = \lambda_2 - \lambda_3 = 2\lambda_2 + \lambda_1, \tag{36}$$

where we have used that $I = e_1 \otimes e_1 + e_2 \otimes e_2 + e_3 \otimes e_3$. Without loss of generality, $r = 0$ in the uniaxial state (since $\lambda_2 = \lambda_3$ Ref. [57]), but r is nonzero in the biaxial state.

According to the standard thermodynamic principles, the equilibrium value of Q corresponds to a minimum of a free energy functional. We thus need an expression for the free energy directly expressed in terms of Q (rather than in terms of the distribution f as discussed in Section (2.1)). As a starting point, we consider the famous Landau–de Gennes free energy (see Refs. [58,59]), which in the absence of external aligning fields and surfaces is given as

$$F_{LG}[Q] = \int_{\Omega} \left(\frac{a(T)}{2} \text{tr}(Q^2) - \frac{b}{3} \text{tr}(Q^3) + \frac{c}{4} (\text{tr}(Q^2))^2 \right) \tag{37a}$$

$$+ \frac{L_1}{2} |\nabla Q|^2 + \frac{L_2}{2} \sum_{i=1}^3 \text{tr}(\nabla Q_i \nabla Q_i) + \frac{L_3}{2} |\nabla \cdot Q|^2 \tag{37b}$$

$$+ \frac{L_4}{2} \sum_{i=1}^3 Q_i \cdot \nabla \times Q_i + \frac{L_5}{2} \sum_{i=1}^3 \text{tr}(\nabla Q_i Q_i (\nabla Q_i)^T) dx. \tag{37c}$$

The first line on the right-hand side of Eq. (37a) describes the bulk free energy density, assuming that the latter can be written as a polynomial in the Q tensor. The coefficients b and c are usually considered as state-independent material constants, whereas a depends on the temperature or composition (for a thermotropic or lyotropic system, respectively). Specifically, a change of the sign of a induces the isotropic-nematic transition. Note that all of the terms appearing in the bulk free energy are constructed to be rotationally invariant, as required for a physically meaningful (that is, scalar) free energy F . This requirement also enters into the remaining terms in Eq. (37) which contain gradient terms and thus describe the “elastic part” of the free energy, that is, the free energy due to elastic distortions. Here, the notation Q_i is used to describe the i th row of the Q -tensor (regarded as a column vector), and the parameters L_1, \dots, L_5 are material constants. A frequent assumption is the one-constant approximation, where $L_2 = L_3 = L_4 = L_5 = 0$ (see Ref. [54]).

At this point it seems natural to ask about the relationship between the free energy functionals for the Q tensor, such as the Landau–de Gennes ansatz defined in Eq. (37), and the “microscopic” free energy functionals for the full probability distribution considered in Section 2. Indeed, both type of functionals are assumed to yield the *same* equilibrium state (described by f or Q) by minimization! A systematic strategy to derive a Q -dependent free energy is as follows: One first expresses the full distribution f as a power series in terms of orientational order parameters (involving Q and higher-order moments). Inserting and expanding

the logarithmic (entropic) and interaction parts of the free energy up to the lowest vanishing terms (which involve some closure approximation for the moments), one then obtains an expression for the bulk free energy (for a recent application of this strategy, see Ref. [60]). The elastic contribution can then be derived by performing an additional gradient expansion.

Here we restrict ourselves to illustrating the relation between the Q - and the f -dependent functional at the example of the Maier–Saupe interaction functional. The latter is given in Eq. (10); it represents the interaction part of the full f -dependent functional F in Eq. (14). Neglecting any spatial and temporal dependence of f , we find that

$$\begin{aligned} & - \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} (\mathbf{n} \cdot \hat{\mathbf{n}})^2 f(\mathbf{n}) f(\hat{\mathbf{n}}) d\mathbf{n} d\hat{\mathbf{n}} \\ &= - \left(\int_{\mathbb{S}^2} \mathbf{n} \otimes \mathbf{n} f(\mathbf{n}) d\mathbf{n} \right) : \left(\int_{\mathbb{S}^2} \hat{\mathbf{n}} \otimes \hat{\mathbf{n}} f(\hat{\mathbf{n}}) d\hat{\mathbf{n}} \right) \\ &= - \left(\int_{\mathbb{S}^2} (\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I) f(\mathbf{n}) d\mathbf{n} \right) : \left(\int_{\mathbb{S}^2} (\hat{\mathbf{n}} \otimes \hat{\mathbf{n}} - \frac{1}{3}I) f(\hat{\mathbf{n}}) d\hat{\mathbf{n}} \right) \\ & \quad + \frac{1}{3} \int_{\mathbb{S}^2} \hat{\mathbf{n}} \cdot \hat{\mathbf{n}} f(\hat{\mathbf{n}}) d\hat{\mathbf{n}} + \frac{1}{3} \int_{\mathbb{S}^2} \mathbf{n} \cdot \mathbf{n} f(\mathbf{n}) d\mathbf{n} - \frac{1}{9} = -|Q|^2 + \frac{5}{9}. \end{aligned} \tag{38}$$

The free energy then takes the form

$$F_{MS}[f] \sim \int_{\mathbb{S}^2} f(\mathbf{n}) (\ln f(\mathbf{n}) - 1) d\mathbf{n} - \alpha |Q|^2 + \frac{5}{9} \alpha, \tag{39}$$

where we have not yet touched the entropic part (first term). The additive constants $\int_{\mathbb{S}^2} f(\mathbf{n}) d\mathbf{n}$ and $(5\alpha)/9$ (with α being a constant related to the coupling strength, see also Eq. (9)) can be neglected since the physical (equilibrium) behavior is determined by the derivative of F rather than by F itself. The important point of (Eq. (39)) is that the (Maier–Saupe) interaction contribution is simply expressed as the square of the norm of the order parameter. Historically, this was one of the motivating ideas to construct a Q -dependent free energy.

At the end of this section on the stationary Q -tensor theory, we point the reader to a quite omnipresent problem of the Landau–de Gennes free energy functional: Minimization of F_{LG} (see Eq. (37)) can yield solutions for Q , whose eigenvalues λ_i violate the constraints given in Eq. (33) (see Mottram and Newton [56]). To circumvent this problem, Ball and Majumdar [58] proposed the following strategy, which is based on the free energy F_{MS} given in Eq. (39). The idea is to minimize F_{MS} over all probability densities f for a fixed Q -tensor (which has the required properties). To this end, one first defines the set of probability densities related to a given Q -tensor via

$$\begin{aligned} \mathcal{A}_Q &:= \left\{ f : \mathbb{S}^2 \rightarrow \mathbb{R}, f \geq 0, \int_{\mathbb{S}^2} f(\mathbf{n}) d\mathbf{n} = 1; \right. \\ & \quad \left. Q = \int_{\mathbb{S}^2} \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I \right) f(\mathbf{n}) d\mathbf{n} \right\}. \end{aligned} \tag{40}$$

For this set \mathcal{A}_Q , the authors of Ref. [58] considered the minimization problem associated to the energy (39) and defined the function

$$g(Q) := \begin{cases} \min_{f \in \mathcal{A}_Q} \int_{\mathbb{S}^2} f(\mathbf{n}) \ln f(\mathbf{n}) d\mathbf{n} & \text{if } -\frac{1}{3} \leq \lambda_i(Q) \leq \frac{2}{3} \quad i = 1, 2, 3, \\ \infty & \text{otherwise.} \end{cases} \tag{41}$$

The function g is finite if the eigenvalues of the given Q -tensor fulfill the constraints in Eq. (33) (see Ref. [58]). One then obtains a new bulk free energy density (replacing that in Eq. (37a)), which is defined as

$$\psi_B(Q) = Tg(Q) - \alpha |Q|^2, \tag{42}$$

where T denotes the absolute temperature and α the coupling strength (see Eq. (39)). Ball and Majumdar [58] have investigated in detail the analytical properties of $\psi_B(Q)$, like smoothness, convexity, isotropy, boundedness from below and logarithmic blow-ups at the boundary of

the domain (see also Ref. [55]). This paves the way to usage of this functional in stationary and nonstationary problems. Moreover, the functional can be easily extended toward inhomogeneous situations. Specifically, in the one-constant approximation one obtains

$$F_{BM}[Q] := \int_{\Omega} (L_1 |\nabla Q|^2 + \psi_B(Q)) dx. \quad (43)$$

An alternative strategy to “cure” the problem of obtaining eigenvalues of Q beyond a prescribed range has been suggested by Heidenreich et al. [61]. They proposed an “amended” free energy functional which coincides with the Landau–de Gennes ansatz for small degree of ordering, but includes a correction term becoming effective for stronger nematic order. The correction can be motivated by an expansion of the Onsager excluded-volume potential. The amended free energy potential is given by (see Ref. [61])

$$F[Q] = \int_{\Omega} \left(\frac{a(T)}{2} |Q|^2 - \frac{b}{3} \text{tr}(Q^3) - \frac{c_{\max}^4}{2} \ln \left(1 - \frac{|Q|^4}{c_{\max}^4} \right) \right) dx. \quad (44)$$

The potential induces logarithmic blow-ups when the sum of the squares of the eigenvalues of Q approaches a certain threshold c_{\max} , i.e. $(\sum_{i=1}^3 \lambda_i^2) \rightarrow c_{\max}^2$. Choosing the norm in the definition (44) differently, taking rather the spectral than the Frobenius norm in the logarithmic term, would guarantee blow ups for Q -tensors with eigenvalues leaving the physical range (33). The associated functional is given by

$$F[Q] = \int_{\Omega} \left(\frac{a(T)}{2} |Q|^2 - \frac{b}{3} \text{tr}(Q^3) - \frac{1}{8} \ln \left(1 - 4 \left\| Q + \frac{1}{6} I \right\|_2^4 \right) \right) dx, \quad (45)$$

where the spectral norm $\|A\|_2^2$ of a symmetric matrix $A \in \mathbb{R}^{3 \times 3}$ is just the largest absolute value of the eigenvalues. This formulation leads to minimizers fulfilling the physical condition (33). In this way we avoid the infinite-dimensional minimization problem in (41), which involves a special set of function (see Eq. (40)).

