Conservation-Dissipation Formalism for soft matter physics: II. Application to non-isothermal nematic liquid crystals

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Abstract. For most existing non-equilibrium theories, the modeling of non-isothermal processes is a hard task. Intrinsic difficulties involve the non-equilibrium temperature, the coexistence of conserved energy and dissipative entropy, etc. In this paper, by taking the non-isothermal flow of nematic liquid crystals as a typical example, we illustrate that thermodynamically consistent models in either vectorial or tensorial forms can be constructed within the framework of the Conservation-Dissipation Formalism (CDF). And the classical isothermal Ericksen-Leslie model and Qian-Sheng model are shown to be special cases of our new vectorial and tensorial models in the isothermal, incompressible and stationary limit. Most importantly, from the above examples, it is known that CDF can easily solve the issues relating with non-isothermal situations in a systematic way. The first and second laws of thermodynamics are satisfied simultaneously. The non-equilibrium temperature is defined self-consistently as a partial derivative of the entropy function. Relaxation-type constitutive relations are constructed, which give rise to classical linear constitutive relations, like Newton’s law and Fourier’s law, in stationary limits. Therefore, CDF is expected to have a broad scope of applications in soft matter physics, especially under complicated situations, such as non-isothermal, compressible and nanoscale systems.

1 Introduction

Liquid crystals are intermediate states of materials between solids and liquids. According to their different molecular symmetries, liquid crystals are loosely classified into nematics, cholesterics and smectics. Among them, the nematic liquid crystals, which are usually composed of long, thin, rod-like molecules with long axes of neighbouring molecules aligned roughly parallel to each other, are the most studied ones [1].

Based on scales of description, theories for nematic liquid crystals can be categorized into three different but closely related types: the Doi-Onsager theory, Landau-de Gennes theory and Ericksen-Leslie theory. The first one belongs to a molecular model, which focuses on the distribution function of molecular orientations. The second one is a tensorial model, in which a symmetric traceless tensor ($Q$-tensor) is utilized to describe the orientational properties of molecules. The last one is a vectorial model, which uses a unit vector to characterize the average direction of molecules [2]. Notice that the second moment of the orientational distribution function corresponds to the $Q$-tensor, while the uniaxial form of the $Q$-tensor reduces to the director vector in the Ericksen-Leslie theory. As a consequence, models for liquid crystals in different scales are connected to each other under certain limit processes. It was rigorously shown in mathematics that [2,3] the Doi-Onsager equation could be simplified to the $Q$-tensor theory by the Bingham closure and Taylor expansion, while the Ericksen-Leslie equation could be derived from the $Q$-tensor theory by expansion near the local equilibrium.

Pioneering works on the macroscopic continuum modeling of nematic liquid crystals can be dated back to Ericksen [4] and Leslie [5,6] in the 1960s, who established rather general conservation laws and constitutive equations from a hydrodynamical point of view. The Ericksen-Leslie (E-L) theory is shown to be successful in modeling and explaining many intrinsic physical phenomena of the nematics, including the flow alignment, electric and magnetic induced flows in display devices [1,6,7] etc.
Due to the complexity of E-L theory in mathematical analysis, Lin and Liu [8, 9] tried to simplify it by introducing a penalty approximation to relax the nonlinear constraint of the director and by reducing the Oseen-Frank energy into a single term. The global existence of weak solutions of the simplified isothermal model was proved rigorously. Later, a similar model was derived by Sun and Liu [10] within a general energetic variational framework, and by us with the Conservation-Dissipation Formalism (CDF) in the first paper of this series [11]. For recent developments on mathematical models for the hydrodynamic flows of nematic liquid crystals, see refs. [12, 13] for details.

The classical E-L theory presumes the liquid crystal is at constant temperature and the director is of constant length. However, the non-isothermal and compressible nematic liquid crystals are far more interesting and important in industry. A key reason is that for nematics of thermotropic type the most usual operation to induce a phase transition is to change the temperature. Furthermore, mixtures of different nematics are widely used in the display industry in order to obtain a low melting point [1]. In contrast to isothermal E-L models, results for non-isothermal cases are not so fruitful. The generalized E-L model in non-isothermal situations was presented, by Hieber and Prüss [14, 15] based on the principle of thermodynamical consistency, in the incompressible case by Feireisl, Rocca and Schimperna [16], and by De Anna and Liu [17] with a generalized Oseen-Frank energy.

On the other hand, one can discuss the hydrodynamic behaviour of liquid crystals based on the Landau-de Gennes (LdG) theory [1]. The LdG theory shares the same variables of density and velocity as the E-L theory. A fundamental difference between them lies on the choice of order parameters. To account for states of nematics at time $t$ and position $x$, the E-L theory adopts the director vector $d(x, t)$, which is sufficient to describe the nematic dynamics of low-molar mass, while the LdG theory considers a traceless symmetric tensor $Q(x, t)$ that is more accurate in the presence of high disclination density [18]. As to the $Q$-tensor theory, there are plenty of different models, based on the orientational distribution function [2], derived from variational principles [19, 20], and recently for non-isothermal nematics [21, 22]. However, a general dynamical theory that takes non-isothermal and compressible effects into account for liquid crystals described by $Q$-tensor is still lacking [23].

In this paper, we concentrate on the applications of CDF to non-isothermal flows of nematic liquid crystals. New generalized vectorial (E-L) theory and tensorial ($Q$-tensor) theory for non-isothermal and compressible situations are constructed. Concrete expressions of the entropy flux and entropy production rate of the system, as well as constitutive relations for the stress tensor, director/$Q$-tensor body torque, director/$Q$-tensor surface torque and heat flux are derived. Especially, under the isothermal and incompressible condition, the classical E-L theory or Qian-Sheng model are shown to be special cases of our vectorial and tensorial models in the stationary limit.

2 Vectorial models for non-isothermal flows of nematic liquid crystals

2.1 Conservation laws

In this part, we consider non-isothermal flows of liquid crystals in the nematic phase. For simplicity, external electric and magnetic fields are not taken into consideration. The conservation laws of mass, momentum, angular momentum and total energy take the following form:

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho v) = 0, \quad (1)$$

$$\frac{\partial}{\partial t}(\rho v) + \nabla \cdot (\rho v \otimes v) = \xi + \nabla \cdot \sigma, \quad (2)$$

$$\frac{\partial}{\partial t}(\rho w) + \nabla \cdot (\rho v \otimes w) = g + \nabla \cdot \pi, \quad (3)$$

$$\frac{\partial}{\partial t}(\rho v \otimes w) + \nabla \cdot (\rho ve) = \xi \cdot v + \nabla \cdot (\sigma \cdot v + \pi \cdot w - q). \quad (4)$$

Here $\rho$ is the density of liquid crystals, $v \in \mathbb{R}^3$ is the velocity, $\xi$ is the external body force per unit volume, $\sigma$ is the stress tensor. In eq. (3), $\rho_1 = \rho |r|^2$ is the density of inertia moment, where $r$ is the effective position vector. Its norm $|r|$ is assumed to be constant in what follows. $d \in \mathbb{R}^3$ is the director vector which describes the preferred orientation of molecules. The material derivative of $d$ gives the director velocity $v \equiv \frac{d}{dt}(d)$. $\pi$ is the director surface torque, $g$ is the intrinsic body torque acting on the director. Both are measured per unit volume, describing effects of macroscopic flows on the microscopic structure. In eq. (4), $e = u + \frac{1}{2} v^2 + \frac{2}{27} w^2$ denotes the specific total energy density, including both translational and rotational kinetic energies as $\frac{1}{2} v^2$ and $\frac{2}{27} w^2$, and the internal energy as $u$. $q$ represents the heat flux. The symbol $\otimes$ denotes the tensor product, $(a \otimes b)_{ij} = a_i b_j$ for $a, b \in \mathbb{R}^3$.

In general, the stress tensor can be decomposed into four parts based on their different origins

$$\sigma = -pI + \sigma_V + \sigma_E + \sigma_L, \quad (5)$$

where $p$, $\sigma_V$, $\sigma_E$, $\sigma_L$ denote the thermodynamic pressure, viscous stress, Ericksen stress for the static state and Leslie stress for the non-equilibrium state, respectively. From the perspective of viscous-elastic fluids, $\sigma_E$ is induced by elastic distortions, $(\sigma_V + \sigma_L)$ together composes the stress induced by viscosity effects, in which $\sigma_V$ is the viscous stress for homogenous fluid flows, and $\sigma_L$ is the orientation-induced viscous stress. A similar decomposition was introduced by Hieber and Prüß [15]. However, in their work, constitutive relations of stresses were given directly and without a clear physical interpretation. Analogously, the director surface torque $\pi$ and body torque $g$ can be separated as

$$\pi = \pi_V + \pi_E + \pi_L, \quad g = g_V + g_E + g_L, \quad (6)$$

with the subscript $V$, $E$, $L$ denoting the viscous, Ericksen and Leslie parts, respectively.
Remark 1. Note in many cases the left-hand side of eq. (3) is neglected for simplicity. However, when the anisotropic axis is subjected to large accelerations [6, 24], the director inertial term will play an important role. And it is kept in the current study to preserve the elegant mathematical structure of local conservation laws.

Remark 2. In most previous works, the director vector \( \mathbf{d} \) was assumed to be uniform and was simplified as a unit vector in a unit sphere \( S^2 \). It is necessary to emphasize that, here we introduce \( \mathbf{d} \in \mathbb{R}^3 \) as a 3-dimensional vector, to account for both the preferred orientation and the average length \([25]\) of rod-like molecules. In this way, the vectorial theory can be extended to the case of mixtures of molecules with varied lengths \([25–27]\).

Remark 3. In eqs. (1)–(4), the local conservation laws of \((\rho, \mathbf{v}, \mathbf{w}, \mathbf{c})\) are directly introduced. Physically, they are a straightforward consequence of the first law of thermodynamics (or the energy conservation law) and the Galilean principle \([28]\).

