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Modelling of Nematic Liquid Crystals in Electromagnetic Fields

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Abstract

The paper elaborates a dynamic scheme which accounts for the evolution of nematic liquid crystals. The liquid crystal is allowed to be compressible and subject to the action of mechanical and electromagnetic forces. The temperature is also involved and is allowed to vary in space and time. The equation of macroscopic motion and the evolution equation for the degree of orientation, the director and the temperature are derived. The approach is developed within a thermodynamic framework by regarding the degree of orientation and the director as internal variables. This implies that the evolution functions follow as a consequence of the requirements placed by thermodynamics and without any appeal to ad-hoc balance equations.

Keywords: Nematics, degree of orientation, evolution equation, electromagnetic field

1 Introduction

Nematic liquid crystals are aggregates of molecules which possess orientational order and are made of elongated, rod-like molecules or of disc-like molecules which share the common property that the central ellipsoid of inertia is a spheroid [4, 3]. The orientation of a single nematic molecule may then be represented by a unit vector $\mathbf{n}$, called tghe director, parallel to the axis of rotational symmetry of the spheroid. Most molecules possess an head-and-tail symmetry, which means that $\mathbf{n}$ and $-\mathbf{n}$ describe the same physical state. Other molecules, instead, are not invariant under the transformation $\mathbf{n} \to -\mathbf{n}$.

The aggregate of nematic molecules may become isotropic, which corresponds to the complete absence of order. We then need a degree of orientation, s [5]. We let $s \in [0, 1]$ and say that $s = 0$ corresponds to the isotropic configuration, $s = 1$ to the nematic configuration, where all molecules have the same orientation.

The purpose of this paper is to elaborate a dynamic scheme accounting for the evolution of the nematic liquid, which is allowed to be compressible, under the action of mechanical and electromagnetic forces. The temperature θ is also involved and the objective is to determine the equation of macroscopic motion and the evolution equation for $s, \mathbf{n}, \theta$. This purpose is realized by means of a systematic thermodynamic framework where s, $\mathbf{n}$ and the time derivative of $\mathbf{n}$ are regarded as internal variables. This implies that the evolution functions follow as a consequence of the requirements placed by thermodynamics. The head-and-tail symmetry is modelled by the dependence on $\mathbf{n}$ through the dyadic product $\mathbf{n} \otimes \mathbf{n}$. The absence of symmetry is accounted by a direct dependence on $\mathbf{n}$. Both schemes are established and the main consequences are derived. A brief analysis is also given of the generalizations and differences relative to relevant papers on the dynamics of nematic liquid crystals.

2 Electromagnetism and balance equations

2.1 Maxwell's equations in media

Let $\Omega \subseteq \mathbb{R}^3$ be the (possibly time-dependent) region occupied by the body. The fields considered throughout have $\Omega \times \mathbb{R}$ as their common space-time domain.

Let $\mathbf{E}$ be the electric field, $\mathbf{B}$ the magnetic induction, $\mathbf{D}$ the electric displacement and $\mathbf{H}$ the magnetic field. Also, let ϱ be the charge density, $\mathbf{J}$ the electric current density, $\mathbf{v}$ the velocity field. The magnetization $\mathbf{M}$ and the polarization $\mathbf{P}$ are defined by

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}, \qquad \mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}).$$

Under Galilean transformations $\mathbf{P}$ is invariant as well as the Lorentz magnetization $\boldsymbol{\mathcal{M}} = \mathbf{M} + \mathbf{v} \times \mathbf{P}$. Further, $\boldsymbol{\mathcal{J}} = \mathbf{J} - \varrho\mathbf{v}$, $\boldsymbol{\mathcal{H}} = \mathbf{H} - \mathbf{v} \times \mathbf{D}$, $\boldsymbol{\mathcal{E}} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$ are invariant.

The superposed dot denotes the material time derivative and ∇ is the gradient operator. Hence, for any vector field $\mathbf{w}$ on $\Omega \times \mathbb{R}$, we have

$$\dot{\mathbf{w}} = \partial_t \mathbf{w} + (\mathbf{v} \cdot \nabla)\mathbf{w}.$$

We denote by $\overset{*}{\mathbf{w}}$ the flux derivative (or convected time derivative) of $\mathbf{w}$,

$$\overset{*}{\mathbf{w}} = \dot{\mathbf{w}} + \mathbf{w}\nabla \cdot \mathbf{v} - (\mathbf{w} \cdot \nabla)\mathbf{v}. \tag{2.1}$$

Maxwell's equations can then be written in the form

$$\nabla \times \boldsymbol{\mathcal{E}} = -\overset{*}{\mathbf{B}}, \qquad \nabla \times \boldsymbol{\mathcal{H}} = \overset{*}{\mathbf{D}} + \boldsymbol{\mathcal{J}}, \tag{2.2}$$

$$\nabla \cdot \mathbf{B} = 0, \qquad \nabla \cdot \mathbf{D} = \varrho. \tag{2.3}$$

The continuity condition for charge takes the form

$$\partial_t \varrho + \nabla \cdot \boldsymbol{\mathcal{J}} = 0. \tag{2.4}$$

For later convenience, we consider the Poynting vector $\boldsymbol{\mathcal{E}} \times \boldsymbol{\mathcal{H}}$ and say that, by means of (2.2), we have

$$\nabla \cdot (\boldsymbol{\mathcal{E}} \times \boldsymbol{\mathcal{H}}) = -\boldsymbol{\mathcal{H}} \cdot \overset{*}{\mathbf{B}} - \boldsymbol{\mathcal{E}} \cdot \overset{*}{\mathbf{D}} - \boldsymbol{\mathcal{E}} \cdot \boldsymbol{\mathcal{J}}. \tag{2.5}$$

2.2 Balance equations

The liquid crystal is allowed to be compressible. The mass density ρ and the velocity $\mathbf{v}$ satisfy the continuity equation

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0, \tag{2.6}$$

at any posizion $\mathbf{x} \in \Omega$ and time $t \in \mathbb{R}$. Let $\mathbf{L}$ be the velocity gradient, in components $L_{ij} = \partial v_i / \partial x_j$, $i, j = 1, 2, 3$. Substitution of $\nabla \cdot \mathbf{v}$ from (2.6) in (2.1) gives

$$\overset{*}{\mathbf{w}} = \rho \, \dot{\overline{\mathbf{w}/\rho}} - \mathbf{L}\mathbf{w}. \tag{2.7}$$

Let $\mathbf{T}$ denote the stress tensor and $\mathbf{b}$ the body force (per unit volume). Both $\mathbf{T}$ and $\mathbf{b}$ may account also for electromagnetic effects. For instance, $\mathbf{b}$ comprises the Lorentz force $\varrho \boldsymbol{\mathcal{E}} = \varrho(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. The balance of linear momentum is written in the form

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \mathbf{b}. \tag{2.8}$$

Owing to the internal structure and the occurrence of electromagnetic fields we let $\mathbf{T}$ be non-symmetric.

