

## Director Theories

We have seen in Chapter 1 that the nematic phase is most naturally described by two order parameter tensors  $\mathbf{Q}$  and  $\mathbf{B}$  that can be obtained as macroscopic averages of molecular tensors. However, different phenomenological theories were first developed motivated by the unique optical properties of the nematic phase. We postpone to Chapter 4 the investigation of continuum theories based on the order tensors and begin here by looking at *director* theories that are motivated by the observation that a nematic, although liquid, behaves like a crystal in that it exhibits optically distinguished local directions. These directions are the main protagonists of director theories.

The optical properties of a crystal are primarily determined by the nature of the relationship between an electric field  $\mathbf{E}$  and the displacement  $\mathbf{D}$  it induces. In general, this relationship can be written as [175]

$$\mathbf{D} = \epsilon(\omega)\mathbf{E}, \quad (3.1)$$

where the dielectric tensor  $\epsilon$  normally depends on the frequency  $\omega$  of the electric field. In the limit as  $\omega$  goes to zero, the dielectric tensor describing the behavior of the crystal in a static electric field is obtained. In the absence of an external magnetic field,  $\epsilon$  is symmetric and hence has three real eigenvalues.

In a crystal with cubic symmetry, all three eigenvalues are equal, and so  $\epsilon$  is simply a multiple of the identity. Such a crystal behaves optically like an isotropic material.

When exactly two eigenvalues of its dielectric tensor are equal, a crystal is optically uniaxial. There exists then a single unique direction, determined by the eigenvector to the third, distinct eigenvalue, along which the crystal behaves like an isotropic material. In a *uniaxial liquid crystal*, this direction can vary in time and space and is described by a unit vector field called the *nematic director*  $\mathbf{n}$ . Because the director can be identified with an eigenvector of  $\epsilon$ , it merely describes an axis and as such is a “headless” vector. This fact, that  $\mathbf{n}$  is to be identified with  $-\mathbf{n}$ , is termed the *nematic symmetry*. Mathematically, it means that  $\mathbf{n}$  is to be regarded not as an element of the unit sphere  $\mathbb{S}^2$  but rather of the real projective plane  $\mathbb{RP}^2$ . Ordinary

nematic liquid crystals are nonpolar materials. In a polar material, there is usually a polarization  $\mathbf{P}$  that contributes to the displacement  $\mathbf{D}$  and that is independent of  $\mathbf{E}$ , so that, in that case, (3.1) is to be replaced by  $\mathbf{D} = \mathbf{P} + \epsilon(\omega)\mathbf{E}$ . If light falls onto a uniaxial crystal along any direction oblique to the optical axis, birefringence (double refraction) occurs: the incoming beam splits into an *ordinary* and an *extraordinary* beam. Two indices of refraction can be defined connected with the velocities of light parallel and perpendicular to the optic axis.

When all three eigenvalues of its dielectric tensor are different, a crystal is optically *biaxial*. The optical behavior in this case is rather complex [175, 33]. There are then three different mutually perpendicular directions associated with the three distinct eigenvalues. While in a solid single crystal these directions are determined by the crystal symmetry, in *biaxial liquid crystals* they vary in space and ultimately depend on the local orientational distribution of the molecules.

In the case of constant scalar order parameter, the dynamical equations for uniaxial nematic liquid crystals have long been established: they were obtained as balance equations for linear and rotational momenta, the latter also including the microstructural contributions [91, 180, 265]. The dynamics of uniaxial nematics with variable order was treated much later by ERICKSEN [99], who posited an additional balance equation for the scalar order parameter. The first theories for biaxial nematics were formulated in terms of a triad of three mutually perpendicular directors [287, 165, 123]. It is sufficient to use just two directors, a route that we follow below.

We start by treating in Section 3.1 the classical uniaxial case with constant scalar order. We then extend our results in two different directions. In Section 3.2 we retain the focus on a uniaxial phase but allow a variable degree of scalar order; in Section 3.3, we introduce a secondary director needed for the description of a biaxial phase while reinstating the assumption of constant scalar order parameters.

### 3.1 The ERICKSEN–LESLIE Theory

The most common nematic liquid crystal is formed by effectively uniaxial molecules. Even if the molecules do not possess perfect cylindrical symmetry, any deviation therefrom does not manifest itself in the macroscopic properties of the phase they form. It is therefore most natural to idealize the molecules and describe their orientation by the single direction in which their main axis points. If this axis is further assumed to be nonpolar, then, as we have seen in Chapter 1, the average orientation of such molecules can be represented by the order tensor  $\mathbf{Q}$ , which can be written in the form (1.91) in terms of two scalar order parameters and three orthonormal vectors. We write it here as

$$\mathbf{Q} = S \left( \mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) + T (\mathbf{m} \otimes \mathbf{m} - \mathbf{l} \otimes \mathbf{l}) \quad (3.2)$$

with the scalar order parameters  $S$  and  $T$  and a set of three orthonormal directors  $\mathbf{n}$ ,  $\mathbf{m}$ , and  $\mathbf{l}$ . The uniaxial nematic phase is characterized by  $T = 0$  and hence can be

described by just  $\mathbf{n}$  and the scalar order parameter  $S$ . Since the order parameter  $S$  is primarily determined by temperature (or by concentration in lyotropic nematics), it is often assumed to be constant, and so the state of the liquid crystal is determined by  $\mathbf{n}$  alone. This is the starting point of the ERICKSEN–LESLIE theory. In accordance with the interpretation of the director  $\mathbf{n}$  as identifying the unique optical axis of symmetry of the nematic, it is defined to be a unit vector and as such needs to satisfy the constraint

$$\mathbf{n} \cdot \mathbf{n} \equiv 1. \quad (3.3)$$

Furthermore, because it represents an axis, the further identification

$$\mathbf{n} \sim -\mathbf{n}, \quad (3.4)$$

known as the nematic symmetry, needs to be made. The nematic symmetry (3.4) will in particular entail invariance of all relevant scalar constitutive functions of the theory under reversal of the orientation of  $\mathbf{n}$ .

The mathematical theory of nematic liquid crystals was first phrased as a variational theory in the seminal works of OSEEN [259] and FRANK [109]: the nematic texture represented by the director field  $\mathbf{n}$  was meant to minimize an elastic distortion energy with density  $W$  per unit volume depending on both  $\mathbf{n}$  and  $\nabla\mathbf{n}$ . Both boundary conditions representing various anchoring mechanisms for  $\mathbf{n}$  and applied electric or magnetic fields are the external agents that would antagonize the natural tendency of a nematic texture to be uniform in space, oriented in whatever direction. FRANK [109] found the most general function  $W$  at most quadratic in  $\nabla\mathbf{n}$  that obeys (3.4). His explicit formula is reproduced below in (3.32); here, as in most of this book, we are more interested in a general infrastructure in which FRANK's theory, like any other, can be phrased.

The classical dynamical theory of nematic liquid crystals resulted from the separate efforts of J.L. ERICKSEN and F.M. LESLIE.<sup>1</sup> ERICKSEN [90] started by proposing the balance equations of a simpler theory for anisotropic fluids with neither couple stress nor intrinsic torque acting on the director. In [92] he also reformulated the variational theory of OSEEN and FRANK in the language of the then revived continuum mechanics and found that his earlier theory for anisotropic fluids does not reduce to OSEEN and FRANK's in the static limit. OSEEN [259] had also advanced a dynamical theory that simply rephrased ANZELIUS's incomplete attempt.<sup>2</sup> Building upon his earlier hydrostatic theory [92], ERICKSEN proposed

<sup>1</sup> Other accounts on this theory, phrased in a mathematical language different from ours, can be found, for example, in [351], [352], and [319].

<sup>2</sup> OSEEN cites the work of A. ANZELIUS as published in 1931 in the Annual of the University of Uppsala with the title *Über die Bewegung der anisotropen Flüssigkeiten*. As explained in [42], this was indeed ANZELIUS's dissertation, written under OSEEN's supervision. A short account on its contents is presented in [42], whence we draw the following appreciation of ANZELIUS's work: "The thesis, which consists of an eighty-four page booklet, represents the only research which Anzelius published on liquid crystals. Nevertheless, this work was the first serious and consistent attempt to derive a dynamical theory for nematics" [42, p. 1271].

in [91] a general system of balance laws that generalized OSEEN's and much inspired LESLIE's theory.<sup>3</sup> LESLIE [179] reexamined the earlier theory of ERICKSEN for anisotropic fluids applying the CLAUSIUS–DUHEM inequality to those constitutive equations. Later, broadening the constitutive assumptions on viscous dissipative actions, LESLIE [180, 181] obtained a general dynamical theory that in the static limit reduces to ERICKSEN's hydrostatics.

LESLIE's viscous torque and stress were postulated independently of any RAY-LEIGH dissipation potential; it was PARODI [265] who first showed how requiring LESLIE's dissipative actions to derive from a dissipation potential embodies a relationship<sup>4</sup> among the six phenomenological viscosity coefficients of the theory.

In the following section we shall start afresh to illustrate how the classical dynamical theory of nematic liquid crystals can be derived from the general dissipation principle posited in Chapter 2. In the closing Sections 3.1.4 and 3.1.5, we shall examine the compatibility of this theory with two extreme neighboring domains: on one side, the original variational theory of OSEEN and FRANK, and on the other, the thermodynamic setting in which we have already placed the NAVIER–STOKES fluid in Section 2.3.3.

### 3.1.1 Nondissipative Dynamics

We first consider a uniaxial nematic in the absence of viscous dissipation. As in the case of the inviscid isotropic fluid of Section 2.3.1, the evolution equations can be derived from D'ALEMBERT's principle that requires that the variation  $\delta\mathcal{W}$  of the total working  $\mathcal{W}$  vanish. The relevant velocities are  $\mathbf{v}$  and the material time derivative of the director  $\dot{\mathbf{n}}$ . The total working  $\mathcal{W}$  in (2.210) takes the form

$$\mathcal{W} = \mathcal{W}^{(a)} + \mathcal{W}^{(c)} - \dot{\mathcal{K}} - \dot{\mathcal{F}}, \quad (3.5)$$

where  $\mathcal{W}^{(a)}$  is the power of the external agents,  $\mathcal{W}^{(c)}$  is the power of the constraints,  $\mathcal{K}$  is the kinetic energy, and  $\mathcal{F}$  is the free energy. We will specify each of these below. Once all the contributions of the power are written in their appropriate form as a product of generalized forces and velocities, the evolution equations can be obtained by requiring that

$$\delta\mathcal{W} = 0, \quad (3.6)$$

where the variation is defined as in (2.231) so that the generalized forces are fixed while the velocities are arbitrarily varied.

Since most processes connected with the reorientation of the director are slow compared with the frequency of sound waves, we consider here the nematic fluid as incompressible so that the mass density  $\varrho$  is constant and  $\text{div } \mathbf{v} = 0$ . The compressible case will be treated within the wider scope of Chapter 5.

<sup>3</sup> See also [97] for an effective summary of these early contributions.

<sup>4</sup> Being such a relation phrased in the then popular language of ONSAGER's reciprocity, it is often called the ONSAGER–PARODI relation, a usage that we do not follow here.

## External Agents

The external power expended on a uniaxial nematic has two contributions. One is the same power as that expended by external forces acting on the material element<sup>5</sup> of an isotropic fluid; see (2.261). In addition to this, power can also be expended on the director, so that the total external power takes the form

$$\mathcal{W}^{(a)}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} (\mathbf{b} \cdot \mathbf{v} + \mathbf{k}_n \cdot \dot{\mathbf{n}}) dV + \int_{\partial^* \mathcal{P}_t} (\mathbf{t} \cdot \mathbf{v} + \mathbf{c}_n \cdot \dot{\mathbf{n}}) dA, \quad (3.7)$$

where  $\mathbf{k}_n$  and  $\mathbf{c}_n$  are generalized body and contact force densities acting on the director  $\mathbf{n}$ . While  $\mathbf{b}$  and  $\mathbf{k}_n$  are assigned sources, generally depending on  $\mathbf{n}$ ,  $\mathbf{t}$  and  $\mathbf{c}_n$  are to be regarded as shape functionals of  $\partial^* \mathcal{P}_t$ , also depending on  $\mathbf{n}$ .