The conservation of total energy in eq. (4) can also be interpreted as the first law of thermodynamics, which states that the internal energy is changed by either doing work or exchanging heat with the environment. The following proposition gives an explicit expression of the first law of thermodynamics for the non-isothermal flows of liquid crystals, which was first considered by Leslie \([5]\) based on rational thermodynamics.

Proposition 1. Assuming that eq. (4) satisfies the principle of material frame-indifference, then the first law of thermodynamics states that, the change in internal energy results from the work done to the system and the heat exchanged with its surroundings:

\[
\rho \frac{du}{dt} = W - \nabla \cdot q, \tag{7}
\]

where the work \( W = \sigma^T : \mathbf{A} + \pi^T : M - g \cdot N \) adopts a bilinear structure as the product of generalized forces \( \sigma, \pi \) and displacements \( \mathbf{A}, \mathbf{M}, \mathbf{N} \), and \( q \) describes the transportation of internal energy by heat flux. Here \( 2A_{ij} = v_{ij} + v_{ji}, \quad 2M_{ij} = v_{ij} - v_{ji}, \quad N_i = w_i - \Omega_i k d_k, \quad M_{ij} = w_{ij} + \Omega_{kj} d_k \).

Proof. By taking scalar product of eq. (2) with \( \mathbf{v} \) and eq. (3) with \( \mathbf{w} \), and using the continuity equation, eq. (4) reduces to the balance law of internal energy

\[
\rho \frac{du}{dt} = \sigma^T : \nabla \mathbf{v} + \pi^T : \nabla \mathbf{w} - g \cdot \mathbf{w} - \nabla \cdot q, \tag{8}
\]

where the superscript \( T \) means transposition, the colon \( : \) is the double inner product between two second-order tensors, i.e., \( \mathbf{A} : \mathbf{B} = \sum_{i,j} A_{ij} B_{ji} \), and \( (\nabla \mathbf{v})_{ij} = \partial v_{ji}/\partial x_i = v_{ji} \).

Notice that quantities \( \rho, \mathbf{u}, q, g \) in eq. (8) are objective and frame indifferent, while \( \nabla \mathbf{v}, \nabla \mathbf{w} \) and \( \mathbf{w} \) are not. To satisfy the principle of material frame-indifference, following Leslie \([5]\), the right-hand side of eq. (8) can be rearranged into a convenient form:

\[
\rho \frac{du}{dt} = \sigma_{ij} v_{j,i} + \pi_{ij} w_{j,i} - g_i w_i - \partial_i q_i = \sigma_{ij}(A_{ij} - \Omega_{ij}) + \pi_{ij}(M_{ij} - \Omega_{ik} d_k),
\]

\[
- g_i (N_i + \Omega_i k d_k) - \partial_i q_i = (\sigma_{ij} A_{ij} + \pi_{ij} M_{ij} - g_i N_i - \partial_i q_i) + (\sigma_{ij} \Omega_{ij} - \pi_{ij} \Omega_{ik} d_k - g_i \Omega_i k d_k)
\]

\[
= \sigma^T : A + \pi^T : M - g \cdot N - \nabla \cdot q + |\sigma - \pi^T : (\nabla d) + g \otimes d| : \Omega = \mu + \pi^T : M - g \cdot N - \nabla \cdot q + \sigma : \Omega, \tag{9}
\]

where \( \mu = \mu_{ij} \) is the double inner product between two second-order tensors, \( \partial_i q_i \) is the double inner product between two first-order tensors, \( A_{ij}, M_{ij}, N_i \) are objective and frame indifferent, while \( g_i \) and \( q_i \) are not. To satisfy the principle of material frame-indifference \([5]\), the underlined term \( \sigma : \Omega = |\sigma - \pi^T \cdot (\nabla d) + g \otimes d| : \Omega \) vanishes in the following derivation. \( \square \)

2.2 Generalized Gibbs relation

To close the system of partial differential equations in (1)–(3) and (7), constitutive relations for \((\sigma, \pi, g, q)\) are needed. Following CDF \([29]\), we introduce a strictly conserved mathematical entropy function

\[
\eta = \rho s(\nu, u, d, \nabla d, C, K, l, h). \tag{10}
\]

Here \( \nu = 1/\rho \) is the specific volume, \( (C, K) \) are tensors with the same size of \((\sigma, \pi)\), and \((l, h)\) are vectors with the same size of \((g, q)\). That is, the unknown variables \( C \) and \( K \) are 3 \times 3 matrices, while the vectors \( l \) and \( h \) are \( \mathbb{R}^3 \). \((C, K, l)\) are used to describe the viscous-elastic effects of nematic liquid crystal flows, and \( h \) characterizes the heat conduction induced by temperature gradients. Notice that \((\nu, u, d, \nabla d)\) represent conserved variables, while \((C, K, l, h)\) represent dissipative variables. In equilibrium, \( C = K = 0, l = h = 0 \), we have

\[
\delta s|_{C=K=0,l=h=0} = s_0(\nu, u, d, \nabla d), \tag{11}
\]

where \( s_0 \) is the equilibrium entropy.

In CDF, instead of directly adopting unknown functions \((\sigma, \pi, g, q)\) appearing in the conservation laws as state variables, alternative conjugate variables \((C, K, l, h)\) are used. \((C, K, l, h)\) are correlated to \((\sigma v, \pi v, g v, q)\) through the partial derivatives of the entropy function, i.e.,

\[
\frac{\partial s}{\partial C} = \sigma v, \quad \frac{\partial s}{\partial K} = \pi v, \quad \frac{\partial s}{\partial l} = g v, \quad \frac{\partial s}{\partial h} = q.
\]
Therefore, once the entropy function \( s \) is specified, a concrete form of \((C, K, l, h)\) are completely determined. Its advantage was shown through a concrete example, the linear and nonlinear Maxwell viscoelastic fluids, by Sun et al. [30] Their main conclusion is that the adoption of conjugate variables is more suitable for constructing genuinely nonlinear constitutive relations.

With the entropy function in hand, the non-equilibrium temperature \( \theta \) and thermodynamic pressure \( p \) are defined by

\[
\theta^{-1} = \frac{\partial s}{\partial q}, \quad \theta^{-1} p = \frac{\partial s}{\partial \rho
}
\]

Consequently, the equilibrium temperature is given by \( T = (\frac{\partial s}{\partial q})^{-1} \). The concept of (equilibrium) temperature is a direct consequence of the zeroth law of thermodynamics. While its absolute value, independent of the material properties of the system under study, is offered by the first and second laws of thermodynamics, like in the Carnots cycle. The framework of equilibrium thermodynamics, including the definition of equilibrium temperature, is directly borrowed by CIT and applied to non-equilibrium conditions by imposing the hypothesis of local equilibrium. According to the Gibbs relation, the (local) equilibrium absolute temperature is defined as \( 1/T = \partial s_0/\partial u \). In contrast, definitions and measurements of temperature and contact temperature based on axiomatic bases [31], the generalized non-equilibrium temperature in EIT [28], the non-equilibrium temperature, their practical applications and possible experiments.

In the next, we are going to examine the entropy evolution. And a manifestation of the second law of thermodynamics will be shown. Firstly, we assume the entropy \( s(\nu, u, d, \nabla d, C, K, l, h) \) to be an isotropic function of \( d \) and \( \nabla d \), or in other words, it is objective with respect to conserved variables. As a direct consequence, the tensor \((\frac{\partial s}{\partial q} \otimes d + \frac{\partial s}{\partial \nabla d} \cdot \nabla d \cdot \frac{\partial s}{\partial \nabla d})\) is symmetric. This result was first pointed out by Ericksen [33] and Leslie [5] in the 1960s, and we represent it as Lemma 2 in appendix A to maintain the self-integrity of formulation.

Secondly, to simplify notations, we employ a differential operator \( D \) as \( Ds = (p s)_l + \nabla \cdot (\nu s) \). Utilizing the continuity equation (1), one deduces that \( Ds = \rho s/dt \). Then, based on the conservation laws (1)–(3) and the balance law (7), it is direct to calculate the entropy evolution as follows:

\[
\eta + \nabla \cdot (\nu s) \equiv Ds(\nu, u, d, \nabla d, C, K, l, h) = \frac{\partial s}{\partial \nu} \partial \nu + \frac{\partial s}{\partial u} \partial u + \frac{\partial s}{\partial d} \cdot \partial d + \frac{\partial s}{\partial C} \cdot \partial C + \frac{\partial s}{\partial K} \cdot \partial K + \frac{\partial s}{\partial t} \partial t \]

\[
\begin{align*}
&= \left( \frac{\partial s}{\partial C} \right) + \left( \frac{\partial s}{\partial K} \right) + \left( \frac{\partial s}{\partial t} \right) + \left( \frac{\partial s}{\partial d} \right) \cdot \partial d + \left( \frac{\partial s}{\partial u} \right) \partial u + \left( \frac{\partial s}{\partial \nu} \right) \partial \nu + \left( \frac{\partial s}{\partial \rho} \right) \partial \rho.
\end{align*}
\]