The internal energy density (per unit mass), e, is allowed to include rotational kinetic energy associated with the motion of $\mathbf{n}$. Denote by $\mathbf{q}$ the heat flux vector and by r the heat supply (per unit volume). For any region $\mathcal{P} \subset \Omega$, moving with the body, we express the balance of energy in the form

$$\frac{d}{dt} \int_{\mathcal{P}} \rho (e + \frac{1}{2} \mathbf{v}^2) dv = \int_{\partial \mathcal{P}} (\mathbf{v}\mathbf{T} - \boldsymbol{\mathcal{E}} \times \boldsymbol{\mathcal{H}} - \mathbf{q}) \cdot \boldsymbol{\nu} \, da + \int_{\mathcal{P}} (\mathbf{b} \cdot \mathbf{v} + r) dv.$$

Because of (2.8) and of the arbitrariness of $\mathcal{P}$ we find the differential form of the energy balance as

$$\rho \dot{e} = \mathbf{T} \cdot \mathbf{L} - \nabla \cdot (\boldsymbol{\mathcal{E}} \times \boldsymbol{\mathcal{H}} + \mathbf{q}) + r. \tag{2.9}$$

Replacing $\nabla \cdot \boldsymbol{\mathcal{E}} \times \boldsymbol{\mathcal{H}}$ from (2.5) and applying (2.7) to $\mathbf{B}$ and $\mathbf{D}$ allow (2.9) to be written

$$\rho \dot{e} = \mathbf{T} \cdot \mathbf{L} - \nabla \cdot \mathbf{q} + r + \rho \boldsymbol{\mathcal{H}} \cdot \dot{\overline{\mathbf{B}/\rho}} + \rho \boldsymbol{\mathcal{E}} \cdot \dot{\overline{\mathbf{D}/\rho}} - (\boldsymbol{\mathcal{H}} \otimes \mathbf{B} + \boldsymbol{\mathcal{E}} \otimes \mathbf{D}) \cdot \mathbf{L} + \boldsymbol{\mathcal{E}} \cdot \boldsymbol{\mathcal{J}}. \tag{2.10}$$

Let η be the entropy density and θ the absolute temperature. The entropy flux need not equal $\mathbf{q}/\theta$. Hence we write the entropy inequality as

$$\rho \dot{\eta} \geq \frac{r}{\theta} - \nabla \cdot (\mathbf{k} + \mathbf{q}/\theta) \tag{2.11}$$

so that $\mathbf{k}$ can be viewed as the extra-entropy flux.

Statement of the second law. *The inequality (2.11) has to hold for any set of functions compatible with the Maxwell equations (2.2)-(2.3), the continuity equation for charge (2.4) and the balance equations (2.6), (2.8), (2.10).*

Substitution of $r - \nabla \cdot \mathbf{q}$ from (2.10) provides

$$\rho(\dot{e} - \theta \dot{\eta}) - \rho \boldsymbol{\mathcal{H}} \cdot \dot{\overline{\mathbf{B}/\rho}} - \rho \boldsymbol{\mathcal{E}} \cdot \dot{\overline{\mathbf{D}/\rho}}$$

$$-(\mathbf{T} - \boldsymbol{\mathcal{H}} \otimes \mathbf{B} - \boldsymbol{\mathcal{E}} \otimes \mathbf{D}) \cdot \mathbf{L} - \boldsymbol{\mathcal{E}} \cdot \boldsymbol{\mathcal{J}} + \frac{1}{\theta} \mathbf{q} \cdot \nabla \theta - \theta \nabla \cdot \mathbf{k} \leq 0.$$

Hence, by means of the free enthalpy density ζ, defined by

$$\rho \zeta = \rho e - \rho \theta \eta - \boldsymbol{\mathcal{H}} \cdot \mathbf{B} - \boldsymbol{\mathcal{E}} \cdot \mathbf{D},$$

we obtain

$$-\rho(\dot{\zeta} + \eta \dot{\theta}) - \mathbf{B} \cdot \dot{\boldsymbol{\mathcal{H}}} - \mathbf{D} \cdot \dot{\boldsymbol{\mathcal{E}}}$$

$$+(\mathbf{T} - \boldsymbol{\mathcal{H}} \otimes \mathbf{B} - \boldsymbol{\mathcal{E}} \otimes \mathbf{D}) \cdot \mathbf{L} + \boldsymbol{\mathcal{E}} \cdot \boldsymbol{\mathcal{J}} - \frac{1}{\theta} \mathbf{q} \cdot \nabla \theta + \theta \nabla \cdot \mathbf{k} \geq 0. \tag{2.12}$$

Some comments are in order. The literature shows various forms of balance laws in electromagnetic deformable media (see, e.g., [6] and refs therein). The present scheme is akin to that of [10] except for the linear momentum density which here is taken in the classical form $\rho \mathbf{v}$ while [10] replaces $\mathbf{v}$ with an undetermined function $\mathbf{g}$. Ericksen's theory [5] assumes that the fluid is incompressible, in which case ρ is constant and $\nabla \cdot \mathbf{v} = 0$.

3 Constitutive equations

Let $\zeta, \eta, \mathbf{B}, \mathbf{D}, \boldsymbol{\mathcal{J}}, \mathbf{q}, \mathbf{k}$ and $\dot{s}, \ddot{\mathbf{N}}$ be given by (constitutive) functions of the set of variables

$$\Gamma_0 = (\theta, \rho, \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{H}}, s, \mathbf{N}, \nabla\theta, \nabla s, \nabla\mathbf{N}, \dot{\mathbf{N}}).$$

The dependence on $\dot{\mathbf{N}}$ is motivated by the fact that e, and hence possibly ζ and η, is allowed to include rotational kinetic energy associated with the motion of $\mathbf{n}$. The vector quantities $\boldsymbol{\mathcal{J}}, \mathbf{q}, \mathbf{k}$ and the time derivatives $\dot{s}, \ddot{\mathbf{N}}$ are allowed to depend also on the higher-order gradients $\nabla\nabla\theta, \nabla\nabla s, \nabla\nabla\mathbf{N}$ and let

$$\Gamma = (\theta, \rho, \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{H}}, s, \mathbf{N}, \nabla\theta, \nabla\rho, \nabla s, \nabla\mathbf{N}, \dot{\mathbf{N}}, \mathbf{L}, \nabla\nabla\theta, \nabla\nabla s, \nabla\nabla\mathbf{N}, \nabla\dot{\mathbf{N}}).$$

We denote by $\mathcal{S}$ and $\boldsymbol{\mathcal{N}}$ the constitutive functions for $\dot{s}$ and $\ddot{\mathbf{N}}$, namely

$$\dot{s} = \mathcal{S}(\Gamma), \qquad \ddot{\mathbf{N}} = \boldsymbol{\mathcal{N}}(\Gamma).$$

No restriction is placed on the constitutive functions $\mathbf{B}, \mathbf{D}, \boldsymbol{\mathcal{J}}$ by (2.2)-(2.3) and (2.4). Such equations hold for any functions $\mathbf{B}, \mathbf{D}, \boldsymbol{\mathcal{J}}$ by letting $\nabla\boldsymbol{\mathcal{E}}, \nabla\boldsymbol{\mathcal{H}}$ and ϱ satisfy them. Also the balance of energy (2.10) holds for any value of $\dot{e}$ by simply letting r be appropriate. As a consequence, we can say that Γ and $\dot{\theta}, \dot{\boldsymbol{\mathcal{E}}}, \dot{\boldsymbol{\mathcal{H}}}, \nabla\dot{\theta}$ can be chosen arbitrarily and meanwhile the balance equations hold.