## Power of the Constraints

In the present setting there are two constraints. One is incompressibility of the material, which leads to the requirement that the velocity fields  $\mathbf{v}$  remain solenoidal. The other is the requirement that the director retain unit length throughout its evolution. Incompressibility is treated as in (2.270) with the pressure  $p$  as a LAGRANGE multiplier. To ensure that  $\mathbf{n}$  remains normalized, we introduce a further LAGRANGE multiplier  $\gamma$ . The power of the constraint (3.3) is obtained by differentiating it with respect to time, which leads to the requirement

$$\mathbf{n} \cdot \dot{\mathbf{n}} \equiv 0, \quad (3.8)$$

which simply implies that  $\dot{\mathbf{n}}$  needs to be orthogonal to  $\mathbf{n}$ . Upon multiplying (3.8) by  $\gamma$  and adding the powers of the constraints, we find their total power  $\mathcal{W}^{(c)}$  to be

$$\begin{aligned} \mathcal{W}^{(c)}(\mathcal{P}_t, \chi) &= \int_{\mathcal{P}_t} (\gamma \mathbf{n} \cdot \dot{\mathbf{n}} + p \operatorname{div} \mathbf{v}) dV \\ &= \int_{\mathcal{P}_t} (\gamma \mathbf{n} \cdot \dot{\mathbf{n}} - \nabla p \cdot \mathbf{v}) dV + \int_{\partial^* \mathcal{P}_t} p \mathbf{v} \cdot \mathbf{v} dA, \end{aligned} \quad (3.9)$$

where the second form follows after the same integration by parts used to arrive at (2.271).

## Kinetic Energy

The kinetic energy density has the usual contribution  $\frac{1}{2} \rho v^2$ , but because the material now has internal structure, there is also *microinertia*. This part of the kinetic energy is related to director rotation, but since the director stems from the average orientation of the constituent molecules, it is not normally possible to recover the complete

---

<sup>5</sup> Here we call generically a body-point that possesses an internal order structure a *material element*.

microinertia from knowledge of the director rotation alone. However, because of the small moment of inertia connected with molecular rotations, the overall microinertia is necessarily small and usually negligible. We take this point of view and neglect microinertia, so that the kinetic energy takes its usual form

$$\mathcal{K}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \frac{1}{2} \varrho \mathbf{v}^2 dV.$$

Accordingly, the rate of change of the kinetic energy is

$$\dot{\mathcal{K}}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \varrho \dot{\mathbf{v}} \cdot \mathbf{v} dV. \quad (3.10)$$

### Elastic Free Energy

In the absence of compressibility, the free energy is independent of the density, and its only contribution stems from the tendency of the director field to oppose local variations. This *curvature elasticity* is usually assumed to have a density  $W$  per unit volume that is a function of the director and its first gradient,<sup>6</sup>  $W = W(\mathbf{n}, \nabla \mathbf{n})$ . For  $W$  to be compatible with the nematic symmetry (3.4), it has to satisfy

$$W(\mathbf{n}, \nabla \mathbf{n}) = W(-\mathbf{n}, -\nabla \mathbf{n}). \quad (3.11)$$

Furthermore, because there is no distinguished direction other than  $\mathbf{n}$  itself, the energy density needs to satisfy

$$W(\mathbf{n}, \nabla \mathbf{n}) = W(\mathbf{R}\mathbf{n}, \mathbf{R}\nabla \mathbf{n}\mathbf{R}^\top), \quad (3.12)$$

where  $\mathbf{R}$  is an arbitrary proper orthogonal transformation.<sup>7</sup> For nonchiral nematic liquid crystals, the requirement (3.12) needs to hold for arbitrary orthogonal transformations  $\mathbf{R}$ . We postpone giving  $W$  a specific form and look at the general case first.

With the total free energy

$$\mathcal{F}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} W(\mathbf{n}, \nabla \mathbf{n}) dV, \quad (3.13)$$

we first observe that, by the transport theorem (2.37) and  $\operatorname{div} \mathbf{v} = 0$ , we simply have

$$\dot{\mathcal{F}}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \dot{W} dV, \quad (3.14)$$

where as usual the dot denotes the material time derivative. By the chain rule,

<sup>6</sup> Here we are guilty of some abuse of notation, since we denote by  $W$  both the elastic free-energy density and the function delivering it. Where there is no risk of confusion, we prefer this venial sin to then unwarranted pedantry.

<sup>7</sup> See also [353, § 3.1.1] and the quotation on p. 139.

$$\dot{W} = \frac{\partial W}{\partial \mathbf{n}} \cdot \dot{\mathbf{n}} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})'. \quad (3.15)$$

To compute  $(\nabla \mathbf{n})'$ , we observe that the material time derivative  $\dot{\mathbf{n}}$  is written in index notation as

$$\frac{d}{dt} n_i = \frac{\partial}{\partial t} n_i + n_{i,k} v_k$$

and its gradient  $\nabla \dot{\mathbf{n}}$  as

$$\left( \frac{d}{dt} n_i \right)_{,j} = \frac{\partial}{\partial t} n_{i,j} + n_{i,kj} v_k + n_{i,k} v_{k,j}.$$

At the same time, the material time derivative of the director gradient  $(\nabla \mathbf{n})'$  reads as

$$\frac{d}{dt} (n_{i,j}) = \frac{\partial}{\partial t} n_{i,j} + n_{i,jk} v_k.$$

Comparing these last two expressions yields, for a twice continuously differentiable director field  $\mathbf{n}$ , the identity

$$(\nabla \mathbf{n})' = \nabla \dot{\mathbf{n}} - (\nabla \mathbf{n}) \nabla \mathbf{v}. \quad (3.16)$$

Using this in equation (3.15), the change in free energy (3.14) becomes

$$\begin{aligned} \dot{\mathcal{F}}(\mathcal{P}_t, \chi) &= \int_{\mathcal{P}_t} \left\{ \left( \frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \cdot \dot{\mathbf{n}} - \left[ (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \right] \cdot \nabla \mathbf{v} \right\} dV \\ &\quad + \int_{\partial^* \mathcal{P}_t} \left( \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \right) \cdot \dot{\mathbf{n}} dA, \end{aligned}$$

where we have performed an integration by parts and used that

$$\frac{\partial W}{\partial \nabla \mathbf{n}} \cdot [(\nabla \mathbf{n}) \nabla \mathbf{v}] = \left[ (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \right] \cdot \nabla \mathbf{v}.$$

After a further integration by parts,  $\dot{\mathcal{F}}$  takes the required form of a product of the generalized velocities  $\mathbf{v}$  and  $\dot{\mathbf{n}}$  and the corresponding generalized forces:

$$\begin{aligned} \dot{\mathcal{F}}(\mathcal{P}_t, \chi) &= \int_{\mathcal{P}_t} \left\{ \left( \frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \cdot \dot{\mathbf{n}} + \operatorname{div} \left[ (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \right] \cdot \mathbf{v} \right\} dV \\ &\quad + \int_{\partial^* \mathcal{P}_t} \left\{ \left( \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \right) \cdot \dot{\mathbf{n}} - \left[ (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \right] \cdot \mathbf{v} \right\} dA. \quad (3.17) \end{aligned}$$

### ERICKSEN's Identity

We show now that the invariance property for the mapping  $W$  stated in (3.12) entails a tensorial consequence that will play a role in Section 3.1.3 shortly below.

By differentiating both sides of equation (3.3), we easily see that a differentiable director field satisfies

$$(\nabla \mathbf{n})^\top \mathbf{n} \equiv \mathbf{0}, \quad (3.18)$$

which is a constraint for  $\nabla \mathbf{n}$ . Thus, letting  $\mathbf{N}$  represent any admissible value of  $\nabla \mathbf{n}$ , for given  $\mathbf{n}$ , we realize that by (3.18) it lives in the linear subspace of  $L(\mathcal{V})$  defined by

$$L(\mathbf{n}, \mathcal{V}) := \{\mathbf{L} \in L(\mathcal{V}) : \mathbf{L}^\top \mathbf{n} = \mathbf{0}\}.$$

Properly, for  $\mathbf{n} \in \mathbb{S}^2$ ,  $W$  is a real-valued mapping defined on  $L(\mathbf{n}, \mathcal{V})$ , for which the requirement (3.12) acquires the following form:

$$W(\mathbf{n}, \mathbf{N}) = W(\mathbf{R}\mathbf{n}, \mathbf{R}\mathbf{N}\mathbf{R}^\top), \quad (3.19)$$

for all  $\mathbf{n} \in \mathcal{V}$ ,  $\mathbf{N} \in L(\mathbf{n}, \mathcal{V})$ , and all proper orthogonal transformations  $\mathbf{R} \in \text{SO}(3)$ .

Let now  $t \mapsto \mathbf{R}(t)$  be a differentiable trajectory in  $\text{SO}(3)$  such that  $\mathbf{R}(0) = \mathbf{I}$ . It follows from (3.19) that the mapping  $w$  defined by

$$w(t) := W(\mathbf{R}(t)\mathbf{n}, \mathbf{R}(t)\mathbf{N}\mathbf{R}^\top(t))$$

is constant. In particular, this implies that its first derivative vanishes at  $t = 0$ , that is, by the chain rule, that

$$\begin{aligned} \dot{w}(0) &= \frac{\partial W}{\partial \mathbf{n}} \cdot \dot{\mathbf{S}}\mathbf{n} + \frac{\partial W}{\partial \mathbf{N}} \cdot (\dot{\mathbf{S}}\mathbf{N} - \mathbf{N}\dot{\mathbf{S}}) \\ &= \mathbf{S} \cdot \left[ \frac{\partial W}{\partial \mathbf{n}} \otimes \mathbf{n} + \frac{\partial W}{\partial \mathbf{N}} \mathbf{N}^\top + \left( \frac{\partial W}{\partial \mathbf{N}} \right)^\top \mathbf{N} \right] = 0, \end{aligned} \quad (3.20)$$

where  $\mathbf{S} := \dot{\mathbf{R}}(0)$ . By differentiating with respect to the parameter  $t$  the identity  $\mathbf{R}(t)\mathbf{R}^\top(t) \equiv \mathbf{I}$  and setting  $t = 0$ , since  $\mathbf{R}(0) = \mathbf{I}$ , we readily see that  $\mathbf{S}$  is a skew-symmetric tensor. Since the trajectory  $t \mapsto \mathbf{R}(t)$  is arbitrary, (3.20) must hold for all skew-symmetric tensors, which is the case, provided that

$$\left[ \frac{\partial W}{\partial \mathbf{n}} \otimes \mathbf{n} + \frac{\partial W}{\partial \mathbf{N}} \mathbf{N}^\top + \left( \frac{\partial W}{\partial \mathbf{N}} \right)^\top \mathbf{N} \right] \in \text{Sym}(\mathcal{V}), \quad (3.21)$$

where  $\text{Sym}(\mathcal{V})$  is the subspace of all symmetric tensors in  $L(\mathcal{V})$  (see Appendix A.1). In components, this condition reads as

$$\epsilon_{ijk} \left( n_j \frac{\partial W}{\partial n_k} + N_{jl} \frac{\partial W}{\partial N_{kl}} + N_{lj} \frac{\partial W}{\partial N_{lk}} \right) = 0. \quad (3.22)$$

Equations (3.21) and (3.22) are equivalent forms of ERICKSEN's identity, which was first derived in [91].

### Variation of the Working

After the preparation of writing the individual power contributions to the working as products of the velocities and generalized forces in the forms (3.17), (3.7), (3.10),



and (3.9), the application of D’ALEMBERT’s principle is straightforward. In these expressions, we merely have to replace the velocities  $\mathbf{v}$  and  $\dot{\mathbf{n}}$  by their variations  $\delta\mathbf{v}$  and  $\delta\dot{\mathbf{n}}$ , so that (3.6) becomes

$$\begin{aligned} \delta\mathcal{W} = & \int_{\mathcal{P}_t} \left\{ \left[ \mathbf{b} - \nabla p - \varrho \dot{\mathbf{v}} - \operatorname{div} \left( (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \right] \cdot \delta \mathbf{v} \right. \\ & + \left[ \mathbf{k}_n + \gamma \mathbf{n} - \frac{\partial W}{\partial \mathbf{n}} + \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} \right] \cdot \delta \dot{\mathbf{n}} \Big\} dV \\ & + \int_{\partial^* \mathcal{P}_t} \left\{ \left[ \mathbf{t} + \left( p \mathbf{I} + (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \mathbf{v} \right] \cdot \delta \mathbf{v} + \left[ \mathbf{c}_n - \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \right] \cdot \delta \dot{\mathbf{n}} \right\} dA. \end{aligned} \quad (3.23)$$

This can vanish identically for arbitrary parts  $\mathcal{P}_t$  only if the terms in the integrands multiplying the variations of the velocities vanish identically. This localization argument implies the equations

$$\varrho \dot{\mathbf{v}} = \mathbf{b} + \operatorname{div} \mathbf{T}, \quad (3.24)$$

$$\frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \mathbf{k}_n = \gamma \mathbf{n} \quad (3.25)$$

in  $\mathcal{P}_t$  and

$$\mathbf{t} = \mathbf{T} \mathbf{v}, \quad (3.26)$$

$$\mathbf{c}_n = \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v}$$

on  $\partial^* \mathcal{P}_t$ . Here, we have set

$$\mathbf{T} = -p \mathbf{I} - (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}}, \quad (3.27)$$

which, as shown by the traction condition (3.26), is CAUCHY’s stress tensor. ERICKSEN [92] interprets the tensor

$$\mathbf{L}_n := \frac{\partial W}{\partial \nabla \mathbf{n}} \quad (3.28)$$

as the *torque stress*<sup>8</sup> introduced by FRANK [109]. It should not be confused with the couple stress, which shall be identified in both equations (3.73) and (3.75) below. Often<sup>9</sup> the field

$$\mathbf{h}_n := \operatorname{div} \mathbf{L}_n - \frac{\partial W}{\partial \mathbf{n}} \quad (3.29)$$

is called the *molecular field*. By use of (3.28) and (3.29), equation (3.25) is also written as

$$\mathbf{h}_n + \mathbf{k}_n = -\gamma \mathbf{n}. \quad (3.30)$$

<sup>8</sup> In more recent literature (see, for example, [182]), it is also known as the *director stress*.