3.2. Nonstationary equations

We now turn to Q -tensor theory for *flowing*, and possibly inhomogeneous, liquid crystals. To this end, various formulations of the equations have been proposed and studied in the literature. The first complete formulation is due to Hess [62,63], who derived the equations using concepts from irreversible thermodynamics (see de Groot and Mazur [64] and showed that they can also be motivated via a Fokker–Planck approach (for a modern derivation, see Hess [12]). A closely related derivation was proposed by Olmstedt and Goldbart [65,66], and by Beris and Edwards [26]. We further mention the equations proposed by Stark and Lubensky [67] derived from the Poisson bracket formalism, and the phenomenologically motivated Q -tensor equations by Pleiner et al. [68].

All of these formulations agree in their general structure (comprising an evolution equation for Q combined with the Navier–Stokes equation for incompressible fluids), but differ in aspects such as the free-energy functional used for the relaxation term, and the types of coupling between the order parameter tensor and the flow profile \mathbf{v} .

In the following we focus on the “hydrodynamical” equations suggested by Edwards and Beris [26], which are widely used in the modern literature as well as in many numerical studies (see, e.g., the Lattice–Boltzmann studies of Yeomans et al. [52]). These equations are given by

$$\frac{\partial Q}{\partial t} + (\mathbf{v} \cdot \nabla) Q - S(Q, \nabla \mathbf{v}) = \Gamma H, \quad (46a)$$

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla p - \nu \Delta \mathbf{v} = \nabla \cdot (\tau + \sigma), \quad (46b)$$

$$\nabla \cdot \mathbf{v} = 0, \quad (46c)$$

where $Q = Q(\mathbf{x}, t)$. In Eq. (46a), the first two terms on the left-hand side form the material derivative of the Q -tensor (including the advection stemming from the flow velocity field \mathbf{v}). The second term S describes

the influence of \mathbf{v} on the spatio-temporal distribution of the order parameter. More specifically, the (tensorial) velocity gradient $\nabla \mathbf{v}$ can lead to stretching of Q , which is imposed by the symmetric part $(\nabla \mathbf{v})_{\text{sym}}$ of the velocity gradient and to a rotation of Q , imposed by the skew-symmetric part $(\nabla \mathbf{v})_{\text{skw}}$. Explicitly, the function S is given by

$$S(Q, \nabla \mathbf{v}) := ((\nabla \mathbf{v})_{\text{skw}} + \xi (\nabla \mathbf{v})_{\text{sym}}) \left(Q + \frac{1}{3} I \right) - \left(Q + \frac{1}{3} I \right) ((\nabla \mathbf{v})_{\text{skw}} - \xi (\nabla \mathbf{v})_{\text{sym}}) - 2\xi \left(Q + \frac{1}{3} I \right) \text{tr}(Q \nabla \mathbf{v}), \quad (47)$$

where the parameter ξ depends on the microscopic properties of the material considered. In the mathematics literature, this parameter is always assumed to be sufficiently small or even zero. Taken altogether, the left-hand side of Eq. (46a) is similar to the Oldroyd derivative of the stress tensor appearing in the description of Oldroyd fluids (see Ref. [69]). The Oldroyd system describes viscoelastic materials by coupling the Navier–Stokes equation with an additional evolution equation for the stress tensor. In this latter equation, the material derivative is consistent with the left-hand side of Eq. (46a) if Q is replaced by the stress and the second line of Eq. (47) is omitted (compare Ref. [69]).

Finally, the right-hand side of (Eq. (46a)) describes the relaxation of Q towards its equilibrium value determined by the minimum of the free energy functional. It thus involves (besides the rotational diffusion constant Γ) the variational derivative of F with respect to the order parameter, that is,

$$H = -\frac{\delta F}{\delta Q}[Q] + \frac{1}{3} \text{tr} \frac{\delta F}{\delta Q}[Q]. \quad (48)$$

The precise form of the function H obviously depends on the choice of the free energy functional F . Common choices in the mathematical literature are the Landau de Gennes functionals F_{LG} (see Eq. (37)) and its modified (constrained) version F_{BM} (see Eq. (43)). From the physical side, most studies concentrate on using F_{LG} .

The second member of (Eq. (46)) describes the interplay between the velocity profile and the orientational ordering. As in the case of the corresponding kinetic equations based on the distribution function f (see, e.g., (Eq. (21))), the coupling is achieved by adding to the standard Navier–Stokes additional stress tensor contributions (note that the isotropic contributions appear already on the left-hand side of (Eq. (46))). The Q -dependent contribution to the stress tensor consists of a symmetric part

$$\tau = -\xi \left(Q + \frac{1}{3} I \right) H - \xi H \left(Q + \frac{1}{3} I \right) + 2\xi \left(Q + \frac{1}{3} I \right) \text{tr}(QH) - \nabla Q : \frac{\partial F}{\partial \nabla Q} \quad (49)$$

and an skew-symmetric part

$$\sigma = QH - HQ, \quad (50)$$

where H is defined as in Eq. (48). In Eq. (49), the last term depends on which terms are included in the elastic part (involving gradient terms) of the free energy, see text below (Eq. (37)). In case of the one-constant approximation, we find that

$$\left(\nabla Q : \frac{\partial F}{\partial \nabla Q} \right)_{ij} := \left(\nabla Q : \frac{\partial(L_1 |\nabla Q|^2)}{\partial \nabla Q} \right)_{ij} = L_1 \sum_{k,l=1}^3 \partial_{x_i} Q_{kl} \partial_{x_j} Q_{kl}. \quad (51)$$

What remains to be calculated is the quantity H , i.e., the functional derivative of the free energy with respect to Q itself (see Eq. (48)). Taking $F = F_{LG}$ (see (Eq. (37))) and using again the one-constant approximation, we obtain

$$H = -a(T)Q + b \left(Q^2 - \frac{1}{3} \text{tr}(Q^2) \right) - cQ \text{tr}(Q^2) + L_1 \Delta Q, \quad (52)$$

where the first three terms on the right-hand side in Eq. (52) stem from the bulk part of the free energy, whereas the last term is due to the elastic part.

Numerical (Lattice–Boltzmann) simulations of the present (Beris–Edwards) Q -tensor model have been studied, among others, by Yeomans

et al. [52,70,71] who focused on the emergence of topological defects and on domain growth. The Q -tensor equations proposed by Hess have been numerically explored in detail in their homogeneous version (see, e.g. Refs. [72,73], who concentrated on the complex time-dependent states appearing at large shear rates), in a simplified inhomogeneous version without back-coupling to the velocity profile (see Ref. [74]) and in the fully coupled inhomogeneous version (see Ref. [75]).

We close this section with some remarks from the mathematical side. The system given by Eqs. (46)–(52), has been studied by Paicu and Zarnescu [76,77] who discussed well-posedness. In Ref. [76], they were able to prove the global existence of weak solutions for the Cauchy problem in dimension three. For the special case that the rotational parameter ξ appearing, e.g., in (Eq. (47)) vanishes, they also demonstrated a certain higher regularity of the solution, as well as weak-strong uniqueness in dimension two. In Ref. [77], the results are extended to non-zero ξ .

The Cauchy problem has also been addressed in Huang and Ding [59] who considered the more general free energy (37) with specific assumptions on the constants L_i ($i = 1, \dots, 5$). Additionally, the authors provided a well-posedness result for small data. Abels et al. [78] studied the Dirichlet and the Neumann problem for the coupled Navier–Stokes/ Q -tensor system involving the Landau–de Gennes free energy (37) in the one-constant approximation (similar to Eq. (43)). They proved global existence of weak solutions as well as local existence of strong solutions together with regularity results.

Further, Wilkinson [55] provided existence results for the case that the free energy functional is chosen to have the form F_{BM} (see Eq. (43)), again with the one-constant approximation. Then H takes the form

$$H := L_1 \Delta Q - T \left(\frac{\partial g}{\partial Q}(Q) - \frac{1}{3} \text{tr} \left(\frac{\partial g}{\partial Q}(Q) \right) I \right) + \alpha Q. \quad (53)$$

The resulting system consists of Eqs. (46)–(50) and Eq. (53). For this case, Wilkinson showed in Ref. [55] global existence of weak solutions in three dimensions for periodic boundary conditions and additional regularity for solutions in two dimensions. We may emphasize that the theory in Ref. [55] predicts Q -tensors as solutions fulfilling the physical constraint (33) (compare to Section 3.1).

Finally, Feireisl et al. [79] considered a nonisothermal variant of system (46) with an extra equation for the temperature and the solution fulfilling an entropy inequality. Existence of weak solutions is proved as well.

4. Ericksen–Leslie theory

As a special case of the Q tensor theory outlined in Section 3, we now consider *uniaxial* nematic states in nonstationary (and possibly inhomogeneous) situations. For an uniaxial (cylindrically symmetric) system, the Q -tensor takes the form

$$Q = s \left(\mathbf{d} \otimes \mathbf{d} - \frac{1}{3} I \right), \quad (54)$$

where \mathbf{d} is the (normalized) eigenvector related to the eigenvalue with the largest absolute value. This eigenvector is unique up to multiplication with -1 ; it has algebraic multiplicity one due to the zero-trace condition (34) of the Q -tensor. Physically speaking, (Eq. (54)) expresses the fact that under the assumption of uniaxiality (which typically holds only for liquid crystals at low molecular weights, see Beris and Edwards [26]), the system’s anisotropy is fully specified by the director \mathbf{d} .