Upon application of the chain rule to $\zeta(\Gamma_0)$ and use of (2.6), (2.12) can be written

$$\begin{aligned}\rho(\zeta_\theta + \eta)\dot{\theta} + (\rho\zeta_{\boldsymbol{\mathcal{E}}} + \mathbf{D}) \cdot \dot{\boldsymbol{\mathcal{E}}} + (\rho\zeta_{\boldsymbol{\mathcal{H}}} + \mathbf{B}) \cdot \dot{\boldsymbol{\mathcal{H}}} + \rho\zeta_s\mathcal{S} + \zeta_{\mathbf{N}} \cdot \dot{\mathbf{N}} + \rho\zeta_{\nabla\theta} \cdot \overline{\nabla\theta}^{\cdot} \\ +\rho\zeta_{\nabla s} \cdot \overline{\nabla s}^{\cdot} + \rho\zeta_{\nabla\mathbf{N}} \cdot \overline{\nabla\mathbf{N}}^{\cdot} + \rho\zeta_{\dot{\mathbf{N}}} \cdot \boldsymbol{\mathcal{N}} - (\mathbf{T} + \rho^2\zeta_\rho\mathbf{1} - \boldsymbol{\mathcal{H}} \otimes \mathbf{B} - \boldsymbol{\mathcal{E}} \otimes \mathbf{D}) \cdot \mathbf{L} \\ -\boldsymbol{\mathcal{J}} \cdot \boldsymbol{\mathcal{E}} + \frac{1}{\theta}\mathbf{q} \cdot \nabla\theta - \theta\nabla \cdot \mathbf{k} \le 0. \qquad (3.1)\end{aligned}$$

The arbitrariness of $\dot{\theta}, \dot{\boldsymbol{\mathcal{E}}}, \dot{\boldsymbol{\mathcal{H}}}, \overline{\nabla\theta}^{\cdot}$ implies that (3.1) holds only if

$$\eta = -\zeta_\theta, \qquad \mathbf{D} = -\rho\zeta_{\boldsymbol{\mathcal{E}}}, \qquad \mathbf{B} = -\rho\zeta_{\boldsymbol{\mathcal{H}}}, \qquad \zeta_{\nabla\theta} = 0. \qquad (3.2)$$

For any scalar or tensor quantity ϕ we have

$$\overline{\nabla\phi}^{\cdot} = \nabla\dot{\phi} - \mathbf{L}^T\nabla\phi.$$

Hence

$$\zeta_{\nabla s} \cdot \overline{\nabla s}^{\cdot} = \nabla \cdot (\zeta_{\nabla s}\dot{s}) - \dot{s}\nabla \cdot \zeta_{\nabla s} - (\nabla s \otimes \zeta_{\nabla s}) \cdot \mathbf{L},$$

$$\zeta_{\nabla\mathbf{N}} \cdot \overline{\nabla\mathbf{N}}^{\cdot} = \nabla \cdot (\zeta_{\nabla\mathbf{N}}\dot{\mathbf{N}}) - \dot{\mathbf{N}}\nabla \cdot \zeta_{\nabla\mathbf{N}} - \boldsymbol{\Xi} \cdot \mathbf{L},$$

where $\boldsymbol{\Xi}$ is a second-order tensor which in components has the form $\Xi_{hk} = N_{ij,h}\zeta_{N_{ij,k}}$. Let

$$\boldsymbol{\mathcal{T}} := \mathbf{T} + \rho^2\zeta_\rho \mathbf{1} - \boldsymbol{\mathcal{H}} \otimes \mathbf{B} - \boldsymbol{\mathcal{E}} \otimes \mathbf{D} + \nabla s \otimes \zeta_{\nabla s} + \boldsymbol{\Xi}.$$

Upon some rearrangements, (3.1) can be written

$$\begin{aligned}(\rho\zeta_s - \nabla\cdot\rho\zeta_{\nabla s})\,\mathcal{S} + (\rho\zeta_{\mathbf{N}} - \nabla\cdot\rho\zeta_{\nabla\mathbf{N}})\cdot\dot{\mathbf{N}} + \rho\zeta_{\dot{\mathbf{N}}}\cdot\boldsymbol{\mathcal{N}} - \boldsymbol{\mathcal{T}}\cdot\mathbf{L} \\ +\nabla\cdot(\rho\zeta_{\nabla s}\dot{s} + \rho\zeta_{\nabla\mathbf{N}}\dot{\mathbf{N}} - \theta\mathbf{k}) - \boldsymbol{\mathcal{J}}\cdot\boldsymbol{\mathcal{E}} + \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta + \mathbf{k}\cdot\nabla\theta \le 0. \qquad (3.3)\end{aligned}$$

Also by analogy with similar contexts [7, 8], the linear dependence on the time derivative of the internal variables suggests that we let

$$\theta\mathbf{k} = \rho\zeta_{\nabla s}\dot{s} + \rho\zeta_{\nabla\mathbf{N}}\dot{\mathbf{N}}. \qquad (3.4)$$

As a consequence we have

$$\begin{aligned}(\rho\zeta_s - \nabla\cdot\rho\zeta_{\nabla s})\,\mathcal{S} + (\rho\zeta_{\mathbf{N}} - \nabla\cdot\rho\zeta_{\nabla\mathbf{N}})\cdot\dot{\mathbf{N}} + \mathbf{k}\cdot\nabla\theta \\ = (\rho\zeta_s - \theta\nabla\cdot\frac{\rho\zeta_{\nabla s}}{\theta})\,\mathcal{S} + (\rho\zeta_{\mathbf{N}} - \theta\nabla\cdot\frac{\rho\zeta_{\nabla\mathbf{N}}}{\theta})\cdot\dot{\mathbf{N}}.\end{aligned}$$

Hence, letting

$$\breve{\zeta} = \frac{\rho\zeta}{\theta}, \qquad \delta_s\zeta := \theta(\breve{\zeta}_s - \nabla\cdot\breve{\zeta}_{\nabla s}), \qquad \delta_{\mathbf{N}}\zeta := \theta(\breve{\zeta}_{\mathbf{N}} - \nabla\cdot\breve{\zeta}_{\nabla\mathbf{N}}),$$

we can write (3.3) in the form

$$\delta_s\zeta\,\mathcal{S} + \delta_{\mathbf{N}}\zeta\cdot\dot{\mathbf{N}} + \zeta_{\dot{\mathbf{N}}}\cdot\boldsymbol{\mathcal{N}} - \boldsymbol{\mathcal{T}}\cdot\mathbf{L} - \boldsymbol{\mathcal{J}}\cdot\boldsymbol{\mathcal{E}} + \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta \le 0. \qquad (3.5)$$

The inequality (3.5) holds if

$$\delta_s\zeta\,\mathcal{S} \le 0, \qquad (3.6)$$

$$\delta_{\mathbf{N}}\zeta\cdot\dot{\mathbf{N}} + \zeta_{\dot{\mathbf{N}}}\cdot\boldsymbol{\mathcal{N}} = -\beta\dot{\mathbf{N}}^2, \qquad (3.7)$$

$$\boldsymbol{\mathcal{T}}\cdot\mathbf{L} + \boldsymbol{\mathcal{J}}\cdot\boldsymbol{\mathcal{E}} - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta \ge 0. \qquad (3.8)$$

We can summarize the results so obtained as follows.

Proposition 1. *The constitutive functions $\zeta, \eta, \mathbf{B}, \mathbf{D}, \boldsymbol{\mathcal{T}}, \boldsymbol{\mathcal{J}}, \mathbf{q}, \mathbf{k}, \mathcal{S}, \boldsymbol{\mathcal{N}}$ satisfy the second law of thermodynamics if (3.2), (3.4), (3.6), (3.7) and (3.8) hold.*

4 Evolution equations

We now look for simple constitutive equations which satisfy the thermodynamic restrictions (3.6)-(3.8).