<sup>9</sup> See, for example, [59, p. 107].

Equation (3.24) is the linear momentum balance, and (3.25) is an equation that we shall soon relate to the balance of torques acting on the director.<sup>10</sup> The part of the stress that depends on the elastic free energy,

$$\mathbf{T}_E := -(\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}}, \quad (3.31)$$

is usually called the ERICKSEN stress. Depending on the actual form of  $W$ , it can fail to be symmetric, in which case the total stress  $\mathbf{T}$  will be asymmetric as well.

As remarked by ERICKSEN [92], in the static limit, where  $\mathbf{v} \equiv \mathbf{0}$ , equations (3.24) and (3.25) become an overdetermined system for the equilibrium of the director  $\mathbf{n}$ . We shall show in Section 3.1.4 how they can be both made consistent with the stationarity requirement for an appropriate energy functional.

### FRANK'S Formula

FRANK [109] derived the most general form of  $W(\mathbf{n}, \nabla \mathbf{n})$  at most quadratic in  $\nabla \mathbf{n}$  that obeys the symmetry requirement (3.11) and is hemitropic, as prescribed by (3.12). He found the following formula, valid for cholesteric liquid crystals:

$$\begin{aligned} W_F(\mathbf{n}, \nabla \mathbf{n}) := & \frac{1}{2} K_1 (\operatorname{div} \mathbf{n})^2 + \frac{1}{2} K_2 (\mathbf{n} \cdot \operatorname{curl} \mathbf{n} + \tau_c)^2 \\ & + \frac{1}{2} K_3 |\mathbf{n} \times \operatorname{curl} \mathbf{n}|^2 + K_{24} [\operatorname{tr}(\nabla \mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2], \end{aligned} \quad (3.32)$$

where  $K_1$ ,  $K_2$ , and  $K_3$  are FRANK's elastic constants and  $\tau_c$  is the characteristic *twist* of the field

$$\mathbf{n}_c = \cos(\tau_c z) \mathbf{e}_x + \sin(\tau_c z) \mathbf{e}_y, \quad (3.33)$$

which in the frame  $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$  represents the generic undistorted orientation of a cholesteric liquid crystal.<sup>11</sup> The field  $\mathbf{n}_c$  describes a helical texture in which the nematic director rotates uniformly along the  $\mathbf{e}_z$  axis; the *pitch*  $p_c$  of the helix, which is defined as

$$p_c := \frac{2\pi}{\tau_c}, \quad (3.34)$$

represents the extension in space needed for  $\mathbf{n}_c$  to perform a complete turn. The elastic constants  $K_1$ ,  $K_2$ , and  $K_3$  are also referred to as the *splay*, *twist*, and *bend* constants, respectively, since they weight the contributions to the elastic energy density  $W_F$  arising from three distinct distortion modes almost pictorially described by these names.<sup>12</sup>

Since  $\operatorname{curl} \mathbf{n}$  is a hemi-indifferent vector, that is, it transforms as in (2.93),  $W_F$  is isotropic only if  $\tau_c = 0$ , in which case  $W_F$  represents the elastic free-energy density of a nematic liquid crystal.

<sup>10</sup> Cf. equation (3.74) below.

<sup>11</sup> See [353, p. 114] for more details on the derivation of (3.32).

<sup>12</sup> These distortion modes are described, for example, in [353, § 3.3].

The last term in (3.32) has a peculiar character: it is a *null Lagrangian*. It was first shown by ERICKSEN [93] that its integral over any shape  $\mathcal{P}_t$  on the reduced boundary  $\partial^*\mathcal{P}_t$  of which  $\mathbf{n}$  is an assigned field  $\mathbf{n}_*$  contributes an energy to  $\mathcal{F}$  that depends only on  $\mathbf{n}_*$ , and so it does not affect the field  $\mathbf{n}$  in  $\mathcal{P}_t$ , as long as  $\mathbf{n}_*$  is kept fixed.<sup>13</sup> For this reason, this term is often omitted from (3.32), especially in the study of bulk properties.<sup>14</sup>

ERICKSEN determined in [94] the conditions that make  $W_F$  positive semidefinite on all admissible director fields, so as to measure the energy required to produce a local distortion starting from a natural, undistorted texture, characteristic of the phase. For nematic liquid crystals, the natural textures with zero energy are all uniform director fields, for which  $\nabla \mathbf{n} \equiv \mathbf{0}$ , whereas for cholesteric liquid crystals the natural textures are all like  $\mathbf{n}_c$  in (3.33) in some appropriate frame.<sup>15</sup> ERICKSEN [94] proved that for nematic liquid crystals,  $W_F$  is positive semidefinite whenever

$$K_1 \geq K_{24}, \quad K_2 \geq K_{24} \geq 0, \quad K_3 \geq 0, \quad (3.35)$$

which are called ERICKSEN's inequalities.<sup>16</sup> For cholesteric liquid crystals, the positive semidefiniteness of  $W_F$  away from all fields  $\mathbf{n}_c$  in the form (3.33) requires in addition that<sup>17</sup>  $K_{24} = 0$ .

### 3.1.2 Dissipative Dynamics

In a uniaxial nematic liquid crystal there are two different velocities that can lead to dissipation: the ordinary material velocity  $\mathbf{v}$  and the rate of change of the director  $\dot{\mathbf{n}}$ . In our setting, outlined in general in Chapter 2, we look for a RAYLEIGH dissipation function that is a quadratic form in these velocities. At the same time, the dissipation function needs to be frame-indifferent, because it describes an objective quantity. In the case of an isotropic viscous fluid, we have seen in Section 2.3.2 how this requirement can be met by constructing the dissipation function as a quadratic form in the stretching  $\mathbf{D} = \frac{1}{2}[\nabla \mathbf{v} + (\nabla \mathbf{v})^\top]$ , which is the simplest indifferent tensorial quantity that is linear in the velocity.

To extend this idea to uniaxial nematics, we need an indifferent time derivative of the director. We use the simplest choice, the corotational time derivative already introduced in (2.83),

$$\dot{\mathbf{n}} = \dot{\mathbf{n}} - \mathbf{W}\mathbf{n}, \quad (3.36)$$

where we recall that

$$\mathbf{W} = \frac{1}{2}[\nabla \mathbf{v} - (\nabla \mathbf{v})^\top] \quad (3.37)$$

is the vorticity tensor. If a different choice of indifferent time derivative is made, the procedure is exactly the same as that outlined below; in the end, this would merely lead to a different grouping of terms in the dissipation.

<sup>13</sup> See also [353, p. 159].

<sup>14</sup> When  $\mathbf{n}$  is not prescribed on the whole of  $\partial^*\mathcal{P}_t$ , such an omission is fully unjustified.

<sup>15</sup> It is easily seen from (3.33) that  $\operatorname{div} \mathbf{n}_c = 0$ ,  $\operatorname{curl} \mathbf{n}_c + \tau_c \mathbf{n}_c = \mathbf{0}$ , and  $(\nabla \mathbf{n}_c)^2 = \mathbf{0}$ .

<sup>16</sup> See also [353, p. 124].

<sup>17</sup> See also [353, § 3.4.2] and [153] for a criticism of this conclusion.

### Generic Dissipation Function

The dissipation function  $R$  is constructed as a function of  $\mathbf{D}$ ,  $\dot{\mathbf{n}}$ , and of  $\mathbf{n}$  itself in such a way that it is a quadratic form in  $(\mathbf{D}, \dot{\mathbf{n}})$ . In view of EULER's theorem on homogeneous functions, this implies that

$$\frac{\partial R}{\partial \mathbf{D}} \cdot \mathbf{D} + \frac{\partial R}{\partial \dot{\mathbf{n}}} \cdot \dot{\mathbf{n}} = 2R.$$

It is easily checked that the pair  $(\nabla \mathbf{v}, \dot{\mathbf{n}})$  depends linearly on the pair  $(\mathbf{D}, \dot{\mathbf{n}})$ , and so it follows that

$$\frac{\partial R}{\partial \nabla \mathbf{v}} \cdot \nabla \mathbf{v} + \frac{\partial R}{\partial \dot{\mathbf{n}}} \cdot \dot{\mathbf{n}} = 2R,$$

which shows that any  $R$  constructed as a quadratic form in  $(\mathbf{D}, \dot{\mathbf{n}})$  is indeed also a quadratic form in  $(\nabla \mathbf{v}, \dot{\mathbf{n}})$ , as required by the dissipation principle.

Before giving a specific form for  $R$  we formally perform the variation of the dissipation functional  $\mathcal{R}$ ,

$$\mathcal{R}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} R(\mathbf{n}; \mathbf{D}, \dot{\mathbf{n}}) dV. \quad (3.38)$$

Although  $R$  is given explicitly as a function of the indifferent rates  $\dot{\mathbf{n}}$  and  $\mathbf{D}$ , the variation needs to be performed with respect to  $\mathbf{v}$  and  $\dot{\mathbf{n}}$ . Thus

$$\begin{aligned} \delta \mathcal{R} &= \int_{\mathcal{P}_t} \left[ \frac{\partial R}{\partial \dot{\mathbf{n}}} \cdot \delta \dot{\mathbf{n}} + \frac{\partial R}{\partial \nabla \mathbf{v}} \cdot \delta \nabla \mathbf{v} \right] dV \\ &= \int_{\mathcal{P}_t} \left[ \frac{\partial R}{\partial \dot{\mathbf{n}}} \cdot \delta \dot{\mathbf{n}} - \operatorname{div} \left( \frac{\partial R}{\partial \nabla \mathbf{v}} \right) \cdot \delta \mathbf{v} \right] dV + \int_{\partial^* \mathcal{P}_t} \left( \frac{\partial R}{\partial \nabla \mathbf{v}} \cdot \mathbf{v} \right) \cdot \delta \mathbf{v} dA. \end{aligned} \quad (3.39)$$

The partial derivatives of  $R$  in this expression can be found using the chain rule, which shows that

$$\frac{\partial R}{\partial \dot{\mathbf{n}}} = \frac{\partial R}{\partial \dot{\mathbf{n}}} \quad (3.40)$$

and

$$\frac{\partial R}{\partial \nabla \mathbf{v}} = \frac{1}{2} \left( \mathbf{n} \otimes \frac{\partial R}{\partial \dot{\mathbf{n}}} - \frac{\partial R}{\partial \dot{\mathbf{n}}} \otimes \mathbf{n} \right) + \frac{\partial R}{\partial \mathbf{D}}. \quad (3.41)$$

### Dynamic Equations

We are now in a position to give the general form of the dynamic equations for the evolution of a uniaxial liquid crystal. The dissipation principle amounts to the requirement (2.232):

$$\delta \mathcal{R} = \delta \mathcal{W}.$$

With the variation  $\delta \mathcal{W}$  as in (3.23) and the variation  $\delta \mathcal{R}$  as in (3.39) together with (3.40) and (3.41) we obtain, as before, the momentum balance in the bulk in the form

$$\rho \dot{\mathbf{v}} = \mathbf{b} + \operatorname{div} \mathbf{T} \quad (3.42)$$

and the traction condition on the boundary as

$$\mathbf{t} = \mathbf{T}\mathbf{v}, \quad (3.43)$$

where now the stress is

$$\mathbf{T} = -p \mathbf{I} - (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} + \frac{1}{2} \left( \mathbf{n} \otimes \frac{\partial R}{\partial \dot{\mathbf{n}}} - \frac{\partial R}{\partial \dot{\mathbf{n}}} \otimes \mathbf{n} \right) + \frac{\partial R}{\partial \mathbf{D}}. \quad (3.44)$$

Apart from a contribution proportional to the identity and the ERICKSEN stress  $\mathbf{T}_E$  as in (3.31), it contains a *viscous* or *dissipative* stress

$$\mathbf{T}_{\text{dis}} := \frac{1}{2} \left( \mathbf{n} \otimes \frac{\partial R}{\partial \dot{\mathbf{n}}} - \frac{\partial R}{\partial \dot{\mathbf{n}}} \otimes \mathbf{n} \right) + \frac{\partial R}{\partial \mathbf{D}}. \quad (3.45)$$

The equation for the director in the bulk becomes

$$\frac{\partial R}{\partial \dot{\mathbf{n}}} + \frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \mathbf{k}_n = \gamma \mathbf{n}, \quad (3.46)$$

and the condition on the boundary, which by (3.28) we now write as

$$\mathbf{c}_n = \mathbf{L}_n \mathbf{v}, \quad (3.47)$$

remains unchanged. This reflects the fact that there is no contribution proportional to  $\dot{\mathbf{n}}$  in the boundary integral in (3.39), which in turn is due to the fact that we did not consider gradients of  $\dot{\mathbf{n}}$  in the dissipation function.