In the 1960s, Ericksen [80,81] and Leslie [82–84] have proposed a set of nonstationary equations describing the director dynamics under shear. This “Ericksen–Leslie” theory is nowadays regarded as a pioneer of the more advanced Q -tensor approach. Besides the assumption of uniaxiality, a further key simplification within the Ericksen–Leslie approach consists of the fact that the degree of order along \mathbf{d} is assumed to be *constant*, specifically, $|\mathbf{d}| = 1$ (similar to the theory of Oseen [85] and Frank [86] for inhomogeneous, stationary nematic states). The resulting set of equations reads, in its most general form (see Ref. [82]),

$$\begin{aligned} \rho_1 \frac{d^2 \mathbf{d}}{dt^2} - \nabla \cdot \left(\frac{\partial F}{\partial \nabla \mathbf{d}} \right) + \frac{\partial F}{\partial \mathbf{d}} - \lambda_1 \left(\frac{\partial \mathbf{d}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{d} + (\nabla \mathbf{v})_{\text{skw}}^T \mathbf{d} \right) \\ + \lambda_2 (\nabla \mathbf{v})_{\text{sym}} \mathbf{d} = \rho_1 \mathbf{G}, \end{aligned} \quad (55a)$$

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla p + \nabla \cdot \left(\nabla \mathbf{d}^T \frac{\partial F}{\partial \nabla \mathbf{d}} \right) - \nabla \cdot \boldsymbol{\sigma} = \mathbf{F}, \quad (55b)$$

$$\nabla \cdot \mathbf{v} = 0, \quad (55c)$$

$$|\mathbf{d}|^2 = 1. \quad (55d)$$

The first term in Eq. (55a) is the second material derivative, where the first one is defined via $d/dt = \partial/\partial t + (\mathbf{v} \cdot \nabla)$, and F is the free energy functional $F = F(\mathbf{d}, \nabla \mathbf{d})$. The vectorial quantities \mathbf{G} and \mathbf{F} appearing on the right-hand sides of Eqs. (55a) and (55b) represent external forces acting on the director and on the velocity field, respectively. Eq. (55b) further involves the so-called “Leslie stress” $\boldsymbol{\sigma}$ that corresponds to the dissipative part of the stress tensor. It is given by

$$\begin{aligned} \boldsymbol{\sigma} := & \mu_1 (\mathbf{d} \cdot (\nabla \mathbf{v})_{\text{sym}} \mathbf{d}) \mathbf{d} \otimes \mathbf{d} + \mu_4 (\nabla \mathbf{v})_{\text{sym}} \\ & + \mu_2 \mathbf{d} \otimes \left(\frac{\partial \mathbf{d}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{d} + (\nabla \mathbf{v})_{\text{skw}} \mathbf{d} \right) \\ & + \mu_3 \left(\frac{\partial \mathbf{d}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{d} + (\nabla \mathbf{v})_{\text{skw}} \mathbf{d} \right) \otimes \mathbf{d} \\ & + \mu_5 \mathbf{d} \otimes \mathbf{d} (\nabla \mathbf{v})_{\text{sym}} + \mu_6 (\nabla \mathbf{v})_{\text{sym}} \mathbf{d} \otimes \mathbf{d}, \end{aligned} \quad (56)$$

where the “Leslie constants” μ_1, \dots, μ_4 are related to those appearing in Eq. (55a) via (see Ref. [82]),

$$\lambda_1 = \mu_2 - \mu_3, \quad \lambda_2 = \mu_5 - \mu_6 = -(\mu_2 + \mu_3). \quad (57)$$

The last equation is often referred to as Parodi’s relation. It is a consequence of the Onsager reciprocal relations (see Ref. [87])

Regarding the free energy F , different choices have been considered. Leslie [82] suggested to use the expression due to Oseen and Frank [86], that is,

$$\begin{aligned} F_{OF}(\mathbf{d}, \nabla \mathbf{d}) := & k_1 (\nabla \cdot \mathbf{d})^2 + k_2 (\mathbf{d} \cdot \nabla \times \mathbf{d} + q)^2 + k_3 |\mathbf{d} \times \nabla \times \mathbf{d}|^2 \\ & + \alpha (\text{tr}(\nabla \mathbf{d})^2 - (\nabla \cdot \mathbf{d})^2), \end{aligned} \quad (58)$$

where k_i ($i = 1, 2, 3$), α and q denote elastic constants. Note that we used the notation $F = F(\mathbf{d}, \nabla \mathbf{d})$ instead of $F[\mathbf{d}]$ to express that we consider F_{OF} as a function in \mathbf{d} and $\nabla \mathbf{d}$ instead of a functional in \mathbf{d} . This is a plausible choice for an inhomogeneous (uniaxial) nematic liquid crystal. However, as proposed by de Gennes [32], the theory can also be used to describe the impact of a magnetic field, disregarding distortion effects. To this end, he proposed the *ansatz*

$$F_H(\mathbf{d}) = -\chi_{\perp} |\mathbf{H}|^2 - (\chi_{\parallel} - \chi_{\perp}) (\mathbf{d} \cdot \mathbf{H})^2, \quad (59)$$

which conforms with the *ansatz* (7) for the effective potential in a corresponding stationary theory. The parameters χ_{\parallel} and χ_{\perp} are the magnetic susceptibility constants for a magnetic field parallel and perpendicular to the director \mathbf{d} , respectively.

4.1. Mathematical studies of the Ericksen–Leslie theory

From the physical side, most of the recent studies of nonequilibrium liquid crystals employ full Q -tensor theories rather than director dynamics since it is well established that the systems of interest are typically *not* uniaxial. From the mathematical perspective, however, the lower-dimensional structure of the Ericksen–Leslie theory, which still carries important aspects of the orientational dynamics, makes this theory somewhat more accessible for rigorous treatments. We thus summarize recent mathematical advances in this area.

To start with, we stress that the full system (55)–(58) of nonlinear partial differential equations involving nonlinear coupling between \mathbf{v} and \mathbf{d} as well as algebraic restrictions is, from the mathematical point

of view, rather difficult. So far results were only achieved under rather strong simplifications. In particular, the second material derivative is nearly always neglected (see Ref. [88] for a first treatment). This seems to be appropriate since the constant ρ_1 , which appears as a prefactor of the second time derivative and is related to the moment of inertia, is typically negligible in a macroscopic viscous system. Moreover, if this second-order term would not be neglected, the first equation would remain of hyperbolic type, what would require a different mathematical approach to existence.

Several important contributions regarding the first-order Ericksen–Leslie theory are due to Lin and Liu [89–91]. In Ref. [89] they considered a system, where the (Oseen–Frank) free energy functional is written in the one-constant approximation (see Eq. (58)). Further, the algebraic restriction $|\mathbf{d}| = 1$ is incorporated by adding a Ginzburg–Landau penalty functional, a trick which was later copied by several other authors. The resulting free energy functional reads

$$F_\varepsilon(\mathbf{d}, \nabla \mathbf{d}) = \frac{1}{2} |\nabla \mathbf{d}|^2 + \frac{1}{4\varepsilon^2} (|\mathbf{d}|^2 - 1)^2. \tag{60}$$

In the dissipative stress tensor σ (see Eq. (56)), Lin and Liu set all Leslie constants to zero except μ_4 , such that $\sigma = \mu_4(\nabla \mathbf{v})_{\text{sym}}$. Further, the external forces appearing on the right-hand sides of Eqs. (55a) and (55b) are neglected, λ_1 is set to one, and λ_2 is set to zero. With this last simplification, translational forces of the fluid onto the director are neglected, which enables to prove a maximum principle for $|\mathbf{d}|^2$ that is essential for the later analysis. The simplified system considered in Lin and Liu [89] then reads

$$\begin{aligned} \frac{\partial \mathbf{d}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{d} &= \Delta \mathbf{d} - \frac{1}{\varepsilon^2} (|\mathbf{d}|^2 - 1) \mathbf{d}, \\ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla p - \frac{\mu_4}{2} \Delta \mathbf{v} &= -\nabla \cdot (\nabla \mathbf{d}^T \nabla \mathbf{d}), \\ \nabla \cdot \mathbf{v} &= 0. \end{aligned} \tag{61}$$

Remark that $\mu_4 \nabla \cdot (\nabla \mathbf{v})_{\text{sym}} = (\mu_4/2) \Delta \mathbf{v}$ since \mathbf{v} is solenoidal, (i.e., $\nabla \cdot \mathbf{v} = 0$). For this system (61), Lin and Liu proved global existence of weak solutions and local existence of strong solutions (see Ref. [89]). In Ref. [91], they succeeded in generalizing their results to a system in formal analogy to Eq. (61), but with the full dissipative Leslie stress tensor σ (see Eq. (56)) and not neglecting the nonlinear coupling term $(\nabla \mathbf{v})_{\text{skw}} \mathbf{d}$ in Eq. (55a). This yields

$$\begin{aligned} \frac{\partial \mathbf{d}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{d} + (\nabla \mathbf{v})_{\text{skw}} \mathbf{d} + \frac{\lambda_2}{\lambda_1} (\nabla \mathbf{v})_{\text{sym}} \mathbf{d} &= \Delta \mathbf{d} - \frac{1}{\varepsilon^2} (|\mathbf{d}|^2 - 1) \mathbf{d}, \\ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla p - \sigma' &= -\nabla \cdot (\nabla \mathbf{d}^T \nabla \mathbf{d}), \\ \nabla \cdot \mathbf{v} &= 0. \end{aligned} \tag{62}$$

In treating this system, Lin and Liu [91] again specialized on the case $\lambda_2 = 0$, because the existence results rely essentially on a maximum principle for $|\mathbf{d}|^2$, which does not hold if $\lambda_2 \neq 0$. To illustrate the application of the maximum principle, we multiply the first member of Eqs. (62) (with $\lambda_2 = 0$) with $2\mathbf{d}$, yielding formally an equation for $|\mathbf{d}|^2$,

$$\begin{aligned} \frac{\partial}{\partial t} |\mathbf{d}|^2 + (\mathbf{v} \cdot \nabla) |\mathbf{d}|^2 &= 2\Delta \mathbf{d} \cdot \mathbf{d} - \frac{2}{\varepsilon^2} (|\mathbf{d}|^2 - 1) |\mathbf{d}|^2 \\ &= \Delta |\mathbf{d}|^2 - 2|\nabla \mathbf{d}|^2 - \frac{2}{\varepsilon^2} (|\mathbf{d}|^2 - 1) |\mathbf{d}|^2. \end{aligned} \tag{63}$$

Note that $\mathbf{d} \cdot (\nabla \mathbf{v})_{\text{skw}} \mathbf{d} = 0$. A maximum of the function $|\mathbf{d}|^2$ with respect to time and space implies a maximum of $|\mathbf{d}|$ itself. Moreover, for a maximum of $|\mathbf{d}|^2$, we observe that the first derivatives are zero, such that $\partial_t |\mathbf{d}|^2 + (\mathbf{v} \cdot \nabla) |\mathbf{d}|^2 = 0$ and $\Delta |\mathbf{d}|^2 \leq 0$. The assumption that the maximum is attained at a point where the norm of \mathbf{d} is greater than 1 leads (because of the contribution of the Ginzburg–Landau penalization with $(|\mathbf{d}|^2 - 1) |\mathbf{d}|^2 > 0$ for $|\mathbf{d}| > 1$) to a contradiction. We further mention that Lin and Liu proved in [90] partial regularity of weak solutions to system (71) implying the convergence of the weak solutions of system (61) to a measure-valued solution of the original problem with $|\mathbf{d}| = 1$ as $\varepsilon \rightarrow 0$.