By making use of the following relations (see Lemma 1 in appendix A):

\[
Dd = \rho \left(N + \Omega \cdot d\right),
\]

\[
\begin{align*}
\mathcal{D}(\nabla d) &= \rho \left[M - \nabla \cdot \Omega \cdot (\nabla d) - A \cdot (\nabla d)\right],
\end{align*}
\]

and noticing \( A^T = A, \Omega^T = -\Omega \), we have

\[
\begin{align*}
\frac{\partial s}{\partial d} \cdot Dd + \left( \frac{\partial s}{\partial \nabla d} \right)^T \cdot \mathcal{D}(\nabla d) &= \rho \frac{\partial s}{\partial d} \cdot w_i + \rho \frac{\partial s}{\partial d} \cdot d_{i,j} \\
&= \rho \frac{\partial s}{\partial d_i} \cdot (N_i + \Omega_{k} d_{k}) + \rho \frac{\partial s}{\partial d_{i,j}} \cdot (M_{j,i} - d_{k,j} \Omega_{k}) \\
&+ \Omega_{k} d_{i,k} - A_{i,k} d_{k},
\end{align*}
\]

\[
\begin{align*}
\frac{\partial s}{\partial d} \cdot N_i + \rho \frac{\partial s}{\partial d_{i,j}} \cdot (M_{j,i} - A_{i,k} d_{k}) + \rho \frac{\partial s}{\partial d_{i}} \cdot \Omega_{i,k} d_{k}
\end{align*}
\]

\[
\begin{align*}
= \rho \frac{\partial s}{\partial d} \cdot N + \rho \frac{\partial s}{\partial \nabla d} \cdot \nabla d + \rho \frac{\partial s}{\partial \nabla d} \cdot \nabla d \cdot \frac{\partial s}{\partial \nabla d} : A
\end{align*}
\]

\[
\begin{align*}
&= \rho \frac{\partial s}{\partial d} \cdot N + \rho \frac{\partial s}{\partial \nabla d} \cdot \nabla d: M - \rho \frac{\partial s}{\partial \nabla d} \cdot \nabla d \cdot \frac{\partial s}{\partial \nabla d} : A.
\end{align*}
\]

The underlined term in the fourth step vanishes, since \( \Omega \) is anti-symmetric while \((\frac{\partial s}{\partial \nabla d} \otimes d + \frac{\partial s}{\partial d} \cdot \nabla d \cdot \frac{\partial s}{\partial \nabla d})\) is symmetric by Lemma 2. Substituting the above formula into \( Ds \), we arrive at

\[
Ds = \nabla \cdot (-\theta^{-1} q) + \theta^{-1} (pI + \sigma^T) : A
\]

\[
- \rho \left( \nabla d \cdot \frac{\partial s}{\partial \nabla d} \right) : A + \theta^{-1} \pi^T : M + \rho \frac{\partial s}{\partial \nabla d} : M
\]

\[
- \theta^{-1} q \cdot N + \rho \frac{\partial s}{\partial \nabla d} : N \cdot q \cdot \nabla \theta^{-1} + \frac{\partial s}{\partial C} : DC
\]

\[
+ \frac{\partial s}{\partial K} : DK + \frac{\partial s}{\partial \Omega} \cdot \Omega + \frac{\partial s}{\partial \rho} \cdot \rho
\]

\[
= \nabla \cdot (-\theta^{-1} q) + \theta^{-1} \sigma E - \rho \left( \nabla d \cdot \frac{\partial s}{\partial \nabla d} \right) : A
\]

\[
+ \left( \theta^{-1} \pi^T + \rho \frac{\partial s}{\partial \nabla d} \right) : M - \theta^{-1} q E - \rho \frac{\partial s}{\partial \nabla d} \cdot N.
\]
2.3 Decomposition of entropy production rate

Notice that the decomposition of the entropy production rate $\Sigma^f$ is not unique. In this paper, we adopt a straightforward decomposition mainly based on the different physical origins of variables, including the Ericksen (static) part, the Leslie (non-equilibrium) part and the viscous part.

Remember that the subscript $E$ denotes the static deformation value, i.e., the Ericksen part, which as a consequence makes no contribution to the entropy production rate:

$$epr_0 = \left[ \theta^{-1} \sigma^E_T - \rho \left( \nabla d \cdot \frac{\partial s}{\partial \nabla d} \right) \right] : A$$

$$+ \left( \theta^{-1} \pi^E_T + \rho \frac{\partial s}{\partial \nabla d} \right) : M$$

$$- \left( \theta^{-1} g_E - \rho \frac{\partial s}{\partial \nabla d} \right) : N = 0. \tag{15}$$

Due to the arbitrariness of $A$, $M$ and $N$, the Ericksen parts of the stress tensor, director surface torque, and director body torque become

$$\sigma^E = \rho \theta \left( \nabla d \cdot \frac{\partial s}{\partial \nabla d} \right)^T, \quad \pi^E = -\rho \theta \left( \frac{\partial s}{\partial \nabla d} \right)^T, \quad g^E = \rho \theta \frac{\partial s}{\partial \nabla d}, \tag{16}$$

respectively.

To guarantee the second law of thermodynamics, we further assume the entropy production rates from the classical viscous part and Leslie part are both non-negative

$$epr_1 + epr_2 + epr_3 + epr_4 = (s^E_T : DC + \theta^{-1} \sigma^E_T : A)$$

$$+ (s^K_T : DK + \theta^{-1} \pi^E_T : M)$$

$$+ (s_h : Dh + q \cdot \nabla \theta^{-1}) \geq 0,$$

and $epr_5 \geq 0$. Given the fact that $\sigma^E$, $\pi^E$, $g^E$ and $q$ are conjugate variables of $C$, $K$, $l$ and $h$ with respect to the specific entropy $s$,

$$\frac{\partial s}{\partial C} = \sigma^V, \quad \frac{\partial s}{\partial K} = \pi^V, \quad \frac{\partial s}{\partial l} = g_V, \quad \frac{\partial s}{\partial h} = q, \tag{17}$$

CDF [29] suggests following constitutive equations:

$$\begin{pmatrix}
\rho C^f + \nabla \cdot (\rho v \otimes C) + \theta^{-1} A \\
\rho K^f + \nabla \cdot (\rho v \otimes K) + \theta^{-1} M \\
\rho l^f + \nabla \cdot (\rho v \otimes l) - \theta^{-1} N
\end{pmatrix} = \mathbf{T} \cdot \begin{pmatrix} s_C \\ s_K \\ s_l \end{pmatrix}, \tag{18}$$

where the nonlinear dissipation matrix $\mathbf{T} = \mathbf{T}(\nu, u, d, \nabla d, C, K, l, h)$ is positive definite, and is readily dependent on both conserved and dissipative variables.

Moreover, the remaining Leslie part of the entropy production rate is

$$epr_5 \equiv \theta^{-1} (s^E_T : A + \pi^E_T : M - g_L \cdot N) \geq 0. \tag{19}$$

This is exactly the total entropy production rate in the classical E-L theory, except that the dissipation caused by the director surface torque $\pi^E_T : M$ is also included (see eq. (3.1.21) in ref. [7]). Specifically, by choosing $\pi_L = 0$ and following the same argument of Leslie [5,7], one will arrive at the most widely adopted form of $\sigma_L$ and $g_L$ as follows:

$$\sigma_L = \alpha_1 (d^T A d) \otimes d + \alpha_2 N \otimes d + \alpha_3 d \otimes N + \alpha_4 A$$

$$+ \alpha_5 d \otimes (A \otimes d) + \alpha_6 (A \otimes d) \otimes d, \tag{20}$$

$$g_L = (\alpha_2 - \alpha_3) N + (\alpha_5 - \alpha_6) A \otimes d, \tag{21}$$

where $\alpha_i = \alpha_i(\rho, \theta)$ $(i = 1, \cdots, 6)$ is called the classical Leslie coefficient, depending on the density $\rho$ and nonequilibrium temperature $\theta$. According to Parodi’s relation [7], these coefficients are connected by $\alpha_2 + \alpha_3 = \alpha_5 - \alpha_6$, and the number of independent coefficients reduces to five. In general, the Leslie coefficients cannot be identified separately, except for $\alpha_4$. Fortunately, they are combinations of Miesowicz viscosities, which can be measured accurately. We refer to ref. [24] for the physical interpretation of Leslie coefficients and their relations with experimentally measurable quantities.

By substituting above formulas into $epr_5$, one has

$$\theta \cdot epr_5 = \alpha_1 (d^T A d) + (\alpha_2 + \alpha_3 - \alpha_5)$$

$$+ \alpha_6) (d^T A N) + \alpha_4 |A|^2$$

$$+ (\alpha_5 + \alpha_6) A \otimes d^2 - (\alpha_2 - \alpha_3) |N|^2, \tag{22}$$

where $A^T = A$ was used, and $|A|^2 \equiv A^T A$, $|N|^2 \equiv N^T N$. Since variables $(d, A, N)$ are arbitrary, we have to put restrictions on the Leslie coefficients in order to guarantee the non-negativity of entropy production rate $epr_5$, which is stated as follows.
Theorem 1. The Leslie contribution to the entropy production rate in eq.(5) is non-negative if and only if
\[
\alpha_4 \geq 0, \quad \alpha_5 + \alpha_6 \geq 0, \quad \alpha_3 - \alpha_2 \geq 0, \\
(\alpha_1 + \alpha_5 + \alpha_6) d_1^2 + \alpha_4 \geq 0, \\
4(\alpha_3 - \alpha_2)(\alpha_1 + \alpha_5 + \alpha_6)d_1^2 + 4(\alpha_3 - \alpha_2)\alpha_4 \\
- (\alpha_2 + \alpha_3 - \alpha_5 + \alpha_6)^2 d_1^2 \geq 0, \\
4(\alpha_3 - \alpha_2)((\alpha_1 + \alpha_5 + \alpha_6)d_1^2 + 2\alpha_4) \\
- (\alpha_2 + \alpha_3 - \alpha_5 + \alpha_6)^2 d_1^2 \geq 0,
\]
where \(d_1 \equiv |d| \geq 0\) is the norm of director vector. Above inequalities hold for any \(d_1 \in [d_{\text{min}}, d_{\text{max}}]\), where \([d_{\text{min}}, d_{\text{max}}]\) stands for the length variational range of different liquid crystal molecules when the temperature is changed.

We mention that Ericksen and Leslie imposed restrictions for above coefficients when the nematic liquid crystals were assumed to be isothermal and incompressible. We consider a compressible and non-isothermal system, and thus abandon the assumptions that \(\nabla \cdot \mathbf{v} = 0\) and \(|d| = 1\). Please see Lemma 3 in appendix A.