### General Dissipation Function

The dissipation function  $R$  must also obey the nematic symmetry in (3.4), and so it will be assumed that

$$R(-\mathbf{n}; \mathbf{D}, -\dot{\mathbf{n}}) = R(\mathbf{n}; \mathbf{D}, \dot{\mathbf{n}}). \quad (3.48)$$

The most general quadratic form in  $\dot{\mathbf{n}}$  and  $\mathbf{D}$  that can be constructed in terms of these two rates and the director  $\mathbf{n}$  and that obeys (3.48) has five different terms; we write it as<sup>18</sup>

$$R(\mathbf{n}; \mathbf{D}, \dot{\mathbf{n}}) = \frac{1}{2} \gamma_1 \dot{\mathbf{n}}^2 + \gamma_2 \dot{\mathbf{n}} \cdot \mathbf{D} \mathbf{n} + \frac{1}{2} \gamma_3 (\mathbf{D} \mathbf{n})^2 + \frac{1}{2} \gamma_4 (\mathbf{n} \cdot \mathbf{D} \mathbf{n})^2 + \frac{1}{2} \gamma_5 \operatorname{tr} \mathbf{D}^2, \quad (3.49)$$

where the  $\gamma$ 's are viscosity coefficients.<sup>19</sup> It is easily seen from (3.49) that  $R$  is an isotropic function, since the only hemitropic term quadratic in  $(\mathbf{D}, \dot{\mathbf{n}})$ , namely

<sup>18</sup> See [98] and [184].

<sup>19</sup> These are constitutive constants as long as thermal effects are ignored. We refer the reader to [150] and [77] for studies on the thermal dependence of the viscosity coefficients.

$$R_c := \mathbf{n} \cdot \mathbf{D}\mathbf{n} \times \dot{\mathbf{n}}, \quad (3.50)$$

is ruled out by (3.48). Thus, we conclude that both nematic and cholesteric liquid crystals are represented by a dissipation function  $R$  of one and the same form.

For the function  $R$  to be positive semidefinite, the viscosity coefficients must satisfy appropriate inequalities. We find these by introducing a general representation of  $\mathbf{n}$ ,  $\dot{\mathbf{n}}$ , and  $\mathbf{D}$ . Since  $\mathbf{n}$  and  $\dot{\mathbf{n}}$  must be orthogonal to one another, we let  $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$  denote an orthonormal frame such that

$$\mathbf{n} = \mathbf{e}_1, \quad \dot{\mathbf{n}} = N\mathbf{e}_2, \quad \text{and} \quad \mathbf{D} = A_{ij}\mathbf{e}_i \otimes \mathbf{e}_j, \quad (3.51)$$

where  $N$  is a scalar and the coefficients  $A_{ij}$  satisfy

$$A_{ij} = A_{ji} \quad \text{and} \quad A_{ii} = 0, \quad (3.52)$$

since  $\mathbf{D}$  is a symmetric, traceless tensor. Using both (3.51) and (3.52) in (3.49), we write  $R$  as the sum of four independent quadratic forms:

$$\begin{aligned} R = & \left( \frac{1}{2}\gamma_3 + \gamma_5 \right) A_{13}^2 + \gamma_5 A_{23}^2 \\ & + \frac{1}{2}\gamma_1 N^2 + \gamma_2 N A_{12} + \left( \frac{1}{2}\gamma_3 + \gamma_5 \right) A_{12}^2 \\ & + \frac{1}{2}(\gamma_3 + \gamma_4 + 2\gamma_5) A_{11}^2 + \gamma_5 A_{11} A_{22} + \gamma_5 A_{22}^2. \end{aligned} \quad (3.53)$$

This function is positive semidefinite, provided that

$$\gamma_3 + 2\gamma_5 \geq 0, \quad \gamma_5 \geq 0, \quad (3.54)$$

and the following symmetric matrices are positive semidefinite:

$$H_1 := \begin{bmatrix} \gamma_1 & \gamma_2 \\ \gamma_2 & \gamma_3 + 2\gamma_5 \end{bmatrix}, \quad H_2 := \begin{bmatrix} \gamma_3 + \gamma_4 + 2\gamma_5 & \gamma_5 \\ \gamma_5 & 2\gamma_5 \end{bmatrix}. \quad (3.55)$$

For a  $2 \times 2$  symmetric matrix  $H$  to be positive semidefinite, both elements of its principal diagonal and its determinant must not be negative. For  $H_1$  and  $H_2$  in (3.55), such a criterion reduces to

$$\begin{aligned} \gamma_1 &\geq 0, & \gamma_1(\gamma_3 + 2\gamma_5) - \gamma_2^2 &\geq 0, \\ \gamma_3 + \gamma_4 + 2\gamma_5 &\geq 0, & \gamma_5(2\gamma_3 + 2\gamma_4 + 3\gamma_5) &\geq 0. \end{aligned} \quad (3.56)$$

Since (3.54)<sub>2</sub> and (3.56)<sub>4</sub> imply (3.56)<sub>3</sub>, the independent inequalities that guarantee that  $R$  in (3.49) be positive semidefinite can be collected in the following list:

$$\gamma_1 \geq 0, \quad (3.57a)$$

$$\gamma_3 + 2\gamma_5 \geq 0, \quad (3.57b)$$

$$\gamma_5 \geq 0, \quad (3.57c)$$

$$2(\gamma_3 + \gamma_4) + 3\gamma_5 \geq 0, \quad (3.57d)$$

$$\gamma_1(\gamma_3 + 2\gamma_5) - \gamma_2^2 \geq 0. \quad (3.57e)$$

It readily follows from (3.49) that<sup>20</sup>

$$\frac{\partial R}{\partial \mathbf{D}} = \gamma_2 \overline{\dot{\mathbf{n}} \otimes \mathbf{n}} + \gamma_3 \overline{\mathbf{n} \otimes \mathbf{Dn}} + \gamma_4 (\mathbf{n} \cdot \mathbf{Dn}) \overline{\mathbf{n} \otimes \mathbf{n}} + \gamma_5 \mathbf{D}$$

and

$$\frac{\partial R}{\partial \dot{\mathbf{n}}} = \gamma_1 \dot{\mathbf{n}} + \gamma_2 [\mathbf{Dn} - (\mathbf{Dn} \cdot \mathbf{n})\mathbf{n}]. \quad (3.58)$$

Here,  $\overline{\cdots}$  denotes the symmetric traceless part of a tensor (see also Appendix A.1),

$$\overline{\mathbf{A}} := \frac{1}{2}(\mathbf{A} + \mathbf{A}^\top) - \frac{1}{3}(\text{tr } \mathbf{A})\mathbf{I}, \quad \forall \mathbf{A} \in \mathbf{L}(\mathcal{V}).$$

The viscous stress is thus

$$\begin{aligned} \mathbf{T}_{\text{dis}} = & \gamma_2 \overline{\mathbf{n} \otimes \dot{\mathbf{n}}} + \gamma_3 \overline{\mathbf{n} \otimes \mathbf{Dn}} + \gamma_4 (\mathbf{n} \cdot \mathbf{Dn}) \overline{\mathbf{n} \otimes \mathbf{n}} + \gamma_5 \mathbf{D} \\ & + \gamma_1 \text{skw}(\mathbf{n} \otimes \dot{\mathbf{n}}) + \gamma_2 \text{skw}(\mathbf{n} \otimes \mathbf{Dn}). \end{aligned} \quad (3.59)$$

With (3.58), the director evolution equation (3.46) takes the form

$$\gamma_1 \dot{\mathbf{n}} + \gamma_2 \mathbf{Dn} + \frac{\partial W}{\partial \mathbf{n}} - \text{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \mathbf{k}_n = \gamma \mathbf{n}.$$

### LESLIE Viscosity Coefficients

The form of the viscous stress commonly used is

$$\mathbf{T}_{\text{dis}} = \alpha_1 (\mathbf{n} \cdot \mathbf{Dn}) \mathbf{n} \otimes \mathbf{n} + \alpha_2 \dot{\mathbf{n}} \otimes \mathbf{n} + \alpha_3 \mathbf{n} \otimes \dot{\mathbf{n}} + \alpha_4 \mathbf{D} + \alpha_5 \mathbf{Dn} \otimes \mathbf{n} + \alpha_6 \mathbf{n} \otimes \mathbf{Dn},$$

where the  $\alpha$ 's are LESLIE's coefficients (cf. [185, eq. (4.6)]). This expression is the same as (3.59), provided that

$$\begin{aligned} \alpha_1 &= \gamma_4, & \alpha_2 &= \frac{1}{2}(\gamma_2 - \gamma_1), & \alpha_3 &= \frac{1}{2}(\gamma_2 + \gamma_1), \\ \alpha_4 &= \gamma_5, & \alpha_5 &= \frac{1}{2}(\gamma_3 - \gamma_2), & \alpha_6 &= \frac{1}{2}(\gamma_3 + \gamma_2), \end{aligned} \quad (3.60)$$

whence it follows that

$$\alpha_6 - \alpha_5 = \alpha_2 + \alpha_3, \quad (3.61)$$

which is a relation first derived by PARODI [265]. It is automatically satisfied in our setting because all generalized viscous forces derive here from a potential  $R$ .

For completeness, we also record here the formulas that express the  $\gamma$ 's in terms of the  $\alpha$ 's, which are easily obtained from (3.60) and (3.61):

<sup>20</sup> The derivatives  $\frac{\partial R}{\partial \mathbf{D}}$  and  $\frac{\partial R}{\partial \dot{\mathbf{n}}}$  are to be interpreted in the intrinsic sense (see, for example, [353, p. 133]): the former is a symmetric, traceless tensor, while the latter is a vector everywhere orthogonal to  $\mathbf{n}$ .

$$\gamma_1 = \alpha_3 - \alpha_2, \quad (3.62a)$$

$$\gamma_2 = \alpha_3 + \alpha_2, \quad (3.62b)$$

$$\gamma_3 = \alpha_2 + \alpha_3 + 2\alpha_5, \quad (3.62c)$$

$$\gamma_4 = \alpha_1, \quad (3.62d)$$

$$\gamma_5 = \alpha_4. \quad (3.62e)$$

Use of these formulas in inequalities (3.57) transforms them into the inequalities for the LESLIE viscosities that are reproduced below to ease the comparison with those derived in [319, p. 146]:

$$\alpha_3 \geq \alpha_2, \quad (3.63a)$$

$$\alpha_4 \geq 0, \quad (3.63b)$$

$$\alpha_2 + \alpha_3 + 2\alpha_4 + 2\alpha_5 \geq 0, \quad (3.63c)$$

$$2(\alpha_1 + \alpha_2 + \alpha_3) + 3\alpha_4 + 4\alpha_5 \geq 0, \quad (3.63d)$$

$$(\alpha_3 - \alpha_2)(\alpha_2 + \alpha_3 + 2\alpha_4 + 2\alpha_5) \geq (\alpha_2 + \alpha_3)^2. \quad (3.63e)$$

### 3.1.3 Rotational Momentum and Couple Stress

We have derived the dynamic equations of nematic director theory using generalized forces acting on the generalized velocity  $\dot{\mathbf{n}}$ . We eventually obtained two coupled balance equations, (3.42) and (3.46), one for the linear momentum and the other for the orientational order. The format we used is quite general and can be applied in a similar manner to a wide variety of ordered media [311, 312]. In the present case, if one takes the naïve view that the director represents a rigid body capable both of being conveyed by the flow and of rotating relative to it, the director balance is equivalent to the balance of rotational momentum. Correspondingly, in such a kinematic interpretation, we may attribute two rotational velocities to  $\mathbf{n}$  in one and the same frame: one is the spin vector  $\mathbf{w}$  of the flow, that is, the axial vector associated with the vorticity tensor  $\mathbf{W}$  in (3.37), and the other will be denoted by  $\mathbf{w}_n$ . We write

$$\dot{\mathbf{n}} = \mathbf{w} \times \mathbf{n}$$

in the first case and

$$\dot{\mathbf{n}} = \mathbf{w}_n \times \mathbf{n} \quad (3.64)$$

in the second case. In the former, by (3.36),

$$\overset{\circ}{\mathbf{n}} = \mathbf{0},$$

while in the latter,

$$\overset{\circ}{\mathbf{n}} = (\mathbf{w}_n - \mathbf{w}) \times \mathbf{n}. \quad (3.65)$$

As LESLIE [185] has shown, it is indeed possible to formulate the theory based on the classical balances without resorting to generalized velocities and forces.