After the work of Lin and Liu, many other studies have appeared focusing on slightly more complicated models. For example, Cavaterra

et al. [92] considered model (62) with $\lambda_2 \neq 0$. They demonstrated global existence of weak solutions without a maximum principle and, additionally, local existence of classical solutions for periodic boundary conditions. Wu et al. [93] studied the importance of Parodi’s relation (last equation in (57)) for the well-posedness and stability of the system. The long-time behavior for a similar model was investigated in Petzeltová et al. [94], and a nonisothermal model was considered in Feireisl et al. [95]. There is also a first result on the simplified Ericksen–Leslie model (61) driven by multiplicative noise (see [96]).

The restriction of the Ericksen–Leslie theory regarding the constant magnitude of the director has been revisited in an article by Wang et al. [97]. They derived, under specific assumptions for the constants appearing in the Leslie stress, a reformulation of the Ericksen–Leslie system without the Ginzburg–Landau penalization. For this system, they derived various local well-posedness results, as well as global well-posedness for small initial data. We also mention a very recent generalization of the existence theory for the Ericksen–Leslie system (55) by Emmrich and Lasarzik [98]. They showed for a general class of free energies global existence of weak solutions.

5. Cross-Linkages between the different models

Having discussed three major approaches towards the stationary and nonstationary behavior of liquid crystals, one natural question concerns the linkages (if present) between the different models. We start by recalling the (obvious) connections between the dynamical variables of interest. Within the Doi–Hess theory, this is the probability density $f = f(\mathbf{x}, \mathbf{n}, t)$ (see, e.g., Eq. (1)), whose second moment corresponds (up to a constant shift) to the tensorial order parameter $Q = Q(\mathbf{x}, t)$, see Eq. (31). The eigenvector related to the eigenvalue of the Q -tensor with the largest absolute value then represents the director $\mathbf{d} = \mathbf{d}(\mathbf{x}, t)$ in the Ericksen–Leslie theory.

In the case $\mathbf{v} = 0$, all of the approaches discussed here reduce to minimization of a free energy functional. For the Doi–Hess model, one possible choice for the functional $F = F[f]$ is given in Eq. (14). In the Q -tensor and Ericksen–Leslie theory, the minimization is rather carried out with respect to the respective order parameter (Q or \mathbf{d}), and the free energies of interest are given either by the Landau–de Gennes expression F_{LG} (see (37) or alternatively the Maier–Saupe expression (39)), or by the Oseen–Frank energy F_{OF} (see (58)) in the Ericksen–Leslie model Eq. (55).

Are the solutions of these minimization procedures consistent? In this regard it is interesting to note that, according to Majumdar and Zarnescu [57], minimization of the Landau–de Gennes free energy (37) within the one-constant approximation (and for vanishing elastic constant, i.e., $L_1 \rightarrow 0$) can be written in the form

$$Q^* = s \left(\mathbf{d}^* \otimes \mathbf{d}^* - \frac{1}{3} I \right). \tag{64}$$

Here, \mathbf{d}^* is a unit vector minimizing the Oseen–Frank free energy (58) within the one-constant approximation, i.e., $k_1 = k_2 = k_3 = \alpha$.

Not surprisingly, the situation for nonstationary systems is more involved. For the case of a constant velocity field and a spatially homogeneous director \mathbf{d} , Kuzuu and Doi [24] showed that the Doi–Onsager equation and the Ericksen–Leslie equation yield the same results. This is since the time derivative and the convection term in Eqs. (46b) and (55b) vanish, and the Ericksen term $\nabla \cdot \left(\nabla \mathbf{d}^T \frac{\partial F}{\partial \nabla \mathbf{d}} \right)$ in Eq. (55b) becomes zero.

Beris and Edwards [26] have studied the linkages between the full Q -tensor theory and the Ericksen–Leslie. As shown in their monograph [26, Section 11.6.1], the equation of motion (46) for the Q -tensor reduces to equation (55) for the director in the uniaxial case.

Based on this earlier work, Wang et al. [99] have generalized the derivation of the Ericksen–Leslie equations from the Doi–Hess theory towards an inhomogeneous systems. To do this they formulated the problem as a limiting problem for vanishing Deborah number using a Hilbert

expansion. The connection between the Doi–Hess model (18)–(21) and the nonstationary equations for the Q-tensor (46) was investigated by Han et al. [100] They derived the system of Eq. (46) from Eqs. (18) to (21) using the so-called Bingham closure (see Ref. [101]). The latter provides a strategy to approximate higher order moments of the probability density f based on the second moment of f (i.e., Q).

A rigorous derivation of the Ericksen Leslie system (55) with the Oseen–Frank energy (58) starting from the Q-tensor theory for vanishing elastic constants ($L_i \rightarrow 0$ for $i = 1, 2, 3$ and $L_4 \equiv 0$ in the Landau–de Gennes energy (37)) was shown by Wang et al. [102] again by using a Hilbert expansion method.

6. Relative energy estimates for nonconvex energies

In view of the highly complex (and often nonlinear) evolution equations discussed in this paper, one may ask how different solutions (if present) can be related to one another. Solving this question may provide a new comparing tool for experimental or computational results or the evolution of a time series of a nematic liquid crystal. For probability distribution functions, a modern concept to measure the distance between two solutions involves the “relative entropy”, which is nowadays well established not only in the mathematical community but also in related fields such as information theory [103] and quantum entanglement [104]. The concept goes back to Dafermos [105]. For a strictly convex entropy function $\eta : \mathbb{R} \rightarrow \mathbb{R}$, the relative entropy of two solutions u and \tilde{u} is given by (see Ref. [106, Section 5.3])

$$\mathcal{E}[u|\tilde{u}] := \eta[u] - \eta[\tilde{u}] - \eta'[\tilde{u}](u - \tilde{u}). \tag{65}$$

The strict convexity of η guarantees that \mathcal{E} is nonnegative. Inserting, for example, the entropy function $\eta[u] = u \ln u - u$ (compare Eq. (14)) gives for probability densities u and \tilde{u} on a domain Ω

$$\begin{aligned} \mathcal{E}[u|\tilde{u}] &= \int_{\Omega} (u \ln u - u - \tilde{u} \ln \tilde{u} + \tilde{u} - (\ln \tilde{u})(u - \tilde{u})) dx \\ &= \int_{\Omega} u \ln \left(\frac{u}{\tilde{u}} \right) dx - \int_{\Omega} u dx + \int_{\Omega} \tilde{u} dx \\ &= \int_{\Omega} u \ln \left(\frac{u}{\tilde{u}} \right) dx \end{aligned} \tag{66}$$

since $\int_{\Omega} u dx = \int_{\Omega} \tilde{u} dx = 0$. This is the so-called Kullback–Leibler divergence (see Ref. [107]). Importantly, the concept can also be used in a more general way to measure the distance between two possible solutions (not necessarily distribution functions) of an evolution equation based on a special distance function, the relative entropy. This approach has been used, e.g., to show weak-strong uniqueness property of solutions (see Feireisl and Novotný [108]), the stability of an equilibrium state (see Feireisl [109]), the convergence to a singular limit problem (see Breit, Feireisl and Hofmanova [110] as well as Feireisl [111]), or to derive *a posteriori* estimates of numerical solutions (see Fischer [112]). Another possible application is the definition of a generalized solution concept, the dissipative solutions. The formulation of such a concept relies on an inequality instead of an equality (see Lions [113, Section 4.4]). Weak-strong uniqueness means that, in case of the same initial and boundary values, a generalized solution coincides with the strong solution as long as the latter exists.

In this section, we present a new relative entropy approach for a simplified Ericksen–Leslie model combined with the Oseen–Frank energy. We will show below that the Oseen–Frank free energy is nonconvex. Our approach therefore generalizes the relative entropy approach, which has so far been applied to convex functions, to nonconvex functions. In our context, the main quantities of interest are (free) energies rather than entropies. We therefore refer henceforth to a “relative energy” approach. We exemplify the calculations for the Ericksen–Leslie model but it is likely that the approach can be applied to the Q-tensor model as well. Clearly, such an extension would be highly desirable.

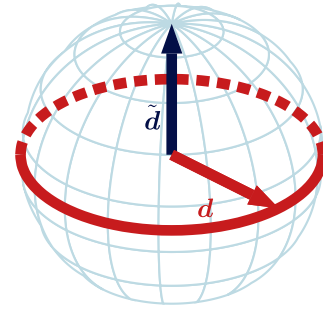


Fig. 2. The function d is given by the arrow, which moves along the equator of the sphere. The function \tilde{d} is the arrow pointing upwards.

Consider the Ericksen–Leslie model (55) with $\rho_1 \equiv 0$, $\lambda_1 = 1$, $F = 0$ and with the free energy

$$F[d] = \frac{k_1}{2} \int_{\Omega} |\nabla d|^2 dx + 2(k_3 - k_1) \int_{\Omega} |(\nabla d)_{\text{skw}} d|^2 dx. \tag{67}$$

We remark that $|\nabla d|^2 = (\nabla \cdot d)^2 + (d \cdot \nabla \times d)^2 + |d \times \nabla \times d|^2 + \nabla \cdot (\nabla d^T d - (\nabla \cdot d)d)$ as long as $|d| = 1$ and $4|(\nabla d)_{\text{skw}} d|^2 = |d \times \nabla \times d|^2$. Thus, the above energy is a simplification of the Oseen–Frank energy (see Eq. (58)) with $k_1 = k_2 = \alpha$ and $q = 0$. We could as well handle the full system and the full Oseen–Frank energy. Here, we simplify the system to keep the calculations readable and to focus on the novelty regarding the nonconvex part of the free energy.