### 2.4 Non-isothermal and compressible vectorial models

In order to derive a concrete model, we present some classical choices of the entropy function and the dissipation matrix as an illustration. We select the specific entropy function as
\[
s(\nu, u, d, \nabla d, C, K, l, h) = s_0(\nu, u, d, \nabla d) - \frac{1}{2} |C|^2 \\
- \frac{1}{2} \frac{|K|^2}{\beta_3} - \frac{1}{2} |l|^2 - \frac{1}{2} \frac{|h|^2}{\beta_4},
\]
where the equilibrium entropy \(s_0(\nu, u, d, \nabla d)\) is a strictly concave function, \(\nu = 1/\rho\), and \(\beta_1, \cdots, \beta_4\) are positive coefficients related to different relaxation times. Since the entropy function depends on non-equilibrium variables in a quadratic form, direct calculations show that
\[
C = -\beta_1 \sigma_V, \quad K = -\beta_2 \pi_V, \quad l = -\beta_3 g_V, \quad h = -\beta_4 q.
\]
With a diagonal and constant matrix \(\mathcal{T} = \frac{1}{\rho} \text{diag}(\frac{\sigma_V}{\theta_1}, \frac{\pi_V}{\theta_2}, \frac{g_V}{\theta_3}, \frac{q}{\theta_4})\), we have
\[
\mathcal{T} \cdot \begin{pmatrix} \sigma_V \\ \pi_V \\ g_V \\ q \end{pmatrix} = \begin{pmatrix} \frac{\sigma_V}{\theta_1} \\ \frac{\pi_V}{\theta_2} \\ \frac{g_V}{\theta_3} \\ \frac{q}{\theta_4} \end{pmatrix},
\]
where the parameters \(\gamma_i\) (\(i = 1, 2, 3, 4\)) are all positive. \(\gamma_1\) and \(\gamma_2\) denote the generalized viscosities, \(\gamma_3\) is the rotational friction coefficient, and \(\gamma_4\) is the thermal conductivity of liquid crystals.

Now it is time to summarize our new vectorial model for non-isothermal and compressible flows of nematic liquid crystals. This model includes the director inertial term and discards the assumption on \(|d| = 1\), and thus is applicable to molecular mixtures. With the above choices of entropy and dissipation matrix, the model reads
\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{v}) = 0, \\
\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = \mathbf{g} + \nabla \cdot \left( -p I + \sigma_V + \sigma_\mathcal{E} + \sigma_L \right), \\
\frac{\partial}{\partial t} (\rho_L u) + \nabla \cdot (\rho_L v \otimes w) = (g_V + g_E + g_L) + \nabla \cdot (\pi_V + \pi_\mathcal{E} + \pi_L), \\
\frac{\partial}{\partial t} (\rho_L w) + \nabla \cdot (\rho_L v \otimes w) = (g_V + g_E + g_L), \\
\beta_1[(\rho \sigma_V)_t + \nabla \cdot (\rho \mathbf{v} \otimes \sigma_V)] - \theta_1 A = -\frac{\sigma_V}{\theta_1}, \\
\beta_2[(\rho \pi_V)_t + \nabla \cdot (\rho \mathbf{v} \otimes \pi_V)] - \theta_1 M = -\frac{\pi_V}{\theta_2}, \\
\beta_3[(\rho g_V)_t + \nabla \cdot (\rho \mathbf{v} \otimes g_V)] + \theta_1 N = \frac{g_V}{\theta_3}, \\
\beta_4[(\rho q)_t + \nabla \cdot (\rho \mathbf{v} \otimes q)] - \theta_1 \gamma_4 = \frac{q}{\theta_4} \gamma_4,
\]
where
\[
\mathbf{g} = \rho \theta \left( \nabla d, \frac{\partial s}{\partial \nabla d} \right)^T, \quad \pi_\mathcal{E} = -\rho \theta \left( \frac{\partial s}{\partial \nabla d} \right)^T, \\
\sigma_\mathcal{E} = \rho \theta \left( \nabla d, \frac{\partial s}{\partial \nabla d} \right)^T, \\
\sigma_L = \alpha_1 (\mathbf{d}^T \cdot \mathbf{d}) \mathbf{d} \otimes \mathbf{d} + \alpha_2 \mathbf{N} \otimes \mathbf{d} + \alpha_3 \mathbf{d} \otimes \mathbf{N} + \alpha_4 \mathbf{A} + \alpha_5 \mathbf{d} \otimes (\mathbf{A} \cdot \mathbf{d}) + \alpha_6 (\mathbf{A} \cdot \mathbf{d}) \otimes \mathbf{d}, \\
\pi_L = 0, \quad \mathbf{g}_L = (\alpha_2 - \alpha_3) \mathbf{N} + (\alpha_5 - \alpha_6) \mathbf{A} \cdot \mathbf{d}.
\]

Here \(2A = (\nabla d)^T + \nabla d, 2\Omega = (\nabla d)^T - \nabla d, N = w - \Omega \cdot d, M = \nabla w + \nabla d, \Omega = \left( \frac{\partial s}{\partial \nabla d} \right)^T\) is the non-equilibrium temperature, and \(p = \theta \left( \frac{\partial s}{\partial \nabla d} \right)^T\) is the thermodynamical pressure. The Leslie coefficients \(\alpha_1, \cdots, \alpha_6\), as functions of density \(\rho\) and non-equilibrium temperature \(\theta\), should also satisfy constraints given in (22).

### 2.5 Isothermal and incompressible vectorial models

In the former section, we have arrived at a general model for nematic liquid crystals under non-isothermal and compressible conditions. When liquid crystals are maintained at constant temperature \(T\), and the director \(d\) is approximated to be of unit length, we arrive at a much simpler model, which has been widely used in previous studies. For this case, \(d(x, t) \in \mathbb{S}^2\), where \(\mathbb{S}^2\) denotes a unit sphere of \(\mathbb{R}^3\).

Notice that the first law of thermodynamics holds automatically under the isothermal condition. As a consequence, the governing equations reduce to the first three conservation laws in (26). To show that the classical E-L theory is a special case of our general model, we set the
density $\rho \equiv 1$ and further assume the inertia moment density is negligible under the isothermal and incompressible condition by setting $\rho_1 \to 0$. The conservation laws of mass, momentum and angular momentum for hydrodynamics of nematic liquid crystals become

$$\nabla \cdot v = 0, \quad \frac{\partial v}{\partial t} + v \cdot \nabla v = -\nabla p + \nabla \cdot (\sigma V + \sigma_E + \sigma_L),$$

$$\left( g_V + g_E + g_L \right) + \nabla \cdot (\pi V + \pi_E + \pi_L) = 0. \quad (29)$$

Under the isothermal condition, the elastic energy (or free energy) function for nematic liquid crystals was first studied by Oseen and Zocher [24] dated back to the 1920s. Later, Frank [34] constructed a concrete energy form based on all possible distortions of the director in 1958. Following the classical Oseen-Frank elastic energy, we have the equilibrium entropy $s_0$ in (23) expressed as

$$s_0(\nu, u, d, \nabla d)|_{\upsilon = 1, \theta = T} = -\frac{1}{T} W_F(d, \nabla d), \quad (30)$$

in which

$$2 W_F(d, \nabla d) = k_1 (\nabla \cdot d)^2 + k_2 [d : (\nabla \times d)^2] + k_3 |d \times (\nabla \times d)|^2 + (k_2 + k_3)|\text{tr}(\nabla d)^2 - (\nabla \cdot d)^2|. \quad (31)$$

Here $k_1, k_2, k_3$ and $(k_2 + k_3)$, depending on the density $\rho$ and temperature $T$, stand for the pure splay, pure twist, pure bend and saddle-splay constants respectively. Furthermore, since the integral of the fourth term of eq. (31)

$$(k_2 + k_3) \int |\text{tr}(\nabla d)^2 - (\nabla \cdot d)^2| dx,$$

depends solely on boundary values of $d$, the saddle-splay term can be discarded for planar boundary conditions [35]. We suggest refs. [36–38] for experimental, theoretical and numerical investigations on the elastic constants $k_i$ ($i = 1, 2, 3, 4$).

In this case, we have $\frac{\partial s_0}{\partial T} = -\frac{1}{T} \frac{\partial W_F}{\partial T}$, $\frac{\partial s_0}{\partial \nabla d} = -\frac{1}{T} \frac{\partial W_F}{\partial \nabla d}$, then the Ericksen parts of the stress tensor, the director surface torque and body torque in eq. (16) become

$$\sigma_E = -\left( \nabla \cdot \frac{\partial W_F}{\partial \nabla d} \right)^T, \quad \pi_E = \left( \frac{\partial W_F}{\partial \nabla d} \right)^T,$$

$$g_E = -\frac{\partial W_F}{\partial d}, \quad (32)$$

by noticing the fact that the non-equilibrium temperature coincides with the equilibrium temperature under isothermal conditions, $\theta = T$. In the stationary limit, $\beta_1, \beta_2, \beta_3 \to 0$, by choosing the dissipation matrix as in eq. (25) and taking Maxwellian iteration, we have

$$\sigma_V = \gamma_1 A, \quad \pi_V = \gamma_2 M, \quad g_V = -\gamma_3 N. \quad (33)$$

Summarizing above equations, we arrive at the classical E-L theory for nematic liquid crystals under the isothermal and incompressible condition as

$$\nabla \cdot v = 0,$$

$$\frac{\partial v}{\partial t} + v \cdot \nabla v = -\nabla p + \nabla \cdot (\sigma V + \sigma_E + \sigma_L),$$

$$\sigma_V + \sigma_E + \sigma_L = -\left( \nabla d \cdot \frac{\partial W_F}{\partial \nabla d} \right)^T + \alpha_1 (d^T \cdot A \cdot d) \delta d + \alpha_2 N \otimes d + \alpha_3 \delta N + (\alpha_4 + \gamma_1) A + \alpha_5 \otimes (A \cdot d) + \alpha_6 (A \cdot d) \otimes d,$$

$$-\frac{\partial W_F}{\partial d} + \nabla \cdot \left( \frac{\partial W_F}{\partial \nabla d} \right)^T - (\alpha_3 - \alpha_2 + \gamma_3) N,$$

except for an additional term $(\gamma_2 \nabla \cdot M)$ in angular momentum equation and two extra terms as $\gamma_1 A$ and $-\gamma_3 N$, which can be absorbed into the classical coefficients as $\alpha_4 + \gamma_1$ and $\alpha_3 - \alpha_2 + \gamma_3$. The first two terms of angular momentum equation are also known as the molecular field of liquid crystals, whose components read $-\frac{\partial W_F}{\partial d} = -\frac{\partial W_F}{\partial \nabla d} + \partial_j \left( \frac{\partial W_F}{\partial \nabla_j} \right)$. The additional term $\partial_j M_{ij} = \partial_j (w_{ij} + \Omega_{kj} d_{kj})$ describes how the spatial gradients of director velocity affect the balance of angular momentum, which is not taken into consideration in the classical E-L equations of liquid crystals [7, 24].