In general, the orientational balance cannot be derived from the balance of rotational momentum; this is obvious if the description of the orientation employs more than three degrees of freedom, as is the case, for example, in the order tensor theories treated in Chapter 4. However, in any event the balance of rotational momentum (2.141) must be satisfied, whether it is equivalent to the orientational balance or not. As shown in [311] for arbitrary tensorial order structure, this is indeed the case provided the kinetic and free energies satisfy appropriate invariance requirements.

We show now how the director balance can be interpreted as a balance of torques on the material element, and we identify the couple stress. Because we have neglected the kinetic energy associated with director rotation, the balance of rotational momentum (2.141) here takes the simpler form

$$2\boldsymbol{\tau} + \operatorname{div} \mathbf{L} + \mathbf{k} = 0, \quad (3.66)$$

where  $\mathbf{L}$  is the couple stress,  $\mathbf{k}$  is a body couple per unit volume, and  $\boldsymbol{\tau}$  is the axial vector associated with the skew-symmetric part of the stress  $\mathbf{T}$  via (2.132). In index notation,

$$2\tau_i = \epsilon_{ijk} T_{kj}. \quad (3.67)$$

Thus  $\boldsymbol{\tau}$  is determined by our knowledge of the stress tensor (3.44), and we will now use this to identify  $\mathbf{L}$  and  $\mathbf{k}$  via the rotational momentum balance (3.66).

We start by giving the director balance a different form. Defining

$$\mathbf{g}_n := -\frac{\partial R}{\partial \mathbf{n}} \quad (3.68)$$

and taking the vector product of  $\mathbf{n}$  with (3.46), we find that

$$\mathbf{n} \times \left( \mathbf{g}_n - \frac{\partial W}{\partial \mathbf{n}} + \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} + \mathbf{k}_n \right) = \mathbf{0}, \quad (3.69)$$

which, by (3.29), also acquires the more compact form

$$\mathbf{n} \times (\mathbf{g}_n + \mathbf{h}_n + \mathbf{k}_n) = \mathbf{0}. \quad (3.70)$$

Computing explicitly (3.67) with the stress (3.44) yields

$$2\tau_i = \epsilon_{ijk} \left( n_j g_{nk} + n_{l,j} \frac{\partial W}{\partial n_{l,k}} \right),$$

where we have denoted by  $g_{nk}$  the Cartesian components of  $\mathbf{g}_n$  and<sup>21</sup> by  $\frac{\partial W}{\partial n_{l,k}}$  those of  $\mathbf{L}_n$ . ERICKSEN's identity in the form (3.22) allows us to write  $2\boldsymbol{\tau}$  as

$$\begin{aligned} 2\tau_i &= \epsilon_{ijk} \left( n_j g_{nk} - n_j \frac{\partial W}{\partial n_k} - n_{j,l} \frac{\partial W}{\partial n_{k,l}} \right) \\ &= \epsilon_{ijk} \left( -n_j k_{nk} - n_j \left[ \frac{\partial W}{\partial n_{k,l}} \right]_{,l} - n_{j,l} \frac{\partial W}{\partial n_{k,l}} \right) \\ &= \epsilon_{ijk} \left( -n_j k_{nk} - \left[ n_j \frac{\partial W}{\partial n_{k,l}} \right]_{,l} \right), \end{aligned} \quad (3.71)$$

<sup>21</sup> With a common abuse of notation.

where the director balance (3.69) was used to obtain the second line. Comparing (3.71) with (3.66) shows that the latter is satisfied if we interpret

$$\mathbf{k} = \mathbf{n} \times \mathbf{k}_n \quad (3.72)$$

as the body couple and

$$\mathbf{L} = \epsilon_{ijk} n_j \frac{\partial W}{\partial n_{k,l}} \mathbf{e}_i \otimes \mathbf{e}_l \quad (3.73)$$

as the couple stress, where  $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$  is any orthonormal positively oriented basis.<sup>22</sup> With (3.72) we can regard (3.69) as a balance of torques if we interpret

$$\mathbf{n} \times \mathbf{g}_n = -\mathbf{n} \times \frac{\partial R}{\partial \mathbf{n}}$$

as a viscous torque and

$$\mathbf{n} \times \mathbf{h}_n = \mathbf{n} \times \left( \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \frac{\partial W}{\partial \mathbf{n}} \right)$$

as an elastic torque. Thus, in the inviscid limit, equation (3.25), which can equivalently be rewritten as

$$\mathbf{n} \times (\mathbf{k}_n + \mathbf{h}_n) = \mathbf{n} \times \left( \mathbf{k}_n + \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \frac{\partial W}{\partial \mathbf{n}} \right) = \mathbf{0}, \quad (3.74)$$

is interpreted as a balance of elastic and body couples.

Finally, the traction condition for the director (3.47) allows us to identify the surface couple as

$$\mathbf{c} = \mathbf{n} \times \mathbf{c}_n,$$

which is consistent with  $\mathbf{c} = \mathbf{L}\mathbf{v}$ . It readily follows from (3.73) that  $\mathbf{L}$  can be characterized by its action on any vector  $\mathbf{u} \in \mathcal{V}$  as

$$\mathbf{L}\mathbf{u} = \mathbf{n} \times \left( \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \mathbf{u} = \mathbf{n} \times \mathbf{L}_n \mathbf{u}. \quad (3.75)$$

Since by (2.92), the vector product of two indifferent vectors is hemi-indifferent, it follows from (3.75) that

$$\begin{aligned} \mathbf{L}^* \mathbf{u}^* &= \mathbf{L}^* \mathbf{R} \mathbf{u} = (\det \mathbf{R}) \mathbf{R} \mathbf{L} \mathbf{u} = (\det \mathbf{R}) \mathbf{R} \mathbf{L} \mathbf{R}^\top \mathbf{R} \mathbf{u} \\ &= (\det \mathbf{R}) \mathbf{R} \mathbf{L} \mathbf{R}^\top \mathbf{u}^*, \end{aligned} \quad (3.76)$$

where  $\mathbf{R}$  is the orthogonal tensor representing a change of frame. By the arbitrariness of  $\mathbf{u}^*$ , it follows from (3.76) that the constitutive law (3.73) for the couple stress is hemitropic, as it should be.

<sup>22</sup> Strictly speaking, equation (3.44) determines  $\mathbf{L}$  to within a divergence-free tensor. We shall see in Section 3.1.4 how this indeterminacy can be removed.

If the director is thought of as rotating independently from the flow, its time derivative is given by (3.64), where the rotational velocity  $\mathbf{w}_n$  may differ from the spin vector  $\mathbf{w}$  of the flow and by (3.65), in general,  $\dot{\mathbf{n}} \neq \mathbf{0}$ . With (3.72) and (3.64) we have

$$\mathbf{k}_n \cdot \dot{\mathbf{n}} = \mathbf{k}_n \cdot (\mathbf{w}_n \times \mathbf{n}) = \mathbf{w}_n \cdot (\mathbf{n} \times \mathbf{k}_n) = \mathbf{k} \cdot \mathbf{w}_n.$$

Similarly,

$$\mathbf{c}_n \cdot \dot{\mathbf{n}} = \mathbf{c} \cdot \mathbf{w}_n,$$

and so the power of the external agents (3.7) can be equivalently written as

$$\mathcal{W}^{(a)}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} (\mathbf{b} \cdot \mathbf{v} + \mathbf{k} \cdot \mathbf{w}_n) dV + \int_{\partial^* \mathcal{P}_t} (\mathbf{t} \cdot \mathbf{v} + \mathbf{c} \cdot \mathbf{w}_n) dA,$$

which reduces to (2.142) only if  $\mathbf{w}_n = \mathbf{w}$ , so that  $\dot{\mathbf{n}} = \mathbf{0}$ .

### 3.1.4 Variational Compatibility

In this section, following essentially ERICKSEN [92], we establish the condition under which the static limit of the balance equations (3.66) and (3.25) can be related to the EULER–LAGRANGE equation for the stationarity of an energy functional, thus justifying the purely variational approach to the statics of liquid crystals, which was the first theory proposed by OSEEN [259] and FRANK [109].

#### Principle of Virtual Power

Our starting point here will be a principle of virtual power, which is actually the conceptual antecedent of D’ALEMBERT’s principle, which in Section 3.1.1 served as a foundation for inviscid dynamics. Imagine any subbody  $\mathcal{P}$  carved from the body  $\mathcal{B}$ , subject on its reduced boundary  $\partial^* \mathcal{P}$  to a system of generalized tractions  $(\mathbf{t}, \mathbf{c}_n)$  and, in its interior  $\mathring{\mathcal{P}}$ , to a system of generalized body forces  $(\mathbf{b}, \mathbf{k}_n)$  expending power on any virtual motion described by the generalized velocities  $(\mathbf{v}, \dot{\mathbf{n}})$ , so that (3.7) still formally applies, though no real motion  $\chi$  exists here:<sup>23</sup>

$$\mathcal{W}^{(a)}(\mathcal{P}) = \int_{\mathcal{P}} (\mathbf{b} \cdot \mathbf{v} + \mathbf{k}_n \cdot \dot{\mathbf{n}}) dV + \int_{\partial^* \mathcal{P}} (\mathbf{t} \cdot \mathbf{v} + \mathbf{c}_n \cdot \dot{\mathbf{n}}) dA. \quad (3.77)$$

As above,  $\mathbf{b}$  and  $\mathbf{k}_n$  are assigned sources, whereas  $\mathbf{t}$  and  $\mathbf{c}_n$  are shape functionals to be determined so as to comply with equilibrium. Like any real flow, the virtual flow  $\mathbf{v}$  is also required to preserve the volume of any arbitrary subbody  $\mathcal{P}$ , since it is a means to mimic any admissible isochoric deformation of  $\mathcal{P}$ , possibly accompanied by an equally admissible change in the director distortion. Thus, the virtual flow  $\mathbf{v}$  will also be subject to the kinematic constraint

<sup>23</sup> For notational coherence, we should denote the virtual flow by  $\delta \mathbf{v}$ , instead of  $\mathbf{v}$ , which is usually reserved for the real motion. However, no confusion is likely to arise here, since the only motion present is virtual.

$$\operatorname{div} \mathbf{v} = 0. \quad (3.78)$$

Similarly, denoting now by  $\dot{\mathcal{F}}$  the virtual rate of change of the free energy  $\mathcal{F}$  in (3.13), by the transport theorem (2.37) applied to a virtual motion, in complete analogy with (3.14), we write

$$\dot{\mathcal{F}}(\mathcal{P}) = \int_{\mathcal{P}} \dot{W} dV. \quad (3.79)$$

The principle of virtual power prescribes that at equilibrium an incompressible liquid crystal in  $\mathcal{B}$  with elastic energy density (per unit volume)  $W$  and subject to the traction system  $(\mathbf{t}, \mathbf{c}_n)$  and to the body force system  $(\mathbf{b}, \mathbf{k}_n)$  satisfies the requirement

$$\dot{\mathcal{F}}(\mathcal{P}) = \mathcal{W}^{(a)}(\mathcal{P}) + \mathcal{W}^{(c)}(\mathcal{P}) \quad (3.80)$$

for all subbodies  $\mathcal{P}$  of  $\mathcal{B}$  and for all systems of virtual generalized velocities  $(\mathbf{v}, \dot{\mathbf{n}})$ , where  $\mathcal{W}^{(c)}(\mathcal{P})$  is the power of the constraints<sup>24</sup> (3.78) and (3.8),

$$\mathcal{W}^{(c)}(\mathcal{P}) = \int_{\mathcal{P}} (p \operatorname{div} \mathbf{v} + \gamma \mathbf{n} \cdot \dot{\mathbf{n}}) dV.$$

Virtually with no change in the formal development of Section 3.1.1, we give  $\dot{\mathcal{F}}$  in (3.79) the following form:

$$\dot{\mathcal{F}}(\mathcal{P}) = \int_{\partial^* \mathcal{P}} (\mathbf{T} \mathbf{v} \cdot \mathbf{v} + \mathbf{L}_n \mathbf{v} \cdot \dot{\mathbf{n}}) dA - \int_{\mathcal{P}} (\operatorname{div} \mathbf{T} \cdot \mathbf{v} + \mathbf{h}_n \cdot \dot{\mathbf{n}}) dV,$$

where  $\mathbf{h}_n$  is the molecular field defined in (3.29),  $\mathbf{L}_n$  is the torque stress (3.28), and  $\mathbf{T}$  is the stress tensor as in (3.27). Thus, by (3.77) and (3.79), enforcing (3.80) requires the following equations to be satisfied:

$$\mathbf{b} + \operatorname{div} \mathbf{T} = \mathbf{0} \quad \text{and} \quad \mathbf{h}_n + \mathbf{k}_n + \gamma \mathbf{n} = \mathbf{0}, \quad (3.81a)$$

which hold in  $\mathcal{B}$ , and

$$\mathbf{t} = \mathbf{T} \mathbf{v} \quad \text{and} \quad \mathbf{c}_n = \mathbf{L}_n \mathbf{v}, \quad (3.81b)$$

which specify the generalized tractions as special functionals of  $\partial^* \mathcal{P}$ .