First, we reason that the free energy in Eq. (67) is indeed nonconvex. To this end, we give an example, which violates the convexity condition $F[\lambda d + (1 - \lambda)\tilde{d}] \leq \lambda F[d] + (1 - \lambda)F[\tilde{d}]$ for a $\lambda \in (0, 1)$. Consider the two functions $d, \tilde{d} : \mathbb{R}^3 \supseteq \Omega \rightarrow \mathbb{S}^2$ given by $d(x, y, z) = (\sin(z), \cos(z), 0)$ and $\tilde{d}(x, y, z) = (0, 0, 1)$ (see Fig. 2). Calculating the free energy functional for both functions d and \tilde{d} yields

$$F[d] = \frac{k_1}{2} |\Omega| \quad \text{and} \quad F[\tilde{d}] = 0, \tag{68}$$

where $|\Omega|$ denotes the volume measure of the domain Ω . Since $2(\nabla d)\tilde{d} = (\cos(z), -\sin(z), 0)$, we find for the free energy functional evaluated at a convex combination of d and \tilde{d} that

$$F[\lambda d + (1 - \lambda)\tilde{d}] = \lambda^2 \frac{k_1}{2} |\Omega| + \lambda^2 (1 - \lambda)^2 \frac{(k_3 - k_1)}{2} |\Omega|. \tag{69}$$

Choosing now $(k_3 - k_1) = 5k_1$ and $\lambda = 1/2$ leads to

$$\begin{aligned} F\left[\frac{1}{2}d + \frac{1}{2}\tilde{d}\right] &= \frac{1}{4} \frac{k_1}{2} |\Omega| + \frac{5}{16} \frac{k_1}{2} |\Omega| = \frac{9}{16} \frac{k_1}{2} |\Omega| \\ &> \frac{1}{2} \frac{k_1}{2} |\Omega| = \frac{1}{2} F[d] + \frac{1}{2} F[\tilde{d}], \end{aligned} \tag{70}$$

which proves that the free energy F (see Eq. (67)) is indeed not convex.

In the following we choose $k_1 = (k_1 - k_3) = 1$ for brevity of notations. In addition, we assume that a constant velocity is prescribed, $\mathbf{v} \equiv \text{const}$. The equation of motion (55) then simplifies to

$$\begin{aligned} \partial_t d + (\mathbf{v} \cdot \nabla) d &= - \frac{\delta F}{\delta d} [d] = \nabla \cdot \left(\frac{\partial F_{OF}}{\partial \nabla d} (d, \nabla d) \right) - \frac{\partial F_{OF}}{\partial d} (d, \nabla d) \\ &= \nabla \cdot (\nabla d + ((\nabla d)_{\text{skw}} d \otimes d)_{\text{skw}}) - (\nabla d)_{\text{skw}}^T (\nabla d)_{\text{skw}} d \\ &= \Delta d + \nabla \cdot ((\nabla d)_{\text{skw}} d \otimes d)_{\text{skw}} - (\nabla d)_{\text{skw}}^T (\nabla d)_{\text{skw}} d. \end{aligned} \tag{71}$$

By F_{OF} we denote the potential (58) of the Oseen–Frank energy for the simplified case of Energy (67). Since \mathbf{v} is constant, an integration by parts shows formally that

$$\begin{aligned} \int_{\Omega} (\mathbf{v} \cdot \nabla) d \cdot \frac{\delta F}{\delta d} [d] dx &= \int_{\Omega} (\mathbf{v} \cdot \nabla) d \cdot \left(-\nabla \cdot \left(\frac{\partial F_{OF}}{\partial \nabla d} (d, \nabla d) \right) + \frac{\partial F_{OF}}{\partial d} (d, \nabla d) \right) dx \end{aligned}$$

$$\begin{aligned}
 &= \int_{\Omega} \left((\mathbf{v} \cdot \nabla) \nabla \mathbf{d} : \frac{\partial F_{OF}}{\partial \nabla \mathbf{d}}(\mathbf{d}, \nabla \mathbf{d}) + (\mathbf{v} \cdot \nabla) \mathbf{d} \cdot \frac{\partial F_{OF}}{\partial \mathbf{d}}(\mathbf{d}, \nabla \mathbf{d}) \right) dx \\
 &= \int_{\Omega} (\mathbf{v} \cdot \nabla) F_{OF}(\mathbf{d}, \nabla \mathbf{d}) dx = 0
 \end{aligned} \tag{72}$$

for every solution \mathbf{d} of Eq. (71). The last equation in the Calculation (72) holds since \mathbf{v} is assumed to be solenoidal and fulfill homogeneous Dirichlet boundary conditions. Testing Eq. (71) with the variational derivative of the solution \mathbf{d} , i.e., multiplying Eq. (71) with $\delta F / \delta \mathbf{d}$ and integrating over $\Omega \times (0, t)$, yields with $\int_{\Omega} \partial_t \mathbf{d} \cdot (\delta F / \delta \mathbf{d}) dx = \partial_t F[\mathbf{d}]$ formally the energy equality

$$F[\mathbf{d}(t)] + \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}(s)] \right|^2 dx ds = F[\mathbf{d}(0)] \quad \text{for } t \in (0, T). \tag{73}$$

The generalization of the concept of relative energies to nonconvex functionals relies on a suitable definition of the relative energy. If a functional η is nonconvex, the relative energy defined by (65) is not necessarily positive anymore. Here we introduce a new way to define the relative energy for nonconvex functions, which is nonnegative and allows to show an associated relative energy inequality (see inequality (75)). The proof of this inequality is carried out in Proposition 6.1.

The relative energy is given by

$$\begin{aligned}
 \mathcal{E}[\mathbf{d}(t)|\tilde{\mathbf{d}}(t)] &:= \frac{1}{2} \int_{\Omega} |\nabla \mathbf{d}(t) - \nabla \tilde{\mathbf{d}}(t)|^2 dx \\
 &\quad + \frac{1}{2} \int_{\Omega} |(\nabla \mathbf{d}(t))_{\text{skw}} \mathbf{d}(t) - (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t)|^2 dx.
 \end{aligned} \tag{74}$$

The following proposition gives an estimate of the relative energy and thus a measure of the distance of two solutions.

Proposition 6.1. *Let \mathbf{d} and $\tilde{\mathbf{d}}$ be two sufficiently smooth solutions to Eq. (71) fulfilling the same Dirichlet boundary conditions with boundary values that are constant in time. Then there holds for $t \in (0, T)$*

$$\begin{aligned}
 \mathcal{E}[\mathbf{d}(t)|\tilde{\mathbf{d}}(t)] &\leq 2 \left(\mathcal{E}[\mathbf{d}(0)|\tilde{\mathbf{d}}(0)] \right. \\
 &\quad + \max_{(x,t) \in \Omega \times [0,T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^2 \int_{\Omega} |\mathbf{d}(0) - \tilde{\mathbf{d}}(0)|^2 dx \\
 &\quad \left. + \int_{\Omega} |(\mathbf{d}(0) - \tilde{\mathbf{d}}(0)) \cdot ((\nabla \mathbf{d}(0) - \nabla \tilde{\mathbf{d}}(0))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0)| dx \right) \exp(\mathcal{K}(t)),
 \end{aligned} \tag{75}$$

where

$$\begin{aligned}
 \mathcal{K}(t) &= 4ct \max_{(x,t) \in \Omega \times [0,T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^4 \\
 &\quad + 2(1+c) \int_0^t \max_{x \in \Omega} (|\tilde{\mathbf{d}}(\mathbf{x})| |\nabla \partial_t \tilde{\mathbf{d}}(\mathbf{x})| + |\nabla \tilde{\mathbf{d}}(\mathbf{x})| |\partial_t \tilde{\mathbf{d}}(\mathbf{x})| \\
 &\quad + |\nabla \partial_t \tilde{\mathbf{d}}(\mathbf{x})| + |\partial_t \tilde{\mathbf{d}}(\mathbf{x})| + |\mathbf{v}(\mathbf{x})|^2) ds.
 \end{aligned} \tag{76}$$

Both solutions coincide if $\mathbf{d}(0) = \tilde{\mathbf{d}}(0)$. Here c denotes the constant of the Poincaré inequality (see Eq. (98)).

The proof of this result is deferred to the appendix. Proposition 6.1 guarantees that the difference of two possible solutions \mathbf{d} and $\tilde{\mathbf{d}}$ of Eq. (71) measured by the relative energy (74) depends continuously on the difference of their initial values. The growth of the relative energy is controlled only by the difference of the initial values and one of the two solutions, i.e., $\tilde{\mathbf{d}}$ and the prescribed velocity field \mathbf{v} . One consequence is the weak-strong uniqueness property of the system, i.e., the solutions must coincide if one is sufficiently regular (compare with Eq. (76)) and both emanate from the same initial data.

Finally, we would like to comment on the novelty and impact of the presented approach: The mathematical theory on global existence of generalized solutions, which is essential to prove global convergence of numerical schemes, and their uniqueness is so far restricted to non-stationary systems equipped with the one-constant approximation of the Oseen–Frank energy. To capture anisotropic elastic effects the one-constant approximation does not seem to resemble the actual material

properties (see Ref. [32, Section 3.1.3]). In Refs. [98,114–116], we extended the mathematical research towards systems equipped with the full Oseen–Frank energy and thus nonconvex energies. An essential tool in this context is the relative energy inequality (see in particular Refs. [115,116]). Beside the mathematical applications mentioned above, we think that our relative energy approach can be of interest for more applied investigations as well, since the relative energy serves as a natural measure for the distance between different alignment fields.

7. Open problems

In view of the substantial research progress discussed in the previous sections, it seems appropriate to close this article by pointing out some open problems and challenging questions for the future.

We start by taking the mathematical perspective. Whereas the stationary problem seems under control (as summarized, e.g., by Ball [117]), the dynamical behavior has many aspects for which a detailed mathematical treatment is still missing (see, e.g., Zhou et al. [13]). All dynamical models presented in this article consist of an evolution equation for the quantity describing the anisotropy (distribution function, Q-tensor, director), which is then coupled to the Navier–Stokes equations (see Eqs. (18)–(21), (46) and (55)). Showing the well-posedness for the Navier–Stokes equations alone is still a Millennium problem (see Fefferman [118]) that seems to be out of reach (see Tao [119]). Consequently, one cannot hope to show well-posedness of the coupled systems discussed in this article. However, as already indicated in the previous sections, there are recent mathematical achievements from which future investigations could start.