### 3 Extension to the tensorial theory

In the previous section, a generalized vectorial model for non-isothermal flows of nematic liquid crystals is derived, which includes the classical E-L model as a special case under the isothermal condition. In this part, we focus on CDF for the generalized Qian-Sheng (Q-S) model [20], and the Beris-Edwards model [19, 39] can be treated in a similar way. From the multi-scale thermodynamic [40] point of view, the E-L like vectorial theory belongs to a description of lower level, while the tensorial theory contains more details in the internal structure of liquid crystals, and thus belongs to a higher level. CDF provides a unified and elegant framework for describing non-isothermal systems for both vectorial and tensorial models. To avoid lengthy derivations, here only the key results for the tensorial model are included. Interested readers may refer to the Electronic Supplemental Material (ESM) for details.

In the tensorial theory, the conservation laws of mass and momentum for non-isothermal compressible flows of nematic liquid crystals are the same as those for the vectorial model, while the angular momentum and total energy conservation laws are different, which read

$$\frac{\partial}{\partial t} (\rho_1 \dot{Q}) + \nabla \cdot (\rho_1 v \otimes \dot{Q}) = g + \nabla \cdot \pi,$$

$$\frac{\partial}{\partial t} (\rho e ) + \nabla \cdot (\rho v e) = \xi \cdot v + \nabla \cdot (\sigma \cdot v + \pi : \dot{Q} - q),$$

where the second-order tensor $g$ is body torque and the third-order tensor $\pi$ is surface torque. The total energy includes internal energy, translational kinetic energy and
rotational kinetic energy as \( \rho e = \rho u + \frac{1}{2} \rho v^2 + \frac{1}{2} \rho_1 \dot{Q}^2 \). In analogy with eq. (5) in the vectorial theory, the stress tensor, \( Q \)-tensor body torque and surface torque can be separated into \( \sigma = -\rho \dot{l} + \sigma_E + \sigma_{QS} + \sigma_V, \quad g = E + g_{QS} + G \) and \( \pi = \pi_E + \pi_{QS} + \pi_V \), respectively.

Supposing the balance equation of internal energy to satisfy the principle of objectivity, direct calculations yield

\[
\rho \frac{du}{dt} = \sigma^T : \nabla v + g : \dot{Q} + \nabla^T \dot{\nabla} Q - \nabla \cdot q,
\]

where \( \pi^T \nabla \dot{Q} = (\pi^T)_{ijkl} \partial_k (\tilde{Q}_{ij}) \) is the triple scalar product between the third-order tensors \((\pi^T)_{ijkl}\) and \( \partial_k \tilde{Q}_{ij} = \partial \tilde{Q}_{ij}/\partial x_k \). The second-order tensor \( Y = \dot{Q} - \Omega \cdot \dot{Q} + \dot{Q} \cdot \Omega \) is the Jaumann derivative of \( Q \), representing the change rate of \( Q \) relative to the fluid angular velocity. In terms of Cartesian coordinates, the third-order tensor \( M \) is defined as

\[
M_{klj} = \partial_k \tilde{Q}_{lj} + \partial_k \tilde{Q}_{llj} - \partial_l \tilde{Q}_{lj},
\]

which is shown to be objective in Lemma 4. The terms which violate the principle of frame-indifference in eq. (37) are neglected. The third-order tensors \( \pi \) and \( M \) in eqs. (35)–(37), accounting for the contributions of the surface torque to the angular momentum and energy, are not found in the existing literature as far as we know.

In order to find constitutive relations for \((\sigma, \pi, g, q)\), we follow CDF and specify a strictly concave mathematical entropy function

\[
\eta = \rho s(u, v, Q, \nabla Q, \tilde{C}, \tilde{K}, \tilde{l}, \tilde{h}),
\]

where \( \nu = 1/\rho \). \((\nu, u, Q, \nabla Q)\) denote the conserved variables, while \((\tilde{C}, \tilde{K}, \tilde{l}, \tilde{h})\) are specified according to \( \frac{\partial \sigma}{\partial \eta} = \pi_v, \quad \frac{\partial M}{\partial \eta} = \pi_V \) and \( \frac{\partial q}{\partial \eta} = q \). According to the generalized Gibbs relation and Lemma 5, we derive the time evolution equation of the entropy \( \eta \) as

\[
D_s(u, v, Q, \nabla Q, \tilde{C}, \tilde{K}, \tilde{l}, \tilde{h}) = -\nabla \cdot J^f + \Sigma^f,
\]

where \( J^f = \theta^{-1} q \) and

\[
\Sigma^f = \left( \theta^{-1} \sigma^T_E - \rho \nabla Q \right) : \frac{\partial s}{\partial \nabla Q} \cdot \left[ \frac{\partial s}{\partial \nabla Q} + \theta^{-1} \pi^T_E + \rho \left( \frac{\partial s}{\partial \nabla Q} \right)^T \right] : M
\]

\[
+ \frac{\partial s}{\partial \Omega} \left( \frac{\partial s}{\partial \Omega} \right)^T : \tilde{C} + \theta^{-1} \sigma^T_V : A + \left( \frac{\partial s}{\partial \Omega} \right)^T : \tilde{h}
\]

\[
- \theta^{-1} \nabla \cdot g : \left( \frac{\partial s}{\partial \Omega} \right)^T : \tilde{C} + \theta^{-1} \pi^T_V : M
\]

\[
+ \frac{\partial s}{\partial \Omega} \cdot \nabla q + q \cdot \nabla \theta^{-1}
\]

\[
+ \theta^{-1} \left( \sigma^T_{QS} : A - g_{QS} : Y + \pi^T_{QS} : M \right).
\]

Following basically the same procedure taken in the vectorial theory, we arrive at a new system of constitutive equations for the non-isothermal tensorial model as

\[
\begin{align*}
\sigma_E &= \rho \theta \left( \nabla Q : \frac{\partial s}{\partial \nabla Q} \right)^T, \\
\pi_E &= -\rho \theta \left( \frac{\partial s}{\partial \nabla Q} \right)^T, \\
\left[ (\rho \dot{C})_t + \nabla \cdot (\rho v \otimes \tilde{C}) \right] + \theta^{-1} A = \frac{\sigma_V}{\theta \gamma_1}, \\
\left[ (\rho \dot{h})_t + \nabla \cdot (\rho v \otimes \tilde{h}) \right] - \theta^{-1} Y = \frac{\pi_V}{\theta \gamma_2}, \\
\left[ (\rho \tilde{K})_t + \nabla \cdot (\rho v \otimes \tilde{K}) \right] + \theta^{-1} M = \frac{\sigma_{QS}}{\theta \gamma_3}, \\
\left[ (\rho \tilde{h})_t + \nabla \cdot (\rho v \otimes \tilde{h}) \right] + \theta^{-1} q = \frac{\pi_{QS}}{\theta \gamma_4}, \\
\sigma_{QS} &= \tilde{a}_1 (Q \cdot A) Q + \tilde{a}_4 A + \tilde{a}_5 Q : A + \tilde{a}_6 A \cdot Q + \frac{1}{2} \mu_2 Y - \mu_1 Q \cdot Y + \mu_1 (Q \cdot Y)^2 \\
&+ \tilde{a}_7 \text{tr}(A) (I + \alpha \text{tr}(A)) Q : Q, \\
g_{QS} &= -\frac{1}{2} \mu_2 A - \mu_1 Y, \quad \pi_{QS} = 0,
\end{align*}
\]

where \( \tilde{a}_1, \tilde{a}_4, \tilde{a}_5, \mu_1, \mu_2, \tilde{a}_7 \) and \( \tilde{a}_8 \) are material- and temperature-dependent viscosity coefficients of liquid crystals, and \( \tilde{a}_6 \leq \tilde{a}_5 \leq \mu_2 \). We adopt \( \tilde{a}_7 \) and \( \tilde{a}_8 \) to describe the compressible effects on the stress tensor, which will vanish if the system is incompressible. In that case, the expression of \( \sigma_{QS} \) reduces to the classical constitutive equations in ref. [20].

Now, the total entropy production rate of system (40) is readily obtained as

\[
\Sigma^f = \frac{1}{\theta \gamma_1} |\sigma_V|^2 + \frac{1}{\theta \gamma_2} |\pi_V|^2 + \frac{1}{\theta \gamma_3} |\nabla U|^2 + \frac{1}{\theta \gamma_4} |\pi_{QS}|^2 + \tilde{a}_7 \text{tr}(A)^2 + \tilde{a}_8 \text{tr}(A) Q : (Q \cdot A)^2 \\
+ \tilde{a}_1 (Q \cdot A)^2 + \tilde{a}_4 A^2 + (\tilde{a}_5 + \tilde{a}_6) (Q \cdot A) : A + \mu_2 Y : A + \mu_1 |Y|^2
\]

where the first four terms \((epr1 + epr2 + epr3 + epr4) \geq 0\) are produced by relaxation processes. The underlined residual terms, denoted as \( epr5 \), correspond to the classical Qian-Sheng theory. In order to guarantee the non-negativeness of \( epr5 \), the phenomenological coefficients \( \tilde{a} \)'s and \( \mu \)'s shall satisfy further restrictions, similar to Theorem 1 in the vectorial model. Considering the complexity of tensor calculations, we present a non-trivial sufficient condition for \( epr5 \geq 0 \) as

\[
\tilde{a}_8 = 0, \quad \tilde{a}_7 \geq 0, \quad \tilde{a}_4 \geq 0, \quad \mu_1 \geq 0, \quad \tilde{a}_1 \geq 0, \quad 4 \tilde{a}_4 \mu_2 - \mu_1^2 \geq 0, \quad 4 \tilde{a}_4 \tilde{a}_1 - (\tilde{a}_5 + \tilde{a}_6)^2 \geq 0,
\]

\[
4 \tilde{a}_1 \tilde{a}_4 \mu_1 - \tilde{a}_1 \mu_2^2 - \mu_1 (\tilde{a}_5 + \tilde{a}_6)^2 \geq 0.
\]

Please see Lemma 6 for a proof on the sufficiency.