The first equation in (3.81a) is the static limit of the balance equation of linear momentum (3.66) in the inviscid case, while the second equation coincides with (3.30); both have been reobtained<sup>25</sup> within an alternative, independent formulation of statics. Since both these vectorial equations are in the single unknown field  $\mathbf{n}$ , they apparently overdetermine it. We shall see below how such an overdetermination can in general be resolved.

<sup>24</sup> Here, as in (3.9),  $p$  and  $\gamma$  are unknown LAGRANGE multipliers, with precisely the same mechanical meaning.

<sup>25</sup> There is more than a pedagogical reason in favor of such a derivation. The method illustrated here will guide us to obtain the appropriate equilibrium equations when in Section 5.2.1 we move in less traditional territories.

Now we pause briefly to consider other consequences of the principle of virtual power, which must hold whenever equations (3.81) do, though some might require more labor to be derived directly from these.<sup>26</sup>

### Special Virtual Motions

The first of such consequences follows from taking as virtual motion a rigid motion, described by the system of generalized velocities  $(\mathbf{v}_R, \dot{\mathbf{n}}_R)$ . Paraphrasing (2.71), we write  $\mathbf{v}_R$  as

$$\mathbf{v}_R(x) = \mathbf{v}_o + \mathbf{W}(x - o), \quad (3.82)$$

where  $\mathbf{v}_o$  is an arbitrary vector, representing the virtual velocity of the point  $o$ , and  $\mathbf{W}$  is an arbitrary skew-symmetric tensor. Moreover, we set

$$\dot{\mathbf{n}}_R := \mathbf{W}\mathbf{n}, \quad (3.83)$$

which, by (3.36), means that  $\dot{\mathbf{n}} = \mathbf{0}$ , and so the director  $\mathbf{n}$  is conveyed along with the fluid and remains at rest relative to it. By requiring  $\dot{\mathcal{F}}(\mathcal{P})$  to vanish for all  $\mathcal{P}$  along a rigid motion, which is a kinematic consequence of  $\mathcal{F}(\mathcal{P})$  being frame-indifferent, with the aid of (3.79) and since  $\mathbf{v}_R$  satisfies (3.78), we reobtain ERICKSEN's identity (3.21), as the reader will easily verify.

Since  $\dot{\mathcal{F}}(\mathcal{P})$  vanishes on all virtual rigid motions, (3.80) requires that  $\mathcal{W}^{(a)}(\mathcal{P}) + \mathcal{W}^{(c)}(\mathcal{P})$  vanish as well. Use of (3.82) and (3.83), by the arbitrariness of  $\mathbf{v}_o \in \mathcal{V}$  and  $\mathbf{W} \in \text{Skw}(\mathcal{V})$ , yields

$$\int_{\mathcal{P}} \mathbf{b} \, dV + \int_{\partial^*\mathcal{P}} \mathbf{t} \, dA = \mathbf{0}, \quad (3.84a)$$

$$\int_{\mathcal{P}} [(x - o) \otimes \mathbf{b} + \mathbf{n} \otimes \mathbf{k}_n] dV + \int_{\partial^*\mathcal{P}} [(x - o) \otimes \mathbf{t} + \mathbf{n} \otimes \mathbf{c}_n] dA \in \text{Sym}(\mathcal{V}). \quad (3.84b)$$

While (3.84a), easily recognized as the balance of all forces acting on the subbody  $\mathcal{P}$  in equilibrium, is an immediate consequence of (3.81a)<sub>1</sub> and (3.81b)<sub>1</sub>, (3.84b) can be employed to establish more directly formula (3.75) for the couple stress tensor  $\mathbf{L}$ .

By requiring the skew-symmetric part of the tensor in (3.84b) to vanish and using the fact that the axial vector of the tensor  $(\mathbf{b} \otimes \mathbf{a} - \mathbf{a} \otimes \mathbf{b})$  is  $\mathbf{a} \times \mathbf{b}$  (see also Appendix A.1), we give (3.84b) the following equivalent form:

$$\int_{\mathcal{P}} [(x - o) \times \mathbf{b} + \mathbf{n} \times \mathbf{k}_n] dV + \int_{\partial^*\mathcal{P}} [(x - o) \times \mathbf{T}\mathbf{v} + \mathbf{n} \times \mathbf{L}_n\mathbf{v}] dA = \mathbf{0}, \quad (3.85)$$

where use has also been made of (3.81b). Equation (3.85) clearly indicates that the tensor  $\mathbf{L}$  defined as in (3.75) designates the couple stress. Use of (3.75) and the divergence theorem reduces (3.85), valid for all  $\mathcal{P} \in \mathcal{B}$ , to its equivalent local form (3.66), which we need not reproduce here.<sup>27</sup>

<sup>26</sup> This again serves more the purpose of illustrating a method than that of drawing new conclusions.

<sup>27</sup> We thus remove the indeterminacy on  $\mathbf{L}$  signaled on page 182 above.

### Compatibility Potential

Here we write explicitly the condition that must be met to ensure the compatibility of both equations in (3.84). We start from an identity that follows from (3.29) and (3.27),

$$\nabla W + \operatorname{div} \mathbf{T}_E + (\nabla \mathbf{n})^\top \mathbf{h}_n = \mathbf{0}, \quad (3.86)$$

and is more easily proved in indicial notation. By (3.31), we may write

$$w_{,i} - \left( n_{k,i} \frac{\partial W}{\partial n_{k,j}} \right)_{,j} = \frac{\partial W}{\partial n_k} n_{k,i} + \frac{\partial W}{\partial n_{k,j}} n_{k,ji} - n_{k,ij} \frac{\partial W}{\partial n_{k,j}} - n_{k,i} \left( \frac{\partial W}{\partial n_{k,j}} \right)_{,j},$$

whence, since for a smooth director field  $n_{k,ji} = n_{k,ij}$ , we obtain (3.86) in component form. Making use of both equations in (3.81a) and recalling (3.18), we arrive from (3.27) at the following compatibility equation:

$$\nabla W + \nabla p - \mathbf{b} - (\nabla \mathbf{n})^\top \mathbf{k}_n = \mathbf{0}, \quad (3.87)$$

which is equivalently stated by requiring that there be a function  $U = U(x, \mathbf{n})$  of position  $x \in \mathfrak{B}$  in space and orientation  $\mathbf{n} \in \mathbb{S}^2$  such that

$$\mathbf{b} + (\nabla \mathbf{n})^\top \mathbf{k}_n = \nabla U. \quad (3.88)$$

Once (3.88) is met, (3.87) delivers the pressure  $p$  to within a hydrostatic, uniform pressure  $p_0$ :

$$p = p_0 + U - W. \quad (3.89)$$

A way to satisfy (3.88), though presumably it is not the only one, is to assume that

$$\mathbf{b} = \frac{\partial U}{\partial x} \quad \text{and} \quad \mathbf{k}_n = \frac{\partial U}{\partial \mathbf{n}}. \quad (3.90)$$

Here the derivative  $\frac{\partial U}{\partial x}$  is meant to be computed ignoring the possible spatial dependence of  $\mathbf{n}$ . The derivative  $\frac{\partial U}{\partial \mathbf{n}}$  is to be interpreted in the intrinsic sense, made clear for example by Lemma 3.6 of [353, p. 133]: it is by definition a vector orthogonal to  $\mathbf{n}$ . By (3.90) and (3.29), the second equation in (3.84), now compatible with the first, may also be written as

$$\operatorname{div} \left( \frac{\partial W}{\partial \nabla \mathbf{n}} \right) - \frac{\partial W}{\partial \mathbf{n}} + \frac{\partial U}{\partial \mathbf{n}} + \gamma \mathbf{n} = \mathbf{0}, \quad (3.91)$$

which is the EULER-LAGRANGE equation for the energy functional

$$\mathcal{E}[\mathbf{n}] := \int_{\mathfrak{B}} (W - U) dV, \quad (3.92)$$

subject to the constraint (3.3).

Thus we have shown that the static limits of equations (3.24) and (3.25), which can also be obtained independently from a principle of virtual power, are compatible

with a purely variational formulation with energy functional  $\mathcal{E}$  as in (3.92), provided that compatibility condition (3.88) is satisfied. The stress tensor  $\mathbf{T}$  in (3.27), computed with  $p$  as in (3.89) on a solution of (3.91), describes the distribution of internal forces in  $\mathfrak{B}$  at equilibrium. It has also been employed in [115] to compute elastic forces on defects of the director field, a topic that exceeds the scope of this book.<sup>28</sup>

We now illustrate a physically significant case in which both equations in (3.90) hold for a potential  $U$  that can easily be determined.<sup>29</sup> This case arises when the liquid crystal is subject to a magnetic field  $\mathbf{H}$ . According to the explicit computations of LEATHEM [176],  $\mathbf{H}$  exerts both a magnetic body force  $\mathbf{b}_m$  and a body couple  $\mathbf{k}_m$  given by

$$\mathbf{b}_m = (\nabla \mathbf{H})\mathbf{M} \quad \text{and} \quad \mathbf{k}_m = \mathbf{M} \times \mathbf{H}, \quad (3.93)$$

where  $\mathbf{M}$  is now the magnetization induced by  $\mathbf{H}$ . Under the assumption that  $\mathbf{M}$  is linearly related to  $\mathbf{H}$ , a classical symmetry argument (see, for example, [307] and [353, p. 95]) shows that

$$\mathbf{M} = \chi_\perp \mathbf{H} + (\chi_\parallel - \chi_\perp)(\mathbf{H} \cdot \mathbf{n})\mathbf{n}, \quad (3.94)$$

where  $\chi_\parallel$  and  $\chi_\perp$  are the magnetic susceptibilities of the material when  $\mathbf{H}$  is parallel to  $\mathbf{n}$  and when  $\mathbf{H}$  is orthogonal to  $\mathbf{n}$ , respectively.<sup>30</sup> The *diamagnetic anisotropy*, defined by

$$\Delta\chi := \chi_\parallel - \chi_\perp, \quad (3.95)$$

can be either positive or negative, each sign characterizing a different interaction between  $\mathbf{H}$  and  $\mathbf{n}$ , as we shall soon show.

By (3.94), (3.95), and (3.72), we obtain from (3.93) that

$$\mathbf{b}_m = \chi_\perp (\nabla \mathbf{H})\mathbf{H} + \Delta\chi (\mathbf{H} \cdot \mathbf{n})(\nabla \mathbf{H})\mathbf{n}, \quad (3.96a)$$

$$\mathbf{k}_m = \Delta\chi (\mathbf{H} \cdot \mathbf{n})\mathbf{n} \times \mathbf{H} = \mathbf{n} \times \mathbf{k}_n. \quad (3.96b)$$

In particular, (3.96b) shows that for  $\Delta\chi > 0$  the magnetic torque is *aligning*, since it tends to align  $\mathbf{n}$  like  $\mathbf{H}$ , whereas for  $\Delta\chi < 0$  it is *misaligning*, since it tends to align  $\mathbf{n}$  at right angles with  $\mathbf{H}$ . Equation (3.96b) also implies that

$$\mathbf{k}_n = \Delta\chi (\mathbf{H} \cdot \mathbf{n})(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{H}, \quad (3.97)$$

since, by (3.90)<sub>2</sub>,  $\mathbf{k}_n \cdot \mathbf{n} = 0$ . We now show that both (3.96a) and (3.97) agree with (3.90), provided we set

<sup>28</sup> Static defects are singularities in the solutions of equation (3.91). There is a vast literature concerned with them. We cite only the following works, which treat this topic at different levels of generality and rigor: [36, 37, 135, 136, 114, 166, 167, 168, 169, 172, 230, 286, 308, 355]. More recently, defect dynamics has also become the object of mathematical studies. We refer the reader to some papers that may be suggested as first readings: [25, 46, 47, 74, 151, 162, 261, 264, 269, 270, 285, 309, 314, 330, 336].