Specifically, in case of the Doi–Hess model (18)–(21), so far only local existence of weak solutions has been shown (see Zhang and Zhang [42]). Here, global existence of solutions would be helpful for implementing a suitable numerical (finite-element) scheme. For the Q-tensor model and the Ericksen–Leslie model, there are several results on global existence of generalized solutions. However, these have been proved for the special case of a free energy functional involving the one-constant approximation (see, e.g., Paicu and Zarnescu [76] for the Q-tensor model (46) combined with the Landau–de Gennes free energy (37), Wilkinson [55] for the Q-tensor model (46) combined with the Ball–Majumdar free energy (43) and Cavaterra et al. for the Ericksen–Leslie model [92]). Recently, Huang and Ding [59] have suggested a partial generalization for the Q-tensor model (46), and a similar generalization has been carried out in Emmrich and Laszark [98] in case of the Ericksen–Leslie equation. It would be very interesting to extend these analytical results towards more general free energies away from the one-constant approximation such as the full Landau–de Gennes expression (37) for the Q-tensor model or the full Oseen expression Eq. (58) for the Ericksen–Leslie model (see Laszark [114]). Again, for these models global existence of generalized solutions would be desirable.

Progress in these directions is of major importance also from the perspective of soft condensed matter physics. Indeed, as already mentioned in the introduction, there are many studies where equations of the type discussed in this article, and even more complicated variants, are numerically solved without (mathematically confirmed) knowledge about solutions. For example, Q-tensor theories are nowadays often used to model hybrid systems involving additional degrees of freedom, such as liquid crystals with embedded colloids (see Ref. [120]), polar liquid crystals (see Ref. [121]), branched polymers (see Ref. [122]), and ferrogels (see Ref. [123]). Moreover, combining Q-tensor models with activity terms (see Refs. [124,125]) has led to a boost of studies targeting the collective behavior of active systems such as bacterial or artificial microswimmers (see, e.g., Refs. [126,127]). To our knowledge, these extensions of the theory have not been considered by mathematicians at all.

Finally, we briefly comment on future applications of the relative energy approach introduced in Section 6. The presented result (Proposition 6.1) is a first step to generalize the concept of relative en-

ergy inequalities to systems with nonconvex energy functionals. This technique and associated results can hopefully be transferred to other systems with similar properties including Q-tensor theories. A result implicated by the relative energy inequality is the so-called weak-strong uniqueness: In the case that a solution admitting additional regularity exists, it coincides with all other possible generalized solutions emanating from the same initial data. Indeed, it can be immediately inferred from Proposition 6.1 that the relative energy vanishes if the initial values of the two solutions \mathbf{d} and $\tilde{\mathbf{d}}$ coincide and $\tilde{\mathbf{d}}$ fulfills the additional regularity requirements in Eq. (76). Thus, the solutions \mathbf{d} and $\tilde{\mathbf{d}}$ coincide as long as the more regular solution $\tilde{\mathbf{d}}$ exists, which is expected to be the case at least locally in time. Since the uniqueness of solutions only holds locally in time, these models can also exhibit solution multiplicities or bifurcation effects. These effects can be related to phase transitions in liquid crystals (see Ref. [19]) or flow induced instabilities that even multiply. Such motions can be of tumbling, wagging or kayaking type, even chaotic orientational behavior has been detected (see Ref. [53]). It is indeed strongly desirable to investigate these effects in the future.

The relative energy inequality (75) can also be used to derive a weakened solution formalism, the so-called dissipative solution, where only an inequality is assumed to be fulfilled by the solution (see Ref. [113]). Beside these mathematical questions, it is also possible to derive a posteriori estimates to bound modeling errors as well as errors due to numerical approximation (see Ref. [112]). To conclude, we think that the relative energy approach as a measure for the distance between different solutions may serve as a new comparing tool for computational or even experimental results.

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Appendix A

Proof of Proposition 6.1. The relative energy (74) can be explicitly calculated using the binomial formula

$$\begin{aligned} \mathcal{E}[\mathbf{d}(t)|\tilde{\mathbf{d}}(t)] &= F[\mathbf{d}(t)] + F[\tilde{\mathbf{d}}(t)] - \int_{\Omega} \nabla \mathbf{d}(t) : \nabla \tilde{\mathbf{d}}(t) \, dx \\ &\quad - \int_{\Omega} \mathbf{d}(t) \cdot (\nabla \mathbf{d}(t))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx. \end{aligned} \tag{77}$$

Similarly, we calculate the difference of the variational derivatives using the binomial formula

$$\begin{aligned} \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \right|^2 \, dx \, ds &= \\ \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \right|^2 \, dx \, ds + \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \right|^2 \, dx \, ds & \\ - 2 \int_0^t \int_{\Omega} \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \cdot \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \, dx \, ds & \end{aligned} \tag{78}$$

Adding Eqs. (77) and (78) and using the energy equality (73) for the two solutions gives

$$\begin{aligned} \mathcal{E}[\mathbf{d}(t)|\tilde{\mathbf{d}}(t)] + \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \right|^2 \, dx \, ds & \\ = F[\mathbf{d}(0)] + F[\tilde{\mathbf{d}}(0)] - \int_{\Omega} \nabla \mathbf{d}(t) : \nabla \tilde{\mathbf{d}}(t) \, dx & \\ - \int_{\Omega} \mathbf{d}(t) \cdot (\nabla \mathbf{d}(t))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx & \\ - 2 \int_0^t \int_{\Omega} \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \cdot \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \, dx \, ds & \end{aligned} \tag{79}$$

In the following we prove two integration by parts formulas (Eqs. (80) and (89)), which are essential to estimate the relative energy (74). In regard of the third term on the right-hand side of Eq. (79), we observe with the fundamental theorem of calculus and an integration by parts that

$$\begin{aligned} \int_{\Omega} \nabla \mathbf{d}(t) : \nabla \tilde{\mathbf{d}}(t) \, dx - \int_{\Omega} \nabla \mathbf{d}(0) : \nabla \tilde{\mathbf{d}}(0) \, dx & \\ = \int_0^t \int_{\Omega} \partial_s \nabla \mathbf{d}(s) : \nabla \tilde{\mathbf{d}}(s) \, dx \, ds & \\ = \int_0^t \int_{\Omega} \left(\nabla \partial_s \mathbf{d}(s) : \nabla \tilde{\mathbf{d}}(s) + \nabla \mathbf{d}(s) : \nabla \partial_s \tilde{\mathbf{d}}(s) \right) \, dx \, ds & \\ = \int_0^t \int_{\Omega} \left(\partial_s \mathbf{d}(s), -\Delta \tilde{\mathbf{d}}(s) \right) + \left(\partial_s \tilde{\mathbf{d}}(s), -\Delta \mathbf{d}(s) \right) \, dx \, ds. & \end{aligned} \tag{80}$$

The boundary terms disappear since $\partial_s \mathbf{d}$ and $\partial_s \tilde{\mathbf{d}}$ vanish at the boundary. This is due to the fact that the prescribed boundary values are constant in time. Similarly but somehow more involved, we obtain in regard of the fourth term on the right hand side of Eq. (79) that

$$\begin{aligned} \int_{\Omega} \mathbf{d}(t) \cdot (\nabla \mathbf{d}(t))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx & \\ - \int_{\Omega} \mathbf{d}(0) \cdot (\nabla \mathbf{d}(0))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0) \, dx & \\ = \int_0^t \int_{\Omega} \partial_s \mathbf{d}(s) \cdot (\nabla \mathbf{d}(s))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(s))_{\text{skw}} \tilde{\mathbf{d}}(s) \, dx \, ds & \\ = \int_0^t \int_{\Omega} \left(\mathbf{d}(s) \cdot (\nabla \partial_s \mathbf{d}(s))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(s))_{\text{skw}} \tilde{\mathbf{d}}(s) \right. & \\ \quad \left. + \partial_s \mathbf{d}(s) \cdot (\nabla \mathbf{d}(s))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(s))_{\text{skw}} \tilde{\mathbf{d}}(s) \right) \, dx \, ds & \\ + \int_0^t \int_{\Omega} \left(\mathbf{d}(s) \cdot (\nabla \mathbf{d}(s))_{\text{skw}}^T (\nabla \partial_s \tilde{\mathbf{d}}(s))_{\text{skw}} \tilde{\mathbf{d}}(s) \right. & \\ \quad \left. + \mathbf{d}(s) \cdot (\nabla \mathbf{d}(s))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(s))_{\text{skw}} \partial_s \tilde{\mathbf{d}}(s) \right) \, dx \, ds. & \end{aligned} \tag{81}$$

The right-hand side of Eq. (81) is rearranged further on. In the following, we omit the dependence on the integration parameter s for brevity. Adding and simultaneously subtracting the terms

$$\begin{aligned} \int_0^t \int_{\Omega} \left(\tilde{\mathbf{d}} \cdot (\nabla \partial_s \mathbf{d})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} + \partial_s \mathbf{d} \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \mathbf{d})_{\text{skw}} \tilde{\mathbf{d}} \right) \, dx \, ds & \\ + \int_0^t \int_{\Omega} \left(\mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} + \mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \partial_s \tilde{\mathbf{d}} \right) \, dx \, ds & \end{aligned} \tag{82}$$

leads to

$$\begin{aligned} \int_{\Omega} \mathbf{d}(t) \cdot (\nabla \mathbf{d}(t))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx & \\ - \int_{\Omega} \mathbf{d}(0) \cdot (\nabla \mathbf{d}(0))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0) \, dx & \\ = \int_0^t \int_{\Omega} \left(\tilde{\mathbf{d}} \cdot (\nabla \partial_s \mathbf{d})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} + \partial_s \mathbf{d} \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \mathbf{d})_{\text{skw}} \tilde{\mathbf{d}} \right) \, dx \, ds & \\ + \int_0^t \int_{\Omega} \left(\mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} + \mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \partial_s \tilde{\mathbf{d}} \right) \, dx \, ds & \\ + \int_0^t \int_{\Omega} \left((\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \partial_s \mathbf{d})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} \right. & \\ \quad \left. + \partial_s \mathbf{d} \cdot ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}})^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} \right) \, dx \, ds & \\ + \int_0^t \int_{\Omega} \left(\mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}} (\tilde{\mathbf{d}} - \mathbf{d}) \right. & \\ \quad \left. + \mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T ((\nabla \tilde{\mathbf{d}})_{\text{skw}} - (\nabla \mathbf{d})_{\text{skw}}) \partial_s \tilde{\mathbf{d}} \right) \, dx \, ds. & \end{aligned} \tag{83}$$