Especially, under the isothermal condition, the temperature becomes constant \( \theta = T \). Further setting the
density as \( \rho = 1 \), then the classical Landau-de Gennes energy density is expressed as [1]

\[
F_{LdG}(Q, \nabla Q) = -\frac{a}{2}\text{tr}(Q^2) - \frac{b}{3}\text{tr}(Q^3) + \frac{c}{4}\text{tr}(Q^4)
+ \frac{1}{2}(L_1|\nabla Q|^2 + L_2Q_{ij,j}Q_{ik,k}
+ L_3Q_{ij,k}Q_{ik,j} + L_4Q_{ij,l}Q_{kl,j}),
\]

(42)

where the bulk energy includes the phenomenological coefficients \( a, b, c > 0 \), and the elastic coefficients \( L_i \) (\( i = 1, 2, 3, 4 \)). By choosing the entropy function \( s = -F_{LdG}(Q, \nabla Q)/T \), the balance equations of momentum and angular momentum reduce to

\[
\frac{d\vec{v}}{dt} = \xi - \nabla p - \nabla \cdot \left( \nabla Q \cdot \frac{\partial F_{LdG}}{\partial \nabla Q} \right)^T + \dot{\alpha}_1(Q : A)Q
+ (\dot{\alpha}_4 + \gamma_1)A + \dot{\alpha}_5\nabla \cdot A
+ \dot{\alpha}_6A \cdot Q + \frac{1}{2}\mu_2 Y - \mu_1Q \cdot Y + \mu_1(Q \cdot Y)^T,
\]

(43)

\[
\rho \ddot{\vec{Q}} - \frac{\partial F_{LdG}}{\partial Q} + \nabla \cdot \left( \frac{\partial F_{LdG}}{\partial \nabla Q} \right)^T - \frac{1}{2}\mu_2 A
- (\mu_1 - \gamma_2)Y + \gamma_3 \nabla \cdot M.
\]

(44)

The above equations are essentially the same as the Qian-Sheng model [20], except that we have two extra terms \( \gamma_1A, -\gamma_2Y \), and include \( \nabla \cdot M \). The last term \( \partial_kM_{ijkl} = \partial_k(\partial_kQ_{ij} - \Omega_{ik}Q_{lj,k} + Q_{l,ik}\Omega_{lj}) \) is frame indifferent, and describes the effect of the spatial anisotropy of tensorial order parameters on the balance of the angular momentum.

Remark 4. Based on the analysis of length and time scales [20], the E-L equations reflect the long-range and slow-motion limit of the Q-tensor model. By assuming a uniaxial symmetry of Q-tensor,

\[
Q_{ij}(x, t) = \frac{S_0}{2}[3d_i(x, t)d_j(x, t) - \delta_{ij}],
\]

(45)

it was shown that the classical isothermal E-L equations could be recovered from the Qian-Sheng model [2, 20]. A similar conclusion is expected for our generalized non-isothermal tensorial and vectorial models, since both of them can be casted into the framework of CDF.

4 Conclusion and discussion

In the first paper of this series [11], isothermal models for particle diffusion in dilute solutions, polymer phase separation dynamics and simplified Lin-Liu model for isothermal flows of nematic liquid crystals were studied under the guidance of CDF. In the current paper, more complicated non-isothermal and compressible situations are examined by taking nematic liquid crystals as a typical example.

Starting from the fundamental conservation laws, a generalized vectorial model for flows of nematic liquid crystal in a non-isothermal environment is derived within the framework of CDF. The hydrodynamic equations thus deduced are fully consistent with the first and second laws of thermodynamics. A necessary and sufficient condition involving inequalities of Leslie coefficients is obtained to guarantee the non-negativeness of the entropy production rate, with emphasis on different molecular lengths. Under the isothermal and incompressible condition, the classical E-L theory is shown to be a special case of our new vectorial model in the stationary limit. Moreover, all results are readily extended to the tensorial form under non-isothermal and compressible conditions by making use of CDF.

It has been widely recognized that the non-isothermal situations will bring some intrinsic difficulties to the thermodynamics-based mathematical modeling, like proper definitions of the non-equilibrium temperature, non-violation of the first law of thermodynamics, the non-Fourier law for heat conduction, etc. Many non-equilibrium thermodynamic theories or approaches, like the CIT [41], Doi’s variational approach [42], the energetic variational framework [10] and so on, might fail to overcome these obstacles. In contrast, as one of its outstanding merits, CDF has been shown to be able to handle various non-isothermal irreversible processes easily in a systematic way. The first and second laws of thermodynamics are respected in CDF simultaneously. The non-equilibrium temperature and pressure are introduced in a self-consistent way as partial derivatives of the entropy (see ref. [32] for other attempts). Relaxation-type equations for the stress tensor and heat conduction are constructed as direct generalizations of Newton’s law for viscosity and Fourier’s law for heat conduction. All these facts demonstrate that CDF may have a broader scope of applications in soft matter physics.

As we have mentioned, there is a deep connection between CDF and GENERIC [43]. The former is a Conservation-Dissipation formalism as it is named, while the latter is in fact a Hamiltonian-Dissipation formalism (HDF) in some sense. As the Hamiltonian structure has a richer content than the conservation laws, we expect that HDF will lead to stronger restrictions on the constitutive relations than CDF. However, the corresponding mathematical formulation is also much harder. Related works are going on.

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Author contribution statement

LH designed the study. LRP, LH, and YCH carried out the applications and wrote the manuscript. All authors have read and approved the final manuscript.

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Appendix A. Some Lemmas

Lemma 1. (A proof of eq. (13)). The director vector $d$ and its spatial gradient $\nabla d$ satisfy following differential relations:

$$Dd = \rho (N + \Omega \cdot d),$$
$$D(\nabla d) = \rho [M - (\nabla d) \cdot \Omega + \Omega \cdot (\nabla d) - A \cdot (\nabla d)].$$

Proof. Firstly, we have

$$Dd = \frac{\partial}{\partial t} (pd) + \nabla \cdot (vpd) = \rho \left( \frac{\partial}{\partial t} d + v \cdot \nabla d \right) = \rho \frac{d}{dt} d = \rho w = \rho (N + \Omega \cdot d),$$

by recalling the definition of relative angular velocity $N = \omega - \Omega \cdot d$. Secondly, we deduce that

$$D(\nabla d) = \rho \left( \frac{\partial}{\partial t} + v \cdot \nabla \right) (\nabla d) = \rho \nabla \left[ \left( \frac{\partial}{\partial t} + v \cdot \nabla \right) d \right] - \rho \nabla v \cdot \nabla d = \rho [M - (\nabla d) \cdot \Omega + \Omega \cdot (\nabla d) - A \cdot (\nabla d)],$$

where the definition $M = \nabla w + (\nabla d) \cdot \Omega$ was used in the last step. \hfill \Box

The following identity was obtained by Ericksen [33] in 1961, we derive it here to preserve the integrity of contents.

Lemma 2. If $s = s(\nu, u, d, \nabla d, C, K, l, h)$ is objective with respect to conserved variables, the tensor $(\frac{\partial s}{\partial \nu} \otimes d + \frac{\partial s}{\partial v} \cdot \nabla d)$ must be symmetric [33].

Proof. We consider the Euclidean transformation

$$x^*(t) = R(t)x(t) + c(t), \quad (A.1)$$

doing a continuum, here $R = (R_{ij})$ stands for a second-order orthogonal tensor function, i.e., $R^T R = I$. States after rigid motions and original states are denoted by asterisked and unasterisked variables, respectively. Mathematically, we have

$$s(\nu, u, d^*, \nabla d^*, C, K, l, h) = s(\nu, u, d, \nabla d, C, K, l, h),$$

where

$$d^* = R \cdot d, \quad \nabla d^* = R \cdot (\nabla d) \cdot R^T. \quad (A.2)$$

Specifically, we choose arbitrary infinitesimal rotations with

$$R_{ij} = \delta_{ij} + \varepsilon_{ij}, \quad \varepsilon_{ji} = -\varepsilon_{ij}, \quad \varepsilon_{ij} \varepsilon_{kl} \approx 0. \quad (A.3)$$

Substituting the above relations into eq. (A.2), we have

$$d^* - d = \varepsilon \cdot d,$$
$$\nabla d^* - \nabla d = \varepsilon \cdot \nabla d - \varepsilon \cdot \nabla d \cdot \varepsilon = \varepsilon \cdot \nabla d - \varepsilon \cdot \nabla d \cdot \varepsilon + O(\varepsilon^2),$$

where the second equality holds within the leading order of $\varepsilon$. Therefore, one deduces approximately that

$$0 \approx \frac{\partial s}{\partial d} \cdot (d^* - d) + \left[ \frac{\partial s}{\partial \nabla d} \right]^T : [(\nabla d)^* - \nabla d]$$
$$= - \left( \frac{\partial s}{\partial d} \otimes d + \frac{\partial s}{\partial \nabla d} \cdot \nabla d - \nabla d \cdot \frac{\partial s}{\partial \nabla d} : \varepsilon.$$

Since the above equality holds for arbitrary skew-symmetric tensors $\varepsilon$, the tensor in the parenthesis must be symmetric. This completes the proof. \hfill \Box

Lemma 3. (A proof of Theorem 1)