4.1 Evolution of s

The inequality (3.6) holds if and only if

$$\dot{s} = -\alpha(\Gamma)\delta_s\zeta, \qquad \alpha \geq 0. \tag{4.1}$$

Equation (4.1) governs the evolution of s. If, e.g.,

$$\rho\zeta = \rho\tilde{\zeta} + \frac{1}{2}\kappa(\rho,\theta)|\nabla s|^2,$$

where $\tilde{\zeta}$ is independent of ∇s, then (4.1) becomes

$$\dot{s} = -\alpha[\rho\tilde{\zeta}_s - \kappa\Delta s - \theta\nabla s \cdot \nabla\frac{\kappa(\rho,\theta)}{\theta}].$$

4.2 Evolution of $\mathbf{N}$

To exploit the inequality (3.7) we restrict attention to the case

$$\rho\zeta = \Phi(\hat{\Gamma}) + \frac{1}{2}\sigma(\hat{\Gamma})\dot{\mathbf{N}}^2, \qquad \sigma > 0,$$

where $\hat{\Gamma}$ equals Γ deprived of $\dot{\mathbf{N}}$, which amounts to regarding $\sigma(\hat{\Gamma})\dot{\mathbf{N}}^2/2$ as an additive kinetic energy associated with the time dependence of $\mathbf{N}$. Hence we have $\rho\zeta_{\dot{\mathbf{N}}} = \sigma\dot{\mathbf{N}}$ and (3.7) becomes

$$(\delta_{\mathbf{N}}\zeta + \sigma\boldsymbol{\mathcal{N}} + \beta\dot{\mathbf{N}}) \cdot \dot{\mathbf{N}} = 0. \tag{4.2}$$

Because

$$\dot{\mathbf{N}} = \dot{\mathbf{n}} \otimes \mathbf{n} + \mathbf{n} \otimes \dot{\mathbf{n}}$$

and hence

$$\dot{\mathbf{N}} = \dot{\mathbf{N}}^T, \quad \mathrm{tr}\,\dot{\mathbf{N}} = 0, \quad \mathbf{N} \cdot \dot{\mathbf{N}} = 0,$$

eq. (4.2) holds if and only if

$$\sigma\ddot{\mathbf{N}} = -\beta\dot{\mathbf{N}} - \delta_{\mathbf{N}}\zeta + \gamma\mathbf{1} + \nu\mathbf{N} + \boldsymbol{\Omega}, \tag{4.3}$$

where γ and ν are arbitrary scalars while $\boldsymbol{\Omega}$ is a skew-symmetric tensor. We may regard β, γ, ν as functions of $\hat{\Gamma}$.

Since

$$\ddot{\mathbf{N}} = \ddot{\mathbf{n}} \otimes \mathbf{n} + 2\dot{\mathbf{n}} \otimes \dot{\mathbf{n}} + \mathbf{n} \otimes \ddot{\mathbf{n}},$$

it follows that

$$\mathrm{tr}\,\ddot{\mathbf{N}} = 2(\ddot{\mathbf{n}} \cdot \mathbf{n} + |\dot{\mathbf{n}}|^2) = 2\overline{\mathbf{n} \cdot \dot{\mathbf{n}}}^{\,\cdot} = 0$$

whereas $\mathrm{tr}\,\mathbf{N} = 1$. Hence applying the trace operator to (4.3) we obtain

$$-\mathrm{tr}\,\delta_{\mathbf{N}}\zeta + 3\gamma + \nu = 0.$$

In addition, the symmetry of $\mathbf{N}, \dot{\mathbf{N}}, \ddot{\mathbf{N}}$ implies that $\boldsymbol{\Omega}$ must be zero. As a consequence, we can replace γ in (4.3) to obtain the evolution equation for $\mathbf{N}$ in the form

$$\sigma\ddot{\mathbf{N}} = -\beta\dot{\mathbf{N}} - \mathrm{dev}\delta_{\mathbf{N}}\zeta + \nu\mathrm{dev}\mathbf{N}. \tag{4.4}$$

An interesting consequence of (4.4) follows by taking the inner product with $\dot{\mathbf{N}}$. Since $\mathrm{tr}\,\dot{\mathbf{N}} = 0$, for any tensor $\mathbf{A}$

$$(\mathrm{dev}\mathbf{A}) \cdot \dot{\mathbf{N}} = \mathbf{A} \cdot \dot{\mathbf{N}}, \qquad (\mathrm{dev}\mathbf{N}) \cdot \dot{\mathbf{N}} = \mathbf{N} \cdot \dot{\mathbf{N}} = 0.$$

Also, $\boldsymbol{\Omega} \cdot \dot{\mathbf{N}} = 0$. As a consequence the inner product of (4.4) with $\dot{\mathbf{N}}$ gives

$$\frac{1}{2}\sigma\frac{d}{dt}|\dot{\mathbf{N}}|^2 = -\beta|\dot{\mathbf{N}}|^2 - \delta_{\mathbf{N}}\zeta \cdot \dot{\mathbf{N}}. \tag{4.5}$$

As a comment on (4.5), since $\beta/\sigma \geq 0$, the (generalized) force $-\beta\dot{\mathbf{N}}$ in (4.4) may be viewed as a friction term which makes $|\dot{\mathbf{N}}|^2$ to decay in time. The term $-\delta_{\mathbf{N}}\zeta \cdot \dot{\mathbf{N}}$ may be viewed as the power of the external fields, accounted by ζ, on $\mathbf{N}$. In this sense, $\mathrm{dev}\mathbf{N}$ is a force which does no work on $\mathbf{N}$.

4.3 Evolution of n

Applying $\ddot{\mathbf{N}}, \dot{\mathbf{N}}, \mathrm{dev}\mathbf{N}$ to $\mathbf{n}$ provides

$$\ddot{\mathbf{N}}\mathbf{n} = \ddot{\mathbf{n}} - |\dot{\mathbf{n}}|^2\mathbf{n}, \qquad \dot{\mathbf{N}}\mathbf{n} = \dot{\mathbf{n}}, \qquad \mathrm{dev}\mathbf{N}\,\mathbf{n} = \frac{2}{3}\mathbf{n}.$$

Hence applying (4.4) to $\mathbf{n}$ gives

$$\sigma(\ddot{\mathbf{n}} - |\dot{\mathbf{n}}|^2\mathbf{n}) = -\beta\dot{\mathbf{n}} - (\mathrm{dev}\delta_{\mathbf{N}}\zeta)\mathbf{n} + \frac{2\nu}{3}\mathbf{n}.$$

Since

$$\mathrm{dev}\delta_{\mathbf{N}}\zeta = \delta_{\mathbf{N}}\zeta - \frac{1}{3}(\mathrm{tr}\,\delta_{\mathbf{N}}\zeta)\mathbf{1} = \delta_{\mathbf{N}}\zeta - (\gamma + \frac{\nu}{3})\mathbf{1}$$

we have

$$\sigma(\ddot{\mathbf{n}} - |\dot{\mathbf{n}}|^2\mathbf{n}) = -\beta\dot{\mathbf{n}} - (\delta_{\mathbf{N}}\zeta)\mathbf{n} + (\gamma + \nu)\mathbf{n}. \tag{4.6}$$