For the first two terms of the right-hand side of Eq. (83), an integration by parts shows that

$$\begin{aligned}
& \int_0^t \int_{\Omega} (\tilde{\mathbf{d}} \cdot (\nabla \partial_s \mathbf{d})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} + \partial_s \mathbf{d} \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds \\
& + \int_0^t \int_{\Omega} (\mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}} \mathbf{d} + \mathbf{d} \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \mathbf{d})_{\text{skw}} \partial_s \tilde{\mathbf{d}}) \, dx \, ds \\
& = \int_0^t \int_{\Omega} \partial_s \mathbf{d} \cdot (-\nabla \cdot ((\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} \otimes \tilde{\mathbf{d}})_{\text{skw}} + (\nabla \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds \\
& \quad + \int_0^t \int_{\Omega} \partial_s \tilde{\mathbf{d}} \cdot (-\nabla \cdot ((\nabla \mathbf{d})_{\text{skw}} \mathbf{d} \otimes \mathbf{d})_{\text{skw}} + (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \mathbf{d})_{\text{skw}} \mathbf{d}) \, dx \, ds.
\end{aligned} \tag{84}$$

Note that the boundary terms disappear since $\partial_s \mathbf{d}$ and $\partial_s \tilde{\mathbf{d}}$ vanish at the boundary (compare to Eq. (80)). The last two terms on the right-hand side of Eq. (83) are rearranged by adding and subtracting the term

$$\begin{aligned}
& \int_0^t \int_{\Omega} ((\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} \\
& \quad + \partial_s \tilde{\mathbf{d}} \cdot ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}})^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds.
\end{aligned} \tag{85}$$

This leads to

$$\begin{aligned}
& \int_0^t \int_{\Omega} ((\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} \\
& \quad + \partial_s \mathbf{d} \cdot ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}})^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds \\
& + \int_0^t \int_{\Omega} (\mathbf{d} \cdot (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}} (\tilde{\mathbf{d}} - \mathbf{d}) \\
& \quad + \mathbf{d} \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}}^T ((\nabla \tilde{\mathbf{d}})_{\text{skw}} - (\nabla \mathbf{d})_{\text{skw}}) \partial_s \tilde{\mathbf{d}}) \, dx \, ds \\
& = \int_0^t \int_{\Omega} (\partial_s ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) (\mathbf{d} - \tilde{\mathbf{d}}) \\
& \quad + ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) \partial_s (\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds \\
& \quad + \int_0^t \int_{\Omega} ((\nabla \mathbf{d})_{\text{skw}} \mathbf{d} - (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \cdot ((\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}} (\tilde{\mathbf{d}} - \mathbf{d}) \\
& \quad \quad + ((\nabla \tilde{\mathbf{d}})_{\text{skw}} - (\nabla \mathbf{d})_{\text{skw}}) \partial_s \tilde{\mathbf{d}}) \, dx \, ds.
\end{aligned} \tag{86}$$

Using the product rule, the first term on the right-hand side of Eq. (86) can be expressed via

$$\begin{aligned}
& \int_0^t \int_{\Omega} (\partial_s ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) (\mathbf{d} - \tilde{\mathbf{d}}) \\
& \quad + ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) \partial_s (\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds \\
& = \int_0^t \int_{\Omega} \partial_s ((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) (\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} \, dx \, ds \\
& = \int_0^t \int_{\Omega} \partial_s \int_{\Omega} (((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) (\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds \\
& \quad - \int_0^t \int_{\Omega} (((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) (\mathbf{d} - \tilde{\mathbf{d}}) \cdot \partial_s ((\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}})) \, dx \, ds.
\end{aligned} \tag{87}$$

The fundamental theorem of calculus gives for the first term on the right-hand side of Eq. (87) that

$$\begin{aligned}
& \int_0^t \int_{\Omega} \partial_s \int_{\Omega} (((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) (\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds \\
& = \int_{\Omega} (\mathbf{d}(t) - \tilde{\mathbf{d}}(t)) \cdot ((\nabla \mathbf{d}(t))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx \\
& \quad - \int_{\Omega} (\mathbf{d}(0) - \tilde{\mathbf{d}}(0)) \cdot ((\nabla \mathbf{d}(0))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0) \, dx.
\end{aligned} \tag{88}$$

Putting Eqs. (84), (86), (87) and (88) back into (83) finally gives

$$\begin{aligned}
& \int_{\Omega} \mathbf{d}(t) \cdot (\nabla \mathbf{d}(t))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx \\
& \quad - \int_{\Omega} \mathbf{d}(0) \cdot (\nabla \mathbf{d}(0))_{\text{skw}}^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0) \, dx \\
& = \int_0^t \int_{\Omega} \partial_s \mathbf{d} \cdot (-\nabla \cdot ((\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}} \otimes \tilde{\mathbf{d}})_{\text{skw}} + (\nabla \tilde{\mathbf{d}})_{\text{skw}}^T (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \, dx \, ds
\end{aligned}$$

$$\begin{aligned}
& + \int_0^t \int_{\Omega} \partial_s \tilde{\mathbf{d}} \cdot (-\nabla \cdot ((\nabla \mathbf{d})_{\text{skw}} \mathbf{d} \otimes \mathbf{d})_{\text{skw}} + (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \mathbf{d})_{\text{skw}} \mathbf{d}) \, dx \, ds \\
& + \int_{\Omega} (\mathbf{d}(t) - \tilde{\mathbf{d}}(t)) \cdot ((\nabla \mathbf{d}(t))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx \\
& - \int_{\Omega} (\mathbf{d}(0) - \tilde{\mathbf{d}}(0)) \cdot ((\nabla \mathbf{d}(0))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0) \, dx \\
& - \int_0^t \int_{\Omega} (((\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}) (\mathbf{d} - \tilde{\mathbf{d}}) \cdot \partial_s ((\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}})) \, dx \, ds \\
& + \int_0^t \int_{\Omega} ((\nabla \mathbf{d})_{\text{skw}} \mathbf{d} - (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}) \cdot ((\nabla \partial_s \tilde{\mathbf{d}})_{\text{skw}} (\tilde{\mathbf{d}} - \mathbf{d}) \\
& \quad + ((\nabla \tilde{\mathbf{d}})_{\text{skw}} - (\nabla \mathbf{d})_{\text{skw}}) \partial_s \tilde{\mathbf{d}}) \, dx \, ds.
\end{aligned} \tag{89}$$

This is the integration by parts formula needed to estimate the relative energy.

The right-hand side of Eq. (79) is now estimated using Eqs. (80) and (89) as well as Young's inequality (see Ref. [128, Section 4.8]), as follows:

$$\begin{aligned}
& \mathcal{E}[\mathbf{d}(t)|\tilde{\mathbf{d}}(t)] + \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \right|^2 \, dx \, ds \\
& \leq \mathcal{E}[\mathbf{d}(0)|\tilde{\mathbf{d}}(0)] - \int_0^t \int_{\Omega} \left(\partial_s \mathbf{d} + \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \right) \cdot \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \, dx \, ds \\
& \quad - \int_0^t \int_{\Omega} \left(\partial_s \tilde{\mathbf{d}} + \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \right) \cdot \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \, dx \, ds \\
& \quad - \int_{\Omega} (\mathbf{d}(t) - \tilde{\mathbf{d}}(t)) \cdot ((\nabla \mathbf{d}(t))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) \, dx \\
& \quad + \int_{\Omega} (\mathbf{d}(0) - \tilde{\mathbf{d}}(0)) \cdot ((\nabla \mathbf{d}(0))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0) \, dx \\
& \quad + \frac{1}{2} \int_0^t \max_{x \in \Omega} (|\tilde{\mathbf{d}}(x)| |\nabla \partial_s \tilde{\mathbf{d}}(x)| + |\nabla \tilde{\mathbf{d}}(x)| |\partial_s \tilde{\mathbf{d}}(x)|) \\
& \quad \quad \cdot \int_{\Omega} (|(\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}|^2 + |\mathbf{d} - \tilde{\mathbf{d}}|^2) \, dx \, ds \\
& \quad + \frac{1}{2} \int_0^t \max_{x \in \Omega} |\nabla \partial_s \tilde{\mathbf{d}}(x)| \int_{\Omega} (|\mathbf{d} - \tilde{\mathbf{d}}|^2 + |(\nabla \mathbf{d})_{\text{skw}} \mathbf{d} - (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}|^2) \, dx \, ds \\
& \quad + \frac{1}{2} \int_0^t \max_{x \in \Omega} |\partial_s \tilde{\mathbf{d}}(x)| \int_{\Omega} (|(\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}|^2 \\
& \quad \quad + |(\nabla \mathbf{d})_{\text{skw}} \mathbf{d} - (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}|^2) \, dx \, ds.
\end{aligned} \tag{90}$$

The terms in the three last lines of Eq. (90) are estimates of the terms in the two last lines of Eq. (89). To get the right-hand side of inequality (90), we explicitly used that Eq. (77) also holds for $t = 0$ and that the variational derivative is given by

$$\frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] = -\Delta \mathbf{d} - \nabla \cdot ((\nabla \mathbf{d})_{\text{skw}} \mathbf{d} \otimes \mathbf{d})_{\text{skw}} + (\nabla \mathbf{d})_{\text{skw}}^T (\nabla \mathbf{d})_{\text{skw}} \mathbf{d}$$

and similarly for $\tilde{\mathbf{d}}$. Inserting Eq. (71), using that \mathbf{v} is the same for both solutions, yields for the second and third term on the right-hand side of inequality (90) that

$$\begin{aligned}
& - \int_0^t \int_{\Omega} \left(\partial_t \mathbf{d} + \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \right) \cdot \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \, dx \, ds \\
& \quad - \int_0^t \int_{\Omega} \left(\partial_t \tilde{\mathbf{d}} + \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \right) \cdot \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \, dx \, ds \\
& = \int_0^t \int_{\Omega} (\mathbf{v} \cdot \nabla) \mathbf{d} \cdot \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \, dx \, ds + \int_0^t \int_{\Omega} (\mathbf{v} \cdot \nabla) \tilde{\mathbf{d}} \cdot \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \, dx \, ds.
\end{aligned} \tag{91}$$