<sup>29</sup> See also [92] and [183].

<sup>30</sup> Here both  $\chi_\parallel$  and  $\chi_\perp$  are considered to be material constants, uniform in space.

$$U_m = \frac{1}{2} \mathbf{M} \cdot \mathbf{H} = \frac{1}{2} [\chi_\perp (\mathbf{H} \cdot \mathbf{H}) + \Delta\chi (\mathbf{H} \cdot \mathbf{n})^2]. \quad (3.98)$$

While differentiating the magnetic potential  $U_m$  in (3.98) with respect to  $\mathbf{n}$  readily delivers<sup>31</sup> (3.97), to obtain (3.96a) we note that

$$\frac{\partial U_m}{\partial \mathbf{x}} = \chi_\perp (\nabla \mathbf{H})^\top \mathbf{H} + \Delta\chi (\mathbf{H} \cdot \mathbf{n}) (\nabla \mathbf{H})^\top \mathbf{n}, \quad (3.99)$$

since the field  $\mathbf{n}$  is regarded as fixed in computing this derivative. To prove that (3.99) delivers the same body force  $\mathbf{b}$  as (3.96a), we need only remark that  $\mathbf{H}$  is irrotational in  $\mathfrak{B}$ , and so its gradient  $\nabla \mathbf{H}$  is a symmetric tensor.

By (3.92),  $-U_m$  is the magnetic energy that must be minimized together with the elastic energy  $W$  for  $\mathbf{n}$  to attain a stable configuration. It readily follows from (3.98) that for  $\Delta\chi > 0$  the energy  $-U_m$  is minimized when  $\mathbf{n}$  is parallel to  $\mathbf{H}$ , whereas for  $\Delta\chi < 0$  it is minimized for  $\mathbf{n}$  orthogonal to  $\mathbf{H}$ . This shows how a magnetic field interacts with the nematic director. A completely analogous characterization can be derived for the action of an electric field in the linear regime.<sup>32</sup>

### 3.1.5 Thermal Effects

We have so far studied the isothermal dynamics of liquid crystals: all thermal effects have been deliberately neglected. On the other hand, in Section 2.3.3, we have shown already how heat conduction can be incorporated in the theory of isotropic, linearly viscous fluids, including the temperature gradient  $\mathbf{g} := \nabla\theta$  among the local measures of dissipation. Here, following closely the line of thought presented in Section 2.3.3, we set the scene to study thermal effects in liquid crystals: we shall encounter a new torque affecting the director motion, which is imparted by a temperature gradient. We shall see how the polar symmetry of nematics prevents such an action from deploying, so that it will be effective only in cholesteric liquid crystals, proving itself a cause likely to explain an old effect, first observed by LEHMANN [178].

As we first did in (2.282), we allow  $\mathbf{g}$  in the collection  $\mathbf{d}$  of dissipation measures, along with  $\mathbf{D}$  and  $\dot{\mathbf{n}}$ . A quadratic form in  $(\mathbf{g}, \mathbf{D}, \dot{\mathbf{n}})$ , which may also depend on  $\mathbf{n}$  as a parameter, is both hemitropic and even under simultaneous inversion of  $\mathbf{n}$  and  $\dot{\mathbf{n}}$ , only if represented in the form<sup>33</sup>

<sup>31</sup> With the aid of the projection that makes  $\mathbf{k}_n$  obey the condition  $\mathbf{k}_n \cdot \mathbf{n} = 0$ .

<sup>32</sup> MAXWELL's equations have here made only a partial appearance. We have subjected  $\mathbf{H}$  to  $\text{curl } \mathbf{H} = \mathbf{0}$ , but we neglected to enforce  $\text{div } \mathbf{B} = 0$ , where the magnetic induction  $\mathbf{B}$  is related to  $\mathbf{H}$  in a fashion similar to (3.94). An approximation in which the equation for  $\mathbf{B}$  can be ignored is discussed in [353, § 4.1.1], to which we also refer the reader for an analogous discussion on the dielectric interaction.

<sup>33</sup> The two hemitropic, but not isotropic, terms appearing in (3.100) are similar in structure to (3.50), which was ruled out by the nematic symmetry (3.4); the inclusion of  $\mathbf{g}$  in the list  $\mathbf{d}$  of dissipation measures has made these terms available. See also [279].



$$\begin{aligned}
R(\mathbf{n}; \mathbf{g}, \mathbf{D}, \dot{\mathbf{n}}) = & \frac{1}{2}\gamma_1 \dot{\mathbf{n}}^2 + \gamma_2 \dot{\mathbf{n}} \cdot \mathbf{D}\mathbf{n} + \frac{1}{2}\gamma_3 (\mathbf{D}\mathbf{n})^2 + \frac{1}{2}\gamma_4 (\mathbf{n} \cdot \mathbf{D}\mathbf{n})^2 + \frac{1}{2}\gamma_5 \operatorname{tr} \mathbf{D}^2 \\
& + \frac{1}{2}\bar{\kappa}_1 \mathbf{g}^2 + \frac{1}{2}\bar{\kappa}_2 (\mathbf{g} \cdot \mathbf{n})^2 + \bar{\kappa}_3 \mathbf{g} \cdot \mathbf{n} \times \dot{\mathbf{n}} + \bar{\kappa}_4 \mathbf{g} \cdot \mathbf{D}\mathbf{n} \times \mathbf{n},
\end{aligned} \tag{3.100}$$

where the first five terms reproduce the dissipation function in (3.49), the sixth term is the analogue of the thermal term in (2.282), and only the last three terms are new, the first reflecting the anisotropy of the medium and the last two expressing thermal interactions with director relaxation and flow, respectively. Together with the  $\gamma$ 's, the  $\bar{\kappa}$ 's are now functions of the temperature  $\theta$ .

For  $R$  in (3.100) to be positive semidefinite, these functions cannot be arbitrary. Reasoning precisely as we did to obtain the inequalities (3.57), we prove that these must be supplemented by the following to ensure positive semidefiniteness to the extended dissipation in (3.100):

$$\begin{aligned}
\bar{\kappa}_1 + \bar{\kappa}_2 &\geq 0, \\
\bar{\kappa}_1(\gamma_3 + 2\gamma_5) - \bar{\kappa}_3^2 &\geq 0, \\
\gamma_1 \bar{\kappa}_1 - \bar{\kappa}_4^2 &\geq 0, \\
\bar{\kappa}_1[\gamma_1(\gamma_3 + 2\gamma_5) - \gamma_2^2] - 2\gamma \bar{\kappa}_3 \bar{\kappa}_4 - \gamma_1 \bar{\kappa}_3^2 - \bar{\kappa}_4^2(\gamma_3 + 2\gamma_5) &\geq 0.
\end{aligned}$$

Requiring  $R$  in (3.100) to be an isotropic function, so as to comply with the symmetry of nematic liquid crystals, would set both  $\bar{\kappa}_3$  and  $\bar{\kappa}_4$  equal to zero. It will be apparent below how this would simply reduce all thermal effects to an anisotropic heat conduction. Thus, to avoid lessening the consequences of the theory, in this section we shall consider cholesteric liquid crystals.

Allowing for thermal effects, we also need to consider an elastic free-energy density  $W$  depending on the temperature  $\theta$ . That this can be achieved by simply regarding the elastic constants in FRANK's formula (3.32) as functions of  $\theta$  or by resorting to a more general functional dependence is here immaterial: we shall simply assume that  $W = W(\theta, \mathbf{n}, \nabla \mathbf{n})$ , so as to write the time rate of the free energy  $\mathcal{F}$  as

$$\dot{\mathcal{F}}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \left[ \frac{\partial W}{\partial \theta} \dot{\theta} + \frac{\partial W}{\partial \mathbf{n}} \cdot \dot{\mathbf{n}} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n}) \cdot \right] dV. \tag{3.101}$$

Echoing (2.284), we assume that the entropy per unit volume,  $\varrho\eta$ , is a function of  $(\theta, \mathbf{n}, \nabla \mathbf{n})$ :

$$\varrho\eta = H(\theta, \mathbf{n}, \nabla \mathbf{n}), \tag{3.102}$$

so that, by (2.209), the thermal production  $\mathcal{T}$  can be written as

$$\mathcal{T}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \left( H\dot{\theta} + \frac{1}{\theta} \mathbf{q} \cdot \mathbf{g} \right) dV, \tag{3.103}$$

where  $\mathbf{q}$  is the heat flux. According to the general prescription (2.210), the total working  $\mathcal{W}$  in (3.5) here becomes

$$\mathcal{W}^{(t)} = \mathcal{W}^{(a)} + \mathcal{W}^{(c)} - \dot{\mathcal{K}} - \dot{\mathcal{F}} - \mathcal{T},$$

where  $\mathcal{W}^{(a)}$ ,  $\mathcal{W}^{(c)}$ , and  $\dot{\mathcal{K}}$  are still given by (3.7), (3.9), and (3.10), respectively, while  $\dot{\mathcal{F}}$  and  $\mathcal{T}$  are as in (3.101) and (3.103) above.

The form of the principle of minimal reduced dissipation appropriate to the present setting is thus

$$\delta \mathcal{W}^{(t)} = \delta \mathcal{R}, \quad (3.104)$$

where  $\mathcal{R}$  is the functional with density  $R$  in (3.100), formally defined as in (3.38). An easy computation shows that

$$\delta \mathcal{W}^{(t)} = \delta \mathcal{W} - \int_{\mathcal{V}_t} \left( H \delta \dot{\theta} + \frac{1}{\theta} \mathbf{q} \cdot \mathbf{g} \right) dV - \int_{\mathcal{V}_t} \frac{\partial W}{\partial \theta} \delta \dot{\theta} dV,$$

which, by combining (3.23) with the reasoning that in Section 2.3.3 led us to (2.286a) and (2.289), here we conclude that

$$H = -\frac{\partial W}{\partial \theta} \quad (3.105)$$

and

$$\mathbf{q} = -\theta \frac{\partial R}{\partial \mathbf{g}}. \quad (3.106)$$

While the former equation simply restates for liquid crystals the result proved in (2.247) for classical fluids, the latter extends the classical FOURIER's law. It is readily seen from (3.100) that  $\mathbf{q}$  is explicitly given by

$$\mathbf{q} = -\kappa_1 \mathbf{g} - \kappa_2 (\mathbf{g} \cdot \mathbf{n}) \mathbf{n} - \kappa_3 \mathbf{n} \times \dot{\mathbf{n}} - \kappa_4 \mathbf{D} \mathbf{n} \times \mathbf{n},$$

where the functions  $\kappa_i$  of  $\theta$  defined by

$$\kappa_i := \theta \bar{\kappa}_i, \quad i = 1, \dots, 4,$$

represent generalized thermal conductivities.