Due to the simultaneous occurrence of $\sigma|\dot{\mathbf{n}}|^2\mathbf{n}$ and $(\gamma + \nu)\mathbf{n}$, inner multiply (4.6) by $\mathbf{n}$ to obtain

$$-2\sigma|\dot{\mathbf{n}}|^2 = -\mathbf{n} \cdot \delta_{\mathbf{N}}\zeta\, \mathbf{n} + \gamma + \nu.$$

Substitution of $\gamma + \nu$ in (4.6) gives

$$\sigma(\ddot{\mathbf{n}} + |\dot{\mathbf{n}}|^2\mathbf{n}) = -\beta\dot{\mathbf{n}} - [\delta_{\mathbf{N}}\zeta - (\mathbf{n} \cdot \delta_{\mathbf{N}}\zeta\, \mathbf{n})\mathbf{1}]\mathbf{n}. \tag{4.7}$$

Equation (4.7) governs the time evolution of $\mathbf{n}$. The inner product with $\dot{\mathbf{n}}$ provides the evolution of $|\dot{\mathbf{n}}|^2$. Hence, inner multiply (4.7) by $\dot{\mathbf{n}}$ and use the identity

$$\ddot{\mathbf{n}} \cdot \dot{\mathbf{n}} = \frac{1}{2}\frac{d}{dt}|\dot{\mathbf{n}}|^2$$

to obtain

$$\frac{1}{2}\frac{d}{dt}|\dot{\mathbf{n}}|^2 = -\beta|\dot{\mathbf{n}}|^2 - \dot{\mathbf{n}} \cdot \delta_{\mathbf{N}}\zeta\, \mathbf{n}. \tag{4.8}$$

Quite analogously with (4.5), the β-term results in a decay of $|\dot{\mathbf{n}}|^2$ whereas $-\dot{\mathbf{n}} \cdot \delta_{\mathbf{N}}\zeta\, \mathbf{n}$ may be viewed as the appropriate power on $\mathbf{n}$ due to the fields described by ζ.

4.4 Temperature evolution

To derive the evolution equation of the temperature we go back to the energy balance. Let

$$\phi = \zeta - \theta\zeta_\theta.$$

Hence we have

$$\dot{e} = \dot{\phi} + \dot{\boldsymbol{\mathcal{E}}} \cdot \mathbf{D}/\rho + \boldsymbol{\mathcal{E}} \cdot \dot{\overline{\mathbf{D}/\rho}} + \dot{\boldsymbol{\mathcal{H}}} \cdot \mathbf{B}/\rho + \boldsymbol{\mathcal{H}} \cdot \dot{\overline{\mathbf{B}/\rho}}.$$

Look at $\rho\dot{e} - \rho\boldsymbol{\mathcal{E}} \cdot \dot{\overline{\mathbf{D}/\rho}} - \rho\boldsymbol{\mathcal{H}} \cdot \dot{\overline{\mathbf{B}/\rho}}$. By means of (2.10) we obtain

$$\rho\dot{\phi} + \mathbf{D} \cdot \dot{\boldsymbol{\mathcal{E}}} + \mathbf{B} \cdot \dot{\boldsymbol{\mathcal{H}}} = (\mathbf{T} - \boldsymbol{\mathcal{H}} \otimes \mathbf{B} - \boldsymbol{\mathcal{E}} \otimes \mathbf{D}) \cdot \mathbf{L} - \nabla \cdot \mathbf{q} + r + \boldsymbol{\mathcal{E}} \cdot \boldsymbol{\mathcal{J}}. \tag{4.9}$$

Time differentiation of ϕ and use of (3.2) give

$$\rho\dot{\phi} + \mathbf{D} \cdot \dot{\boldsymbol{\mathcal{E}}} + \mathbf{B} \cdot \dot{\boldsymbol{\mathcal{H}}} = -\rho\zeta_{\theta\theta}\dot{\theta} + \rho\phi_\rho\dot{\rho} - \rho\theta\zeta_{\theta\boldsymbol{\mathcal{E}}} \cdot \dot{\boldsymbol{\mathcal{E}}} - \rho\theta\zeta_{\theta\boldsymbol{\mathcal{H}}} \cdot \dot{\boldsymbol{\mathcal{H}}}$$
$$+\rho\phi_s\dot{s} + \rho\phi_{\mathbf{N}} \cdot \dot{\mathbf{N}} + \rho\phi_{\nabla s} \cdot \dot{\overline{\nabla s}} + \rho\phi_{\nabla\mathbf{N}} \cdot \dot{\overline{\nabla\mathbf{N}}} + \rho\phi_{\dot{\mathbf{N}}} \cdot \ddot{\mathbf{N}}.$$

Substitution in (4.9), use of (2.6) and some rearrangements provide

$$\begin{aligned}\rho\zeta_{\theta\theta}\dot{\theta} = -\rho\theta\zeta_{\theta\boldsymbol{\mathcal{E}}}\cdot\dot{\boldsymbol{\mathcal{E}}} - \rho\theta\zeta_{\theta\boldsymbol{\mathcal{H}}}\cdot\dot{\boldsymbol{\mathcal{H}}} + \rho\phi_s\dot{s} + \rho\phi_{\mathbf{N}}\cdot\dot{\mathbf{N}}\\ +\rho\phi_{\nabla s}\cdot\nabla\dot{s} + \rho\phi_{\nabla\mathbf{N}}\cdot\nabla\dot{\mathbf{N}} + \rho\phi_{\dot{\mathbf{N}}}\cdot\ddot{\mathbf{N}} - \tilde{\mathbf{T}} + \nabla\cdot\mathbf{q} - r - \boldsymbol{\mathcal{E}}\cdot\boldsymbol{\mathcal{J}},\end{aligned} \tag{4.10}$$

where

$$\tilde{\mathbf{T}} = \mathbf{T} + \rho^2\phi_\rho\mathbf{1} - \boldsymbol{\mathcal{H}}\otimes\mathbf{B} - \boldsymbol{\mathcal{E}}\otimes\mathbf{D} + \rho\nabla s\otimes\phi_{\nabla s} + \rho\tilde{\boldsymbol{\Xi}}$$

and $\tilde{\Xi}_{jk} = \rho N_{pq,j}\phi_{N_{pq,k}}$.

4.5 First-order system

The whole set of evolution equations may be written as a first-order system. Let

$$f = -\tilde{\mathbf{T}}\cdot\mathbf{L} + \nabla\cdot\mathbf{q} - r - \boldsymbol{\mathcal{E}}\cdot\boldsymbol{\mathcal{J}} - \rho\theta\zeta_{\theta\boldsymbol{\mathcal{E}}}\cdot\dot{\boldsymbol{\mathcal{E}}} - \rho\theta\zeta_{\theta\boldsymbol{\mathcal{H}}}\cdot\dot{\boldsymbol{\mathcal{H}}}.$$

By (4.1), (4.4) and (4.10) we can write the system

$$\dot{s} = -\alpha\delta_s\zeta,$$

$$\dot{\mathbf{N}} = \mathbf{M},$$

$$\sigma\dot{\mathbf{M}} = -\beta\mathbf{M} - \mathrm{dev}\delta_{\mathbf{N}}\zeta + \nu\mathrm{dev}\mathbf{N},$$

$$\theta\zeta_{\theta\theta}\dot{\theta} = \rho\phi_s\dot{s} + \rho\phi_{\mathbf{N}}\cdot\mathbf{M} + \rho\phi_{\nabla s}\cdot\nabla\dot{s} + \rho\phi_{\nabla\mathbf{N}}\cdot\nabla\mathbf{N} + \rho\phi_{\mathbf{M}}\cdot\dot{\mathbf{M}} + f,$$

where $\dot{s}$ and $\dot{\mathbf{N}}$ in the right side are shortands for the corresponding expressions. The dependence of f on the pertinent variables is induced by the constitutive equations of $\phi, \mathbf{T}, \mathbf{B}, \mathbf{D}, \mathbf{q}, \boldsymbol{\mathcal{J}}$.