Due to Eq. (72), we observe for the right-hand side of Eq. (91) that

$$\begin{aligned}
& \int_0^t \int_{\Omega} (\mathbf{v} \cdot \nabla) \mathbf{d} \cdot \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \, dx \, ds + \int_0^t \int_{\Omega} (\mathbf{v} \cdot \nabla) \tilde{\mathbf{d}} \cdot \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \, dx \, ds \\
& = \int_0^t \int_{\Omega} (\mathbf{v} \cdot \nabla) \mathbf{d} \cdot \left(\frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] - \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] \right) \, dx \, ds \\
& \quad + \int_0^t \int_{\Omega} (\mathbf{v} \cdot \nabla) \tilde{\mathbf{d}} \cdot \left(\frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \tilde{\mathbf{d}}}[\tilde{\mathbf{d}}] \right) \, dx \, ds
\end{aligned}$$

$$= \int_0^t \int_{\Omega} \mathbf{v} \cdot (\nabla \mathbf{d} - \nabla \tilde{\mathbf{d}})^T \left(\frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right) dx ds. \quad (92)$$

Hence, the right-hand side of Eq. (91) can be estimated using Young's inequality (see Ref. [128, Section 4.8]),

$$\begin{aligned} & \int_0^t \int_{\Omega} \mathbf{v} \cdot (\nabla \mathbf{d} - \nabla \tilde{\mathbf{d}})^T \left(\frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right) dx ds \\ & \leq \frac{1}{2} \int_0^t \max_{\mathbf{x} \in \Omega} |\mathbf{v}(\mathbf{x})|^2 \int_{\Omega} |\nabla \tilde{\mathbf{d}} - \nabla \mathbf{d}|^2 dx ds \\ & \quad + \frac{1}{2} \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right|^2 dx ds. \end{aligned} \quad (93)$$

For the fourth term on the right-hand side of inequality (90), we observe by Young's inequality (see Ref. [128, Section 4.8])

$$\begin{aligned} & - \int_{\Omega} (\mathbf{d}(t) - \tilde{\mathbf{d}}(t)) \cdot \left((\nabla \mathbf{d}(t))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \right)^T (\nabla \tilde{\mathbf{d}}(t))_{\text{skw}} \tilde{\mathbf{d}}(t) dx \\ & \leq \frac{1}{4} \int_{\Omega} |\nabla \mathbf{d}(t) - \nabla \tilde{\mathbf{d}}(t)|^2 dx \\ & \quad + \max_{(\mathbf{x}, t) \in \Omega \times [0, T]} \left| (\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t) \right|^2 \int_{\Omega} |\mathbf{d}(t) - \tilde{\mathbf{d}}(t)|^2 dx. \end{aligned} \quad (94)$$

With respect to the last term in Eq. (94), we observe with the fundamental theorem of calculus and Eq. (71) that

$$\begin{aligned} & \int_{\Omega} |\mathbf{d}(t) - \tilde{\mathbf{d}}(t)|^2 dx - \int_{\Omega} |\mathbf{d}(0) - \tilde{\mathbf{d}}(0)|^2 dx \\ & = \int_0^t \int_{\Omega} \partial_s |\mathbf{d} - \tilde{\mathbf{d}}|^2 dx ds \\ & = 2 \int_0^t \int_{\Omega} (\partial_s \mathbf{d} - \partial_s \tilde{\mathbf{d}}) \cdot (\mathbf{d} - \tilde{\mathbf{d}}) dx ds \\ & = -2 \int_0^t \int_{\Omega} (\mathbf{v} \cdot \nabla)(\mathbf{d} - \tilde{\mathbf{d}}) \cdot (\mathbf{d} - \tilde{\mathbf{d}}) dx ds \\ & \quad - 2 \int_0^t \int_{\Omega} \left(\frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right) \cdot (\mathbf{d} - \tilde{\mathbf{d}}) dx ds. \end{aligned} \quad (95)$$

The first term on the right-hand side of Eq. (95) vanishes since \mathbf{v} is solenoidal and fulfills homogeneous Dirichlet boundary conditions. With Young's inequality (see Ref. [128, Section 4.8]), we find

$$\begin{aligned} & 2 \max_{(\mathbf{x}, t) \in \Omega \times [0, T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^2 \int_0^t \int_{\Omega} \left(\frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right) \cdot (\mathbf{d} - \tilde{\mathbf{d}}) dx ds \\ & \leq \frac{1}{2} \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right|^2 dx ds \\ & \quad + 2 \max_{(\mathbf{x}, t) \in \Omega \times [0, T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^4 \int_0^t \int_{\Omega} |\mathbf{d} - \tilde{\mathbf{d}}|^2 dx ds. \end{aligned} \quad (96)$$

Inserting Eqs. (91)–(96) back into Eq. (90) gives

$$\begin{aligned} & \mathcal{E}[\mathbf{d}(t)|\tilde{\mathbf{d}}(t)] + \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right|^2 dx ds \\ & \leq \mathcal{E}[\mathbf{d}(0)|\tilde{\mathbf{d}}(0)] + \frac{1}{4} \int_{\Omega} |\nabla \mathbf{d}(t) - \nabla \tilde{\mathbf{d}}(t)|^2 dx + \frac{1}{2} \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right|^2 dx ds \\ & \quad + 2 \max_{(\mathbf{x}, t) \in \Omega \times [0, T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^4 \int_0^t \int_{\Omega} |\mathbf{d} - \tilde{\mathbf{d}}|^2 dx ds \\ & \quad + \max_{(\mathbf{x}, t) \in \Omega \times [0, T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^2 \int_{\Omega} |\mathbf{d}(0) - \tilde{\mathbf{d}}(0)|^2 dx \\ & \quad + \int_{\Omega} (\mathbf{d}(0) - \tilde{\mathbf{d}}(0)) \cdot \left((\nabla \mathbf{d}(0))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \right)^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0) dx \\ & \quad + \frac{1}{2} \int_0^t \max_{\mathbf{x} \in \Omega} |\mathbf{v}(\mathbf{x})|^2 \int_{\Omega} |\nabla \tilde{\mathbf{d}} - \nabla \mathbf{d}|^2 dx ds \\ & \quad + \frac{1}{2} \int_0^t \int_{\Omega} \left| \frac{\delta F}{\delta \mathbf{d}}[\mathbf{d}] - \frac{\delta F}{\delta \mathbf{d}}[\tilde{\mathbf{d}}] \right|^2 dx ds \end{aligned}$$

$$\begin{aligned} & + \frac{1}{2} \int_0^t \max_{\mathbf{x} \in \Omega} (|\tilde{\mathbf{d}}(\mathbf{x})| |\nabla \partial_s \tilde{\mathbf{d}}(\mathbf{x})| + |\nabla \tilde{\mathbf{d}}(\mathbf{x})| |\partial_s \tilde{\mathbf{d}}(\mathbf{x})|) \\ & \quad \times \int_{\Omega} (|(\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}|^2 + |\mathbf{d} - \tilde{\mathbf{d}}|^2) dx ds \\ & + \frac{1}{2} \int_0^t \max_{\mathbf{x} \in \Omega} |\nabla \partial_s \tilde{\mathbf{d}}(\mathbf{x})| \int_{\Omega} (|\mathbf{d} - \tilde{\mathbf{d}}|^2 + |(\nabla \mathbf{d})_{\text{skw}} \mathbf{d} - (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}|^2) dx ds \\ & + \frac{1}{2} \int_0^t \max_{\mathbf{x} \in \Omega} |\partial_s \tilde{\mathbf{d}}(\mathbf{x})| \int_{\Omega} (|(\nabla \mathbf{d})_{\text{skw}} - (\nabla \tilde{\mathbf{d}})_{\text{skw}}|^2 \\ & \quad + |(\nabla \mathbf{d})_{\text{skw}} \mathbf{d} - (\nabla \tilde{\mathbf{d}})_{\text{skw}} \tilde{\mathbf{d}}|^2) dx ds. \end{aligned} \quad (97)$$

The Poincaré inequality ensures that there exists a constant $c > 0$, such that

$$\int_{\Omega} |\mathbf{d} - \tilde{\mathbf{d}}|^2 dx \leq c \int_{\Omega} |\nabla \mathbf{d} - \nabla \tilde{\mathbf{d}}|^2 dx. \quad (98)$$

Note that the Poincaré inequality (see Ref. [129]) is applicable since \mathbf{d} and $\tilde{\mathbf{d}}$ fulfill the same Dirichlet boundary conditions. Using the definition (74) of the relative energy shows that

$$\begin{aligned} & \frac{1}{2} \mathcal{E}[\mathbf{d}(t)|\tilde{\mathbf{d}}(t)] ds \leq \mathcal{E}[\mathbf{d}(0)|\tilde{\mathbf{d}}(0)] + \int_{\Omega} |(\mathbf{d}(0) - \tilde{\mathbf{d}}(0)) \cdot \\ & \quad ((\nabla \mathbf{d}(0))_{\text{skw}} - (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}})^T (\nabla \tilde{\mathbf{d}}(0))_{\text{skw}} \tilde{\mathbf{d}}(0)| dx \\ & \quad + \max_{(\mathbf{x}, t) \in \Omega \times [0, T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^2 \int_{\Omega} |\mathbf{d}(0) - \tilde{\mathbf{d}}(0)|^2 dx \\ & \quad + 2c \max_{(\mathbf{x}, t) \in \Omega \times [0, T]} |(\nabla \tilde{\mathbf{d}}(\mathbf{x}, t))_{\text{skw}} \tilde{\mathbf{d}}(\mathbf{x}, t)|^4 \int_0^t \mathcal{E}[\mathbf{d}|\tilde{\mathbf{d}}] ds \\ & \quad + (1+c) \int_0^t \max_{\mathbf{x} \in \Omega} (|\tilde{\mathbf{d}}(\mathbf{x})| |\nabla \partial_s \tilde{\mathbf{d}}(\mathbf{x})| + |\nabla \tilde{\mathbf{d}}(\mathbf{x})| |\partial_s \tilde{\mathbf{d}}(\mathbf{x})| + |\nabla \partial_s \tilde{\mathbf{d}}(\mathbf{x})| \\ & \quad + |\partial_s \tilde{\mathbf{d}}(\mathbf{x})| + |\mathbf{v}(\mathbf{x})|^2) \mathcal{E}[\mathbf{d}|\tilde{\mathbf{d}}] ds. \end{aligned} \quad (99)$$

Gronwall's estimate (see Ref. [130]) yields the asserted inequality (75). \square

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