Proof. Choose a set of proper orthogonal basis $(e_1, e_2, e_3)$, such that

$$d = d_1 e_1, \quad N = N_1 e_1 + N_2 e_2, \quad A = A_{ij} e_i \otimes e_j,$$

where $d_1 = |d| \geq 0$ is the norm of director vector $d(x, t)$, and the repeated indices are subject to the summation convention. Moreover, two vectors $d$ and $N$ are in a subspace spanned by $(e_1, e_2)$. Inserting the relations of $d, N$ and $A$ into eq. (5), we have

$$\theta \cdot c p r =$$
$$= \alpha_1 d_1^2 A_{11}^2 + (\alpha_2 + \alpha_3 - \alpha_5 + \alpha_6) d_1 (A_{11} N_1 + A_{12} N_2)$$
$$+ \alpha_4 A_{ij} A_{ij}$$
$$+ (\alpha_5 + \alpha_6) d_1^2 (A_{11}^2 + A_{12}^2 + A_{13}^2)$$
$$+ (\alpha_5 - \alpha_2) N_1^2$$
$$+ (\alpha_5 + \alpha_6) d_1^2 (A_{11}^2 + A_{12}^2 + A_{13}^2)$$
$$+ (\alpha_5 - \alpha_2) N_1^2$$
$$+ \alpha_5 A_{ij} A_{ij},$$

where we used the symmetric property of $A$ in the second step. Since $A_{ij}(i \leq j), N_1, N_2$ and $d_1$ are all independent variables, it requires that

$$[(\alpha_1 + \alpha_5 + \alpha_6) d_1^2 + (\alpha_4) A_{11}^2 + (\alpha_2 + \alpha_3 - \alpha_5)$$
$$+ \alpha_6) d_1 A_{11} N_1 + (\alpha_5 - \alpha_2) N_1^2$$
$$+ (\alpha_5 + \alpha_6) d_1^2 + 2 \alpha_4 A_{12}^2 + (\alpha_2 + \alpha_3 - \alpha_5)$$
$$+ \alpha_5) d_1 A_{12} N_2$$
$$+ (\alpha_5 - \alpha_2) N_2^2,$$

$$\alpha_5 A_{ij} A_{ij} \geq 0, \quad \alpha_5 A_{22} \geq 0, \quad 2 \alpha_4 A_{23} \geq 0,$$
$$\alpha_5 A_{33} \geq 0.$$

The last four inequalities yield that

$$\alpha_5 + \alpha_6 \geq 0, \quad \alpha_4 \geq 0. \quad (A.4)$$

Moreover, the left-hand side of the first inequality corresponds to a quadratic form of variables $(A_{11}, A_{12}, N_1, N_2)$, where the associated symmetric matrix reads

see equation on top of the next page.
The matrix $M$ is semi-positive if and only if all leading principal minors have non-negative determinants. Therefore,

$$
M = \begin{pmatrix}
(a_1 + a_5 + a_6)d_1^2 + a_4 & 0 & \frac{(a_2 + a_3 - a_5 + a_6)d_1}{2} & 0 \\
0 & (a_5 + a_6)d_1^2 + 2a_4 & 0 & \frac{(a_2 + a_3 - a_5 + a_6)d_1}{2} \\
* & 0 & a_3 - a_2 & 0 \\
0 & a_3 - a_2 & 0 & a_3 - a_2
\end{pmatrix}.
$$

The substitution of the definition $Y_{ij}^* = \dot{Q}_{ij}^* - \Omega_{ip}^* Q_{pj}^* + \Omega_{ip}^* \Omega_{pj}^*$ gives that

$$
\partial_k^* \dot{Q}_{ij}^* - \Omega_{ip}^* \partial_k^* Q_{pj}^* + \partial_k^* \Omega_{ip}^* \Omega_{pj}^* - \mathcal{R}_{kr} \mathcal{R}_{ip} \mathcal{R}_{jq}(\partial_t \mathcal{Q}_{pq}) \\
- \mathcal{Q}_{pt}(\partial_t \mathcal{Q}_{iq}) + \partial_t \mathcal{Q}_{pt} \mathcal{Q}_{tq}) = \\
\partial_k^* \Omega_{ip}^* Q_{pj}^* - \dot{Q}_{ip}^* \Omega_{pq}^* - \mathcal{R}_{kr} \mathcal{R}_{ip} \mathcal{R}_{jq}(\partial_t \mathcal{Q}_{pt} \mathcal{Q}_{tq}) - \mathcal{Q}_{pt}(\partial_t \mathcal{Q}_{tq}).
$$

The left-hand side is just $M_{ij}^*$, so $M_{ij}^* - \mathcal{R}_{kr} \mathcal{R}_{ip} \mathcal{R}_{jq} \mathcal{M}_{pq}$, which means that the objectivity of $M$ is equivalent to the cancellation of the right-hand side. Actually, we can prove $\partial_t^* \dot{Q}_{pq}^* = \mathcal{R}_{kr} \mathcal{R}_{ip} \mathcal{R}_{jq}(\partial_t \mathcal{Q}_{pq})$, and the other relation follows immediately.

By taking the time derivative of Euclidean transformation $x^*_t = \mathcal{R}_{ij} x^*_j + c$, one has $v^*_t = \dot{R}_{ij} v^*_j + \dot{R}_{ij} x^*_j + \dot{c}$. Further taking spatial gradient, we obtain $\partial_p v^*_t = \mathcal{R}_{pk} \mathcal{R}_{ik} + \mathcal{R}_{pk} \partial_k v^*_j$. It can be readily shown that the anti-symmetric part of velocity gradient is non-objective and transforms like

$$
\Omega_{ip}^* = \mathcal{R}_{is} \mathcal{Q}_{sa} \mathcal{R}_{pa} + \mathcal{R}_{ik} \mathcal{R}_{ph},
$$

via the relation $\mathcal{R}_{ik} \mathcal{R}_{ph} = -\mathcal{R}_{pk} \mathcal{R}_{ik}$. Taking spatial gradients on both sides and multiplying by $Q_{pq}^*$, $\mathcal{Q}_{pq} = \mathcal{Q}_{pt} \mathcal{Q}_{tq}$ (Q is assumed to be objective), we have

$$
\Omega_{ip,k}^* Q_{pj}^* = \mathcal{R}_{is} \mathcal{R}_{pa} \mathcal{R}_{kb} \mathcal{R}_{pt} \mathcal{R}_{jq}(\mathcal{Q}_{sa,k} \mathcal{Q}_{tq}) \\
= \mathcal{Q}_{pt} \mathcal{Q}_{tq} \mathcal{R}_{jk}(\mathcal{Q}_{pt} \mathcal{Q}_{tq}),
$$

where we used the orthogonality $\mathcal{R}_{pa} \mathcal{R}_{pt} = \delta_{at}$ in the second step and relabeled the indices in the last one. This completes the proof.

Lemma 5. In the tensorial theory, by assuming that the entropy function $s(v, u, Q, \nabla Q, \sigma_V, \sigma_V, \pi_V, \pi_V, Q)$ is objective with respect to conserved variables, the tensor $[2Q_{tq}^* \mathcal{M}_{tq} + 2(\partial_t \mathcal{Q}_{tq}) \mathcal{M}_{tq} + \mathcal{Q}_{tq}^* \mathcal{M}_{tq}]$ must be symmetric, and its contraction with the anti-symmetric part of velocity gradient $\Omega$ vanishes.

Proof. As in Lemma 2, we choose arbitrary infinitesimal rotations with

$$
\mathcal{R}_{ij} = \delta_{ij} + \varepsilon_{ij}, \quad \varepsilon_{ji} = -\varepsilon_{ij}, \quad \varepsilon_{ij} \varepsilon_{kl} \approx 0,
$$

and denote variables under the motion $x^*(t) = \mathcal{R}(t)x(t) + c(t)$ by a starred symbol. Taking series expansion of $\varepsilon$ to
the first order, we have
\[ Q^*_{ij} = R_{ip} R_{jq} Q_{pq} = Q_{ij} + \varepsilon_{jq} Q_{iq} + \varepsilon_{ip} Q_{pq} + O(\varepsilon^2), \]
\[ Q^*_{ij,k} = R_{ip} R_{jq} R_{kr} Q_{pq,r} = Q_{ij,k} + \varepsilon_{kr} Q_{ij,r} + \varepsilon_{jq} Q_{iq,k} + \varepsilon_{ip} Q_{pjk} + O(\varepsilon^2). \]
Thus, we have approximately that
\[
0 = s(Q^*_{ij}, Q^*_{ij,k}, \cdots) - s(Q_{ij}, Q_{ij,k}, \cdots) \\
\approx \frac{\partial s}{\partial Q_{ij}} (Q^*_{ij} - Q_{ij}) + \frac{\partial s}{\partial Q_{ij,k}} (Q^*_{ij,k} - Q_{ij,k}) \\
= \frac{\partial s}{\partial Q_{ij}} (\varepsilon_{jq} Q_{iq} + \varepsilon_{ip} Q_{pq}) \\
+ \frac{\partial s}{\partial Q_{ij,k}} (\varepsilon_{kr} Q_{ij,r} + \varepsilon_{jq} Q_{iq,k} + \varepsilon_{ip} Q_{pjk}) \\
= \left[ 2Q_{ik} \frac{\partial s}{\partial Q_{jk}} + 2(\partial_k Q_{il}) \frac{\partial s}{\partial Q_{qkl}} \right] \varepsilon_{ji},
\]
where we used the symmetry of $Q_{ij} = Q_{ji}$ in the last step to relabel indices. Therefore, $[2Q_{ik} \frac{\partial s}{\partial Q_{jk}} + 2(\partial_k Q_{il}) \frac{\partial s}{\partial Q_{qkl}}]$ must be symmetric due to the arbitrariness of the anti-symmetric tensors $\varepsilon$. This completes the proof. \qed

Lemma 6. (A proof on the sufficient condition (41) for $epr 5' \geq 0$)