5 A n-based model

We now regard the director $\mathbf{n}$ as the effective variable, instead of $\mathbf{N}$, which is the case when the physical state of the molecules is not invariant under the transformation $\mathbf{n} \to -\mathbf{n}$. We can then formally repeat the procedure of §3 by replacing $\mathbf{N}$ with $\mathbf{n}$. We obtain

$$\theta\mathbf{k} = \zeta_{\nabla s}\dot{s} + \zeta_{\nabla\mathbf{n}}\dot{\mathbf{n}}$$

and

$$\delta_s\zeta\mathcal{S} + \delta_{\mathbf{n}}\zeta\cdot\dot{\mathbf{n}} + \zeta_{\dot{\mathbf{n}}}\cdot\tilde{\mathbf{n}} - \boldsymbol{\mathcal{T}}\cdot\mathbf{L} - \boldsymbol{\mathcal{J}}\cdot\boldsymbol{\mathcal{E}} + \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta \le 0, \qquad (5.1)$$

where $\tilde{\mathbf{n}}$ is the constitutive function for $\ddot{\mathbf{n}}$, $\boldsymbol{\mathcal{T}}$ is defined as before except for $\mathbf{N}$ replaced by $\mathbf{n}$, and

$$\delta_{\mathbf{n}}\zeta = \theta(\breve{\zeta}_{\mathbf{n}} - \nabla\cdot\breve{\zeta}_{\nabla\mathbf{n}}).$$

Here $\boldsymbol{\mathcal{J}}, \mathbf{q}, \mathbf{k}, \mathcal{S}, \tilde{\mathbf{n}}$ are functions of the list

$$\tilde{\Gamma} = (\theta, \rho, \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{H}}, s, \mathbf{n}, \nabla\theta, \nabla\rho, \nabla s, \nabla\mathbf{n}, \mathbf{L}, \dot{\mathbf{n}}, \nabla\nabla\theta, \nabla\nabla s, \nabla\nabla\mathbf{n}, \nabla\dot{\mathbf{n}}).$$

Sufficient conditions for the validity of (5.1) are

$$\delta_{\mathbf{n}}\xi\cdot\dot{\mathbf{n}} + \zeta_{\dot{\mathbf{n}}}\cdot\tilde{\mathbf{n}} = -\tilde{\beta}|\dot{\mathbf{n}}|^2, \qquad \tilde{\beta}\ge 0, \qquad (5.2)$$

$$-\delta_s\zeta\mathcal{S} + \boldsymbol{\mathcal{T}}\cdot\mathbf{L} \ge 0, \qquad (5.3)$$

$$\boldsymbol{\mathcal{J}}\cdot\boldsymbol{\mathcal{E}} - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta \ge 0. \qquad (5.4)$$

The splitting of (5.1) into (5.2)-(5.4) is motivated by a reasonable simplicity and a more direct comparison with the literature.

As with the dependence on $\dot{\mathbf{N}}$ we let

$$\zeta_{\dot{\mathbf{n}}} = \tilde{\sigma}\dot{\mathbf{n}}$$

so that (5.2) becomes

$$\dot{\mathbf{n}}\cdot(\tilde{\sigma}\ddot{\mathbf{n}} + \tilde{\beta}\dot{\mathbf{n}} + \delta_{\mathbf{n}}\zeta) = 0. \qquad (5.5)$$

A vector perpendicular to $\dot{\mathbf{n}}$ has the form $\omega\mathbf{n} + \mathbf{w}\times\dot{\mathbf{n}}$, the scalar ω and the vector $\mathbf{w}$ being functions of $\tilde{\Gamma}$. Now, $\mathbf{w}$ may be represented as the sum of the parallel and perpendicular parts relative to $\mathbf{n}$, $\mathbf{w} = \mathbf{w}_\parallel + \mathbf{w}_\perp$. Let $\mathbf{w}_\parallel = \xi\mathbf{n}$. The vector product $\mathbf{w}_\perp\times\dot{\mathbf{n}}$ is parallel to $\mathbf{n}$ - possibly $\mathbf{w}_\perp\times\dot{\mathbf{n}} = 0$ - and hence is comprised by $\omega\mathbf{n}$. As a consequence (5.5) implies that

$$\tilde{\sigma}\ddot{\mathbf{n}} = -\tilde{\beta}\dot{\mathbf{n}} - \delta_{\mathbf{n}}\zeta + \omega\mathbf{n} + \xi\mathbf{n}\times\dot{\mathbf{n}}. \qquad (5.6)$$

To obtain the transverse part of $\ddot{\mathbf{n}}$ we apply $\mathbf{1} - \mathbf{n}\otimes\mathbf{n}$ to (5.6). Since

$$(\mathbf{n}\otimes\mathbf{n})\ddot{\mathbf{n}} = (\ddot{\mathbf{n}}\cdot\mathbf{n})\mathbf{n} = -|\dot{\mathbf{n}}|^2\mathbf{n},$$

it follows that

$$\tilde{\sigma}(\ddot{\mathbf{n}} + |\dot{\mathbf{n}}|^2\mathbf{n}) = -\tilde{\beta}\dot{\mathbf{n}} - [\delta_{\mathbf{n}}\zeta - (\mathbf{n}\cdot\delta_{\mathbf{n}}\zeta)\mathbf{n}] + \xi\mathbf{n}\times\dot{\mathbf{n}}. \qquad (5.7)$$

Relative to (4.7), eq. (5.7) shows that, when the head-and-tail symmetry does not occur, also the additive term $\xi\mathbf{n}\times\dot{\mathbf{n}}$ may affect the evolution of $\mathbf{n}$.

5.1 The functions $\mathcal{S}$ and $\boldsymbol{\mathcal{T}}$

Let

$$\mathbf{A} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T), \qquad \mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T), \qquad \mathbf{m} = \dot{\mathbf{n}} - \mathbf{W}\mathbf{n}.$$

Hence $\mathbf{m}$ is the co-rotational derivative of $\mathbf{n}$. Also by analogy with other approaches we let $\boldsymbol{\mathcal{T}}$ be symmetric. Hence (5.3) becomes

$$-\delta_s\zeta\mathcal{S} + \boldsymbol{\mathcal{T}} \cdot \mathbf{A} \geq 0. \tag{5.8}$$

The constitutive equations

$$\dot{s} = -\alpha_1\delta_s\zeta + \alpha_2\mathbf{n} \cdot \mathbf{A}\mathbf{n}, \tag{5.9}$$

$$\begin{aligned}\boldsymbol{\mathcal{T}} = 2\mu_1\mathbf{A} + \mu_2(\mathrm{tr}\,\mathbf{A})\mathbf{1} + \mu_3(\mathbf{n} \otimes \mathbf{A}\mathbf{n} + \mathbf{A}\mathbf{n} \otimes \mathbf{n}) + \mu_4(\mathbf{n} \cdot \mathbf{A}\mathbf{n})\mathbf{n} \otimes \mathbf{n} \\ +\mu_5(\mathbf{m} \otimes \mathbf{A}\mathbf{m} + \mathbf{A}\mathbf{m} \otimes \mathbf{m}) + \alpha_2\delta_s\zeta\,\mathbf{n} \otimes \mathbf{n}\end{aligned}$$

are considered with the coefficients α's and μ's as functions of $\tilde{\Gamma}$. Indeed, substitution makes $-\delta_s\zeta\mathcal{S} + \boldsymbol{\mathcal{T}} \cdot \mathbf{A}$ to be equal to

$$\alpha_1(\delta_s\zeta)^2 + 2\mu_1\mathbf{A} \cdot \mathbf{A} + \mu_2(\mathrm{tr}\,\mathbf{A})^2 + 2\mu_3(\mathbf{A}\mathbf{n})^2 + \mu_4(\mathbf{n} \cdot \mathbf{A}\mathbf{n})^2 + \mu_5(\mathbf{A}\mathbf{m})^2.$$

Hence (5.8) holds if and only if

$$\alpha_1 \geq 0, \quad \mu_1 \geq 0, \quad 2\mu_1 + 3\mu_2 \geq 0, \quad \mu_3 \geq 0, \quad 2\mu_3 + \mu_4 \geq 0, \quad \mu_5 \geq 0.$$

As a consequence, the Cauchy stress $\mathbf{T}$ becomes

$$\begin{aligned}\mathbf{T} = -\rho^2\zeta_\rho\mathbf{1} + \boldsymbol{\mathcal{H}} \otimes \mathbf{B} + \boldsymbol{\mathcal{E}} \otimes \mathbf{D} - \nabla s \otimes \zeta_{\nabla s} - \nabla\mathbf{n} \otimes \zeta_{\nabla\mathbf{n}} \\ +2\mu_1\mathbf{A} + \mu_2(\mathrm{tr}\,\mathbf{A})\mathbf{1} + \mu_3(\mathbf{n} \otimes \mathbf{A}\mathbf{n} + \mathbf{A}\mathbf{n} \otimes \mathbf{n}) + \mu_4(\mathbf{n} \cdot \mathbf{A}\mathbf{n})\mathbf{n} \otimes \mathbf{n} \\ +\mu_5(\mathbf{m} \otimes \mathbf{A}\mathbf{m} + \mathbf{A}\mathbf{m} \otimes \mathbf{m}) + \alpha_2\delta_s\zeta\,\mathbf{n} \otimes \mathbf{n}\end{aligned} \tag{5.10}$$

It is natural to identify $\rho^2\zeta_\rho$ with the pressure and μ_1, μ_2 with the viscosity coefficients.

The possible skew part skw$\mathbf{T}$, of $\mathbf{T}$, in (5.10) is provided by $\boldsymbol{\mathcal{H}} \otimes \mathbf{B}$, $\boldsymbol{\mathcal{E}} \otimes \mathbf{D}$, $\nabla s \otimes \zeta_{\nabla s}$, $\nabla\mathbf{n} \otimes \zeta_{\nabla\mathbf{n}}$. To investigate skw$\mathbf{T}$ it is then convenient to observe that, for any two vectors $\mathbf{u}, \mathbf{v}$, if $\mathbf{v}_\perp$ is perpendicular to $\mathbf{u}$ then

$$\mathrm{skw}(\mathbf{u} \otimes \mathbf{v}) = \mathrm{skw}(\mathbf{u} \otimes \mathbf{v}_\perp).$$

Also by analogy with [4], p. 133, we let

$$\mathbf{D} = \boldsymbol{\epsilon}\boldsymbol{\mathcal{E}}, \qquad \boldsymbol{\epsilon} = \hat{\epsilon}\mathbf{1} + \varepsilon(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1})$$

and the like for the $\mathbf{B}$-$\boldsymbol{\mathcal{H}}$ relation. Hence we have

$$D_n = (\hat{\epsilon} + \frac{2}{3}\varepsilon)\mathcal{E}_n, \qquad \mathbf{D}_\perp = (\hat{\epsilon} - \frac{1}{3}\varepsilon)\boldsymbol{\mathcal{E}}_\perp,$$

where $\mathcal{E}_n, D_n$ are the components along $\mathbf{n}$ whereas $\boldsymbol{\mathcal{E}}_\perp, \mathbf{D}_\perp$ are perpendicular to $\mathbf{n}$. The constitutive equation can also be written

$$\mathbf{D} = \epsilon_\perp \boldsymbol{\mathcal{E}} + (\epsilon_\parallel - \epsilon_\perp)\mathcal{E}_n \mathbf{n},$$

where

$$\epsilon_\parallel = \hat{\epsilon} + \frac{2}{3}\varepsilon, \qquad \epsilon_\perp = \hat{\epsilon} - \frac{1}{3}\varepsilon, \qquad \epsilon_\parallel - \epsilon_\perp =: \epsilon_a.$$

The parameter ϵ_a reflects the anisotropy and is positive or negative according to the structure of the liquid crystal. As a consequence

$$\mathrm{skw}(\boldsymbol{\mathcal{E}} \otimes \mathbf{D}) = \epsilon_a \mathcal{E}_n \mathrm{skw}(\boldsymbol{\mathcal{E}}_\perp \otimes \mathbf{n}) \tag{5.11}$$

and hence $\boldsymbol{\mathcal{E}} \otimes \mathbf{D}$ induces a skew-symmetric part of $\mathbf{T}$ only if $\epsilon_a \neq 0$ and $\mathcal{E}_n \neq 0, \boldsymbol{\mathcal{E}}_\perp \neq 0$ namely when $\boldsymbol{\mathcal{E}}$ is neither parallel nor perpendicular to $\mathbf{n}$.

Similarly, $\nabla s \otimes \zeta_{\nabla s} + \nabla \mathbf{n} \otimes \zeta_{\nabla \mathbf{n}}$ provides a skew-symmetric part if $\zeta_{\nabla s}$ and $\zeta_{\nabla \mathbf{n}}$ are not parallel to ∇s and $\nabla \mathbf{n}$.

5.2 The functions $\boldsymbol{\mathcal{J}}$ and q

The anisotropy induced by $\mathbf{n}$ may affect also $\boldsymbol{\mathcal{J}}$ and $\mathbf{q}$. The functions

$$\boldsymbol{\mathcal{J}} = \sigma_1 \boldsymbol{\mathcal{E}} + \sigma_2 (\boldsymbol{\mathcal{E}} \cdot \mathbf{n})\mathbf{n} + \sigma_3 \nabla\theta + \sigma_4 (\nabla\theta \cdot \mathbf{n})\mathbf{n}, \tag{5.12}$$

$$-\frac{1}{\theta}\mathbf{q} = \kappa_1 \nabla\theta + \kappa_2 (\nabla\theta \cdot \mathbf{n})\mathbf{n} + \kappa_3 \boldsymbol{\mathcal{E}} + \kappa_4 (\boldsymbol{\mathcal{E}} \cdot \mathbf{n})\mathbf{n}, \tag{5.13}$$

where the σ's and the κ's may depend on $\tilde{\Gamma}$, satisfy the inequality (5.4) if and only if

$$\sigma_1 \geq 0, \quad \sigma_1 + \sigma_2 \geq 0, \quad \kappa_1 \geq 0, \quad \kappa_1 + \kappa_2 \geq 0,$$

$$|\sigma_3 + \kappa_3| \leq 4\sigma_1\kappa_1, \qquad |\sigma_4 + \kappa_4| \leq 4(\sigma_1 + \sigma_2)(\kappa_1 + \kappa_2).$$

Accordingly, σ_1 is the transverse electrical conductivity, $\sigma_1 + \sigma_2$ the longitudinal one. Similarly, κ_1 is the transverse thermal conductivity, $\kappa_1 + \kappa_2$ the longitudinal one.