Proof. Assume $\bar{\alpha}_8 = 0, \bar{\alpha}_7 \geq 0$ and denote the residual terms
\[
epr 5' = \bar{\alpha}_4 |A|^2 + \mu_2 Y : A + (\bar{\alpha}_5 + \bar{\alpha}_6) P : A \\
+ \mu_1 |Y|^2 + \bar{\alpha}_1 |P|^2,
\]
as a quadratic form of tensors $A$, $Y$ and $P \equiv Q \cdot A$. Without loss of generality, we firstly choose $A$ as the principle element. By letting $\bar{\alpha}_4 \neq 0$, we have
\[
epr 5' = \bar{\alpha}_4 \left| A + \frac{\mu_2}{2\bar{\alpha}_4} Y + \frac{\bar{\alpha}_5 + \bar{\alpha}_6}{2\bar{\alpha}_4} P \right|^2 \\
+ \left( \mu_1 - \frac{\mu_2}{4\bar{\alpha}_4} \right) |Y|^2 - \frac{\mu_2(\bar{\alpha}_5 + \bar{\alpha}_6)}{4\bar{\alpha}_4} Y : P \\
+ \left( \bar{\alpha}_1 - \frac{(\bar{\alpha}_5 + \bar{\alpha}_6)^2}{4\bar{\alpha}_4} \right) |P|^2 \equiv I_1 + I_2,
\]
where the symmetry property of $A$ (or $Y$) was used to guarantee the commutativity of contractions, $P^T : A = P : A = A^T = P : A$ (or $Y : P^T = Y : P$). Supposing $4\mu_1 \bar{\alpha}_4 \neq \mu_2^2$, the second part of $epr 5'$ becomes
\[
I_2 = \left( \mu_1 - \frac{\mu_2^2}{4\bar{\alpha}_4} \right) |Y|^2 - \frac{\mu_2(\bar{\alpha}_5 + \bar{\alpha}_6)}{4\bar{\alpha}_4} Y : P \\
+ \left[ \bar{\alpha}_1 - \frac{(\bar{\alpha}_5 + \bar{\alpha}_6)^2}{4\bar{\alpha}_4} \right] |P|^2 \\
= \left( \frac{4\mu_1 \bar{\alpha}_4 - \mu_2^2}{4\bar{\alpha}_4} \right) |Y|^2 - \frac{\mu_2(\bar{\alpha}_5 + \bar{\alpha}_6)}{4\bar{\alpha}_4} Y : P \\
+ \left[ \frac{4\bar{\alpha}_1 \bar{\alpha}_4 - (\bar{\alpha}_5 + \bar{\alpha}_6)^2}{4\bar{\alpha}_4} - \frac{\mu_2^2(\bar{\alpha}_5 + \bar{\alpha}_6)^2}{4\bar{\alpha}_4(4\mu_1 \bar{\alpha}_4 - \mu_2^2)} \right] |P|^2 \\
\equiv I_{21} + I_{22}.
\]
Collecting the quadratic terms together, the constraint $epr 5' \geq 0$ yields that
\[
\bar{\alpha}_4 \geq 0, \quad 4\mu_1 \bar{\alpha}_4 - \mu_2^2 \geq 0, \quad \bar{\alpha}_1 \geq 0, \quad 4\bar{\alpha}_1 \bar{\alpha}_4 \mu_1 - \bar{\alpha}_1 \mu_2^2 - \mu_1 (\bar{\alpha}_5 + \bar{\alpha}_6)^2 \geq 0,
\]
from which one deduces that
\[
\bar{\alpha}_4 \geq 0, \quad 4\alpha_4 \mu_1 - \mu_2^2 \geq 0, \quad 4\bar{\alpha}_4 \mu_1 - \bar{\alpha}_1 \mu_2^2 - \mu_1 (\bar{\alpha}_5 + \bar{\alpha}_6)^2 \geq 0.
\]
Repeating above procedures, by choosing principal elements as $Y$ and $P$ separately, we obtain a complete sufficient condition for $epr 5 \geq 0$ as
\[
\bar{\alpha}_8 = 0, \quad \bar{\alpha}_7 \geq 0, \quad \bar{\alpha}_4 \geq 0, \quad \mu_1 \geq 0, \quad \bar{\alpha}_1 \geq 0, \quad 4\bar{\alpha}_4 \mu_1 - \mu_2^2 \geq 0, \quad 4\bar{\alpha}_4 \alpha_4 \mu_1 - \bar{\alpha}_1 \mu_2^2 - \mu_1 (\bar{\alpha}_5 + \bar{\alpha}_6)^2 \geq 0, \quad (A.9)
\]
\[
4\bar{\alpha}_4 \alpha_4 \mu_1 - \bar{\alpha}_1 \mu_2^2 - \mu_1 (\bar{\alpha}_5 + \bar{\alpha}_6)^2 \geq 0.
\]
This completes the proof. \qed

Appendix B. A brief discussion on the angular momentum conservation of liquid crystals

The conservation laws of mass, momentum, angular momentum and total energy play an important role in our mathematical modeling. However, unlike the mass, momentum and energy conservation laws, the conservation of angular momentum is not fully appreciated in the past studies.

In this section, we present a brief discussion on the angular momentum equations, and show that the evolution
equation of $w$ in (3) is a particular solution of the approximate equations for the angular momentum conservation. For nematic liquid crystals, the classical conservation law of the angular momentum takes the following local Eulerian form:

$$\frac{\partial}{\partial t}(pr \times v + \rho_1d \times w) + \nabla \cdot [v \otimes (pr \times v + \rho_1d \times w)] = r - \chi + \nabla \cdot (r \times \sigma + d \times \pi),$$  \tag{B.1}

where $\chi$ and $\pi$ are flow stress tensor and director surface torque, respectively. By applying the continuity equation, it becomes

$$\epsilon_{ijk} \left[ \rho \frac{d}{dt}(r_j v_k) + \rho_1 \frac{d}{dt}(d_j w_k) \right] - \epsilon_{ijk} r_j \chi_k = -\epsilon_{ijk} \partial_t (r_j \sigma_{lk} + d_j \pi_{lk}) = \epsilon_{ijk} (r_j \chi_k - \sigma_{lk} + r_j \sigma_{lk}) + \rho_1 d_j w_k - d_j \pi_{lk} = -d_j \pi_{lk} - \sigma_{jk} = \epsilon_{ijk} [d_j (\rho_1 w_k - \pi_{lk})] - (d_{j,l} \pi_{lk} + \sigma_{jk}) = 0,$$

in the Lagrangian form. Here we used $\epsilon_{ijk} v_j v_k = \epsilon_{ijk} w_j w_k = 0$ and $\epsilon_{ijk} v_j v_k v_k = \epsilon_{ijk} w_j w_k w_k = 0$ in the second step, as well as the momentum conservation in the third step. In the case when $\epsilon_{ijk} (d_j \pi_{lk} + \sigma_{jk})$ can be approximated by $\epsilon_{ijk} d_j g_k$ for a vector function $g$, one deduces that $\epsilon_{ijk} d_j (\rho_1 w_k - \pi_{lk}) - g_k = 0$. A particular solution of the approximate equation is given by

$$\rho_1 w_k - \pi_{lk} - g_k = 0,$$

which is also recognized as Oseen’s equation in the literature [7, 44]. In what follows, we show that this approach can also be extended to the tensorial theory and leads to a generalized hydrodynamic equation for liquid crystals. As to the tensorial theory for liquid crystals, the generalization conservation law of angular momentum becomes

$$\frac{\partial}{\partial t}(pr \times v + \rho_1 Q \times \dot{Q}) + \nabla \cdot [v \otimes (pr \times v + \rho_1 Q \times \dot{Q})] = r - \chi + \nabla \cdot (r \times \sigma + Q \times \pi),$$  \tag{B.2}

where $Q \times \dot{Q} = \epsilon_{ijk} Q_{jm} \pi_{km}$, $Q \times \pi = \epsilon_{ijk} Q_{jm} \pi_{km}$, the third-order tensor $\pi_{km}$ is the surface torque of liquid crystals. By substituting the mass and momentum conservation into (B.2), we obtain

$$\epsilon_{ijk} \left[ \rho \frac{d}{dt}(r_j v_k) + \rho_1 \frac{d}{dt}(Q_{jm} \dot{Q}_{km}) \right] - \epsilon_{ijk} r_j \chi_k = -\epsilon_{ijk} \partial_t (r_j \sigma_{lk} + Q_{jm} \pi_{km}) = \epsilon_{ijk} (r_j \chi_k - \sigma_{lk} + r_j \sigma_{lk}) + Q_{jm} \pi_{km,l} + Q_{jm} \pi_{km,l} = \epsilon_{ijk} r_j (\rho_1 w_k - \chi_k - r_j \pi_{lk}) + \epsilon_{ijk} (Q_{jm} \pi_{km} - \pi_{lk}) = -Q_{jm} \pi_{km,l} - Q_{jm} \pi_{km,l} - \sigma_{jk} = \epsilon_{ijk} \dot{Q}_{jm} (\rho_1 \pi_{km} - \pi_{lm,k}) - \epsilon_{ijk} (Q_{jm} \pi_{lk} + \sigma_{jk}) = 0,$$

where the formula $\rho_1 \dot{w}_k = \chi_k + \sigma_{jk,l}$ was used in the third step. By making a similar approximation that $\epsilon_{ijk} (Q_{jm} \pi_{km} + \sigma_{jk}) = \epsilon_{ijk} Q_{jm} g_{km}$, we have $\epsilon_{ijk} Q_{jm} \pi_{km} - \pi_{km,l} = 0$, where the second-order tensor $(g + \nabla \times \pi)$ is also known as the molecular field of liquid crystals. A particular class of solutions is

$$\rho_1 \hat{Q}_{km} = g_{km} + \partial_t (\pi_{km,l}),$$  \tag{B.3}

which has been employed in eq. (35) as the starting point of our derivation. Clearly, eq. (B.3) is different from the one used by Qian and Sheng [20], in which only the body torque $g$ (or molecular field $h$ in eq. (3) in ref. [20]) is included, while the surface torque $\pi$ is neglected without justification.

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