6 Relation to other approaches

The internal structure of the fluid, represented by the degree of orientation s and the director $\mathbf{n}$, is most often modelled by means of balance equations for scalar and vector generalized momenta. Here we re-visit this view by looking mainly at the Ericksen-Leslie theory [11, 5] and subsequent developments [1, 2]. The fluid is regarded as incompressible in [5, 1] and [2] whereas it is compressible in [11].

Relative to (3.24) of [5] for the stress $\mathbf{T}$, eq. (5.10) is more general because it accounts for the effects of the electromagnetic field through $\boldsymbol{\mathcal{H}}\otimes\mathbf{B}+\boldsymbol{\mathcal{E}}\otimes\mathbf{D}$. The term $\dot{s}\mathbf{n}\otimes\mathbf{n}$ is in fact equivalent to $\delta_s\zeta\mathbf{n}\otimes\mathbf{n}$ in that, by (5.9),

$$\delta_s\zeta\mathbf{n}\otimes\mathbf{n} = -\frac{1}{\alpha_1}\dot{s}\mathbf{n}\otimes\mathbf{n} + \frac{\alpha_2}{\alpha_1}(\mathbf{n}\cdot\mathbf{An})\mathbf{n}\otimes\mathbf{n}.$$

While $\dot{s}\mathbf{n}\otimes\mathbf{n}$ coincides with the same term in (3.24) of [5], the second term provides an equivalent coefficient $\mu_4 + \alpha_2/\alpha_1$, in 5.10), of the $(\mathbf{n}\cdot\mathbf{An})\mathbf{n}\otimes\mathbf{n}$ term. Relative to (3.26) of [5] for $\mathbf{q}$, eqs (5.12)-(5.13) provide a more general scheme for both $\boldsymbol{\mathcal{J}}$ and $\mathbf{q}$ with the cross-coupling terms. Equations (5.12)-(5.13) reduce to (3.26) of [5] if $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{\mathcal{J}}$ are disregarded. The same comments apply to the model in [1].

It is worth remarking that Leslie [11] assumes a balance law for $\rho\dot{\mathbf{n}}$ which amounts to

$$\rho\ddot{\mathbf{n}} = \rho\mathbf{G} + \hat{\mathbf{g}} + \nabla\cdot\boldsymbol{\pi}, \tag{6.1}$$

where $\mathbf{G}$ is the external force on the director, $\hat{\mathbf{g}}$ the intrinsic force, $\boldsymbol{\pi}$ the director stress tensor. The second-order evolution equation for $\mathbf{n}$ is consistent with the present approach and is motivated by a kinetic energy term due to $\dot{\mathbf{n}}$. The distinction between $\mathbf{G}$ and $\hat{\mathbf{g}}$ appears in the energy balance where $\mathbf{G}$ occurs through the power $\mathbf{G}\cdot\dot{\mathbf{n}}$ whereas $\hat{\mathbf{g}}$ does not.

A second-order evolution equation occurs also in [2]. Indeed, they denote by σ the constant director mass density, namely the mass density of mesogens, and let $\mathbf{r} = \sigma\dot{\mathbf{n}}$ be the director momentum density. Hence they assume that

$$\sigma\ddot{\mathbf{n}} = \mathbf{g} + \nabla\cdot\boldsymbol{\pi} \tag{6.2}$$

as a balance equation where $\mathbf{g}$ is the director body force. This assumption is similar to (6.1), of Leslie, except for σ, instead of ρ, being constant. Next they take the energy imbalance, or dissipation inequality, as

$$\rho\dot{\psi} - \boldsymbol{\pi}\cdot\nabla\dot{\mathbf{n}} + \mathbf{g}\cdot\dot{\mathbf{n}} \le 0. \tag{6.3}$$

Such inequality may be motivated by starting from

$$\rho\frac{d}{dt}(e + \sigma|\dot{\mathbf{n}}|^2/2) = \nabla\cdot(\boldsymbol{\pi}\dot{\mathbf{n}}) + h, \tag{6.4}$$

h being the heat supply. By means of (6.2) it follows that

$$\rho \dot{e} = \boldsymbol{\pi} \cdot \nabla \dot{\mathbf{n}} - \mathbf{g} \cdot \dot{\mathbf{n}}.$$

Hence the entropy inequality $\rho \dot{\eta} \geq h/\theta$ and the restriction $\dot{\theta} = 0$ provide (6.3). As a comment, (6.4) does not involve the power $\mathbf{g} \cdot \dot{\mathbf{n}}$. Disregarding the power $\mathbf{g} \cdot \dot{\mathbf{n}}$ in the balance of energy is consistent with [11] and [2] where the intrinsic force does not enter the balance of energy. This, however, is in contrast with the fact that both the couple stress and the body couple occur in the balance of energy for liquid crystals viewed as micropolar continua [6].

If $\psi, \boldsymbol{\pi}, \mathbf{g}$ are functions of $\mathbf{n}$ and $\nabla \mathbf{n}$ then (6.3) holds if

$$\boldsymbol{\pi} = \mathbf{n} \otimes \boldsymbol{\alpha} + \psi_{\nabla \mathbf{n}}, \qquad \mathbf{g} = \lambda \mathbf{n} - (\nabla \mathbf{n}) \boldsymbol{\alpha} - \psi_{\mathbf{n}} - \gamma \dot{\mathbf{n}},$$

where the vector $\boldsymbol{\alpha}$ and the scalars λ, γ ($\gamma \geq 0$) are indeterminate functions of $\mathbf{n}, \nabla \mathbf{n}$. Substitution into (6.2) and use of $\psi_{\nabla \mathbf{n}} \mathbf{n} = 0$, $\psi_{\mathbf{n}} \cdot \mathbf{n} = 0$ [2] yield

$$\sigma(\ddot{\mathbf{n}} + |\dot{\mathbf{n}}|^2 \mathbf{n}) + \gamma \dot{\mathbf{n}} = \nabla \cdot \psi_{\nabla \mathbf{n}} + (\nabla \mathbf{n} \cdot \psi_{\nabla \mathbf{n}}) \mathbf{n} - \psi_{\mathbf{n}}. \tag{6.5}$$

It is of interest that, despite the marked difference between the two approaches, eqs (5.7) and (6.5) are the same once we identify ψ with ζ and σ with ρ and observe that, since the temperature field is not considered in [2], we let θ be constant in (5.7).

7 Conclusions

This paper provides a model of nematic liquid crystals subject to the action of electromagnetic fields. The model is more general, than others appeared in the literature, in that it accounts for compressibility of the fluid, the occurrence of an electromagnetic field, the temperature dependence in the constitutive equations. The evolution equations for the degree of orientation s and the director $\mathbf{n}$ are obtained by regarding $s, \dot{\mathbf{n}}$ as internal variables and by requiring that the evolution functions be compatible with thermodynamics. It seems that such a scheme results in a more systematic approach without any appeal to ad-hoc balance equations.

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