Equations (3.105) and (3.106) followed from the thermal variations  $(\delta \theta, \delta \mathbf{g})$  in (3.104); the mechanical variations  $(\delta \mathbf{v}, \delta \dot{\mathbf{n}})$  are to be performed precisely as they were in Section 3.1.2 above, and they yield formally the same balance equations as in (3.42) and (3.46). However, new thermal contributions can be recognized in both the dissipative stress tensor  $\mathbf{T}_{\text{dis}}$  and the viscous generalized force  $\mathbf{g}_n$ , still delivered by (3.45) and (3.68), but with  $R$  as in (3.100); these are given by

$$\mathbf{T}_{\text{dis}}^{(t)} = \frac{1}{2} \bar{\kappa}_3 [\mathbf{n} \otimes (\mathbf{g} \times \mathbf{n}) + (\mathbf{g} \times \mathbf{n}) \otimes \mathbf{n}] + \bar{\kappa}_4 \overline{(\mathbf{n} \times \mathbf{g}) \otimes \mathbf{n}} \quad (3.107)$$

and

$$\mathbf{g}_n^{(t)} = -\bar{\kappa}_3 \mathbf{g} \times \mathbf{n},$$

respectively. Thus, the stress tensor  $\mathbf{T}$  that enters the balance of linear momentum (3.42) now reads

$$\mathbf{T} = -p\mathbf{I} + \mathbf{T}_E + \mathbf{T}_{\text{dis}}^{(m)} + \mathbf{T}_{\text{dis}}^{(t)},$$

where  $\mathbf{T}_E$  is the ERICKSEN stress (3.31),  $\mathbf{T}_{\text{dis}}^{(m)}$  is the mechanical dissipative stress tensor, still given by (3.59), and  $\mathbf{T}_{\text{dis}}^{(t)}$  is the thermal stress in (3.107). Likewise, the balance of torques expressed by (3.70) now becomes

$$\mathbf{n} \times (\mathbf{g}_n^{(m)} + \mathbf{g}_n^{(t)} + \mathbf{h}_n + \mathbf{k}_n) = \mathbf{0}, \quad (3.108)$$

where  $\mathbf{g}_n^{(m)}$  is the mechanical generalized force, which by (3.58) can still be written as

$$\mathbf{g}_n^{(m)} = -\gamma_1 \dot{\mathbf{n}} - \gamma_2 [\mathbf{D}\mathbf{n} - (\mathbf{D}\mathbf{n} \cdot \mathbf{n})\mathbf{n}],$$

though the viscosities  $\gamma_1$  and  $\gamma_2$  are now functions of temperature. In (3.108),

$$\mathbf{k}^{(t)} := \mathbf{n} \times \mathbf{g}_n^{(t)} = -\bar{\kappa}_3 \mathbf{n} \times (\mathbf{g} \times \mathbf{n}) = -\bar{\kappa}_3 [\mathbf{g} - (\mathbf{g} \cdot \mathbf{n})\mathbf{n}] \quad (3.109)$$

is clearly to be interpreted as the *thermal torque* acting on the director.<sup>34</sup>

LEHMANN [178] first noted a thermal phenomenon in cholesteric liquid crystals that is now traditionally named after him. He observed that an undistorted cholesteric texture like the one represented by equation (3.33) would perform a precessional motion at uniform rotational speed, as though it were a rigid whole, once subjected to a temperature gradient  $\mathbf{g}$  directed along the helical axis  $\mathbf{e}_3$ . No flow appears to sustain the motion, which is ultimately a uniform rotation of all directors  $\mathbf{n}$  about the axis  $\mathbf{e}_3$ . LESLIE [181] showed how the thermal torque in equation (3.109) has the potential to explain LEHMANN's effect:<sup>35</sup> since  $\mathbf{g}$  is orthogonal to  $\mathbf{n}$ , in this case  $\mathbf{k}^{(t)}$  is parallel to  $\mathbf{g}$ ; in general, as shown by (3.109),  $\mathbf{k}^{(t)}$  is proportional to the component of  $\mathbf{g}$  orthogonal to  $\mathbf{n}$ .

As also shown by LESLIE [181], the mechanical balance equations must be supplemented by an equation for the thermal field  $\theta$ : in LEHMANN's problem this equation is solved by a constant  $\mathbf{g}$ , orthogonal to the plates bounding the sample, which

<sup>34</sup> Though  $\mathbf{k}^{(t)}$  is clearly responsible for the thermal effects in cholesteric liquid crystals, the reader should not be induced to believe that it is the only one depending on the temperature: all other torques in (3.108) actually do.

<sup>35</sup> LEHMANN's effect was also referred to by OSEEN [259] as follows: "He [Lehmann] found that in certain cases a substance, spread out between two glass surfaces, would be put into motion, when influenced by a flow of heat coming from below, during which motion the different drops of liquid seemed to be in violent rotation. Further investigations convinced Lehmann that in this case it was not the drop itself, but the structure that moved." It is instructive to read how LESLIE [181] in turn comments about OSEEN's interpretation of LEHMANN's effect: "Oseen goes on to state that he considered that the motion was due to the molecules rotating with uniform speed around vertical axes drawn through their centres of gravity. He claims that his theory provided an explanation of the violent rotation, since his viscous terms vanished for such a motion. However, he offered no explanation of the forces creating the motion." The torques responsible for LEHMANN's effect have the thermal nature first illuminated by LESLIE [181]. We also refer the reader to [182], [34], and [75], where thermomechanical effects in cholesteric liquid crystals are further explored.

are taken at constant, different temperatures. As already shown in Section 2.3.3, such an equation stems from the first law of thermodynamics (2.195). Letting the internal energy per unit volume be denoted by  $W_e$ , by (2.204), (3.102), and (3.105), we set

$$W_e := W + \theta H = W - \theta \frac{\partial W}{\partial \theta}. \quad (3.110)$$

Thus, (2.195) becomes

$$\left( \int_{\mathcal{P}_t} W_e dV \right)' = \mathcal{W}^{(e)}(\mathcal{P}_t, \chi) + \mathcal{Q}(\mathcal{P}_t, \chi), \quad (3.111)$$

where  $\mathcal{W}^{(e)} = \mathcal{W}^{(a)} - \dot{\mathcal{K}}$  is the external power,<sup>36</sup> and  $\mathcal{Q}$  is the heating, which we recall from (2.194),

$$\mathcal{Q}(\mathcal{P}_t, \chi) = - \int_{\partial^* \mathcal{P}_t} \mathbf{q} \cdot \mathbf{v} dA + \int_{\mathcal{P}_t} \sigma dV, \quad (3.112)$$

where  $\sigma$  is the heat supply.

Before deriving from the local form of (3.111) the energy balance equation, we find it instructive to give  $\mathcal{W}^{(e)}$  an equivalent form, valid along the solutions to the mechanical balance equations, thus extending a result obtained in (2.136) for the power stress of classical continuum mechanics. It readily follows from (3.42) and (3.46) that

$$\begin{aligned} \mathcal{W}^{(e)}(\mathcal{P}_t, \chi) &= \int_{\mathcal{P}_t} \left[ -\operatorname{div} \mathbf{T} \cdot \mathbf{v} + \left( \frac{\partial R}{\partial \dot{\mathbf{n}}} + \frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \cdot \dot{\mathbf{n}} \right] dV \\ &\quad + \int_{\partial^* \mathcal{P}_t} \left( \mathbf{T} \mathbf{v} \cdot \mathbf{v} + \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \cdot \dot{\mathbf{n}} \right) dA \\ &= \int_{\mathcal{P}_t} \left[ \mathbf{T} \cdot \nabla \mathbf{n} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot \nabla \dot{\mathbf{n}} + \left( \frac{\partial R}{\partial \dot{\mathbf{n}}} + \frac{\partial W}{\partial \mathbf{n}} \right) \cdot \dot{\mathbf{n}} \right] dV \\ &=: \mathcal{W}^{(i)}(\mathcal{P}_t, \chi), \end{aligned} \quad (3.113)$$

where, as in (2.136),  $\mathcal{W}^{(i)}$  is interpreted as the power of all *internal actions*. Like (2.137), equation (3.113) expresses the balance of power: the power expended in an inertial frame by the external forces applied to a subbody  $\mathcal{P}$  in a motion  $\chi$  is balanced by the power expended by the internal forces and the rate of change of the kinetic energy. Clearly, in this case the viscous, dissipative actions, which also include thermal contributions, are to be reckoned among the internal forces.

Letting

$$W^{(i)} := \mathbf{T} \cdot \nabla \mathbf{v} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot \nabla \dot{\mathbf{n}} + \left( \frac{\partial R}{\partial \dot{\mathbf{n}}} + \frac{\partial W}{\partial \mathbf{n}} \right) \cdot \dot{\mathbf{n}} \quad (3.114)$$

denote the density per unit volume of the internal power  $\mathcal{W}^{(i)}$ , by (3.110) and (3.112), we give (3.111) the following local form:

<sup>36</sup> With  $\mathcal{W}^{(e)}$  and  $\dot{\mathcal{K}}$  as in (3.7) and (3.10), respectively.

$$\left( W - \theta \frac{\partial W}{\partial \theta} \right)^{\cdot} = W^{(i)} - \operatorname{div} \mathbf{q} + \sigma. \quad (3.115)$$

We shall soon give an equivalent, more expressive variant of this equation. Here we pause to remark that, by (3.113),  $\mathscr{W}^{(i)}$  must be frame-indifferent, since  $\mathscr{W}^{(e)}$  is so. On the other hand, the single terms that constitute  $W^{(i)}$  are not frame-indifferent. It is instructive to transform  $W^{(i)}$  in (3.114) into a sum of indifferent terms. To this end, writing  $\nabla \mathbf{v} = \mathbf{D} + \mathbf{W}$  and making use of (3.44), we easily prove that

$$\mathbf{T} \cdot \nabla \mathbf{v} = \mathbf{T} \cdot \mathbf{D} - \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n}) \mathbf{W} + \mathbf{n} \cdot \mathbf{W} \frac{\partial R}{\partial \dot{\mathbf{n}}}. \quad (3.116)$$

Using (3.116), (3.36), and (3.21) in (3.114), we arrive at

$$W^{(i)} = \mathbf{T} \cdot \mathbf{D} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot [\nabla \dot{\mathbf{n}} - \mathbf{W}(\nabla \mathbf{n})] + \left( \frac{\partial R}{\partial \dot{\mathbf{n}}} + \frac{\partial W}{\partial \mathbf{n}} \right) \cdot \dot{\mathbf{n}}. \quad (3.117)$$

While the first and last terms on the right-hand side of (3.117) are clearly frame-indifferent, proving that the tensor  $[\nabla \dot{\mathbf{n}} - \mathbf{W}(\nabla \mathbf{n})]$  is also indifferent is an exercise that at this stage the reader should be able to do with little<sup>37</sup> or no guidance.

Yet another form of  $W^{(i)}$  may be derived, which further simplifies (3.115). Since  $\operatorname{tr} \mathbf{D} = 0$ ,

$$\mathbf{T} \cdot \mathbf{D} = \mathbf{T}_{\text{dis}} \cdot \mathbf{D} - (\nabla \mathbf{n})^{\top} \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot \mathbf{D}, \quad (3.118)$$

where  $\mathbf{T}_{\text{dis}} = \mathbf{T}_{\text{dis}}^{(m)} + \mathbf{T}_{\text{dis}}^{(i)}$  is the total dissipative stress tensor. It follows from inserting (3.118) into (3.117), from making again use of (3.36) and (3.21), and from applying the kinematic identity (3.16) that

$$W^{(i)} = \mathbf{T}_{\text{dis}} \cdot \mathbf{D} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^{\cdot} + \frac{\partial W}{\partial \mathbf{n}} \cdot \dot{\mathbf{n}}. \quad (3.119)$$

Computing  $\dot{W}$  in (3.115) with the aid of the identity

$$\dot{W} = \frac{\partial W}{\partial \theta} \dot{\theta} + \frac{\partial W}{\partial \mathbf{n}} \cdot \dot{\mathbf{n}} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^{\cdot},$$

already implicit in (3.101), we readily obtain from (3.119) that (3.115) reduces to

$$-\left( \frac{\partial W}{\partial \theta} \right)^{\cdot} \theta = \mathbf{T}_{\text{dis}} \cdot \mathbf{D} + \dot{\mathbf{n}} \cdot \frac{\partial R}{\partial \dot{\mathbf{n}}} - \operatorname{div} \mathbf{q} + \sigma, \quad (3.120)$$

where all terms are frame-indifferent and  $\mathbf{q}$  is given by (3.106). Equation (3.120) is the energy balance equation, which must be added to the mechanical balances to determine the evolution of the temperature  $\theta$  along with that of the director  $\mathbf{n}$  and the flow  $\mathbf{v}$ .

<sup>37</sup> The reader is advised to prove first that  $(\nabla \dot{\mathbf{n}})^* = \mathbf{\Omega}(\nabla \mathbf{n})^* + \mathbf{R} \nabla \dot{\mathbf{n}} \mathbf{R}^{\top}$ , where  $\mathbf{\Omega}$  is the spin tensor in (2.50), and then employ (2.63) together with the frame-indifference of  $\nabla \mathbf{n}$ , that is,  $(\nabla \mathbf{n})^* = \mathbf{R} \nabla \mathbf{n} \mathbf{R}^{\top}$ .

One final consequence can be drawn from (3.117) when the director  $\mathbf{n}$  is conveyed by the flow. Whenever this is case,  $\dot{\mathbf{n}}$  vanishes identically and (3.117) reduces to

$$W^{(i)} = \mathbf{T} \cdot \mathbf{D} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot [\nabla \dot{\mathbf{n}} - \mathbf{W}(\nabla \mathbf{n})],$$

where now  $\dot{\mathbf{n}} \equiv \mathbf{W}\mathbf{n}$ . By differentiating in space both sides of this latter identity and applying (3.75), we arrive at

$$W^{(i)} = \mathbf{T} \cdot \mathbf{D} + \mathbf{L} \cdot \nabla \mathbf{w}, \quad (3.121)$$

where  $\mathbf{w}$  is the spin vector. Equation (3.121) coincides with (2.146), thus showing that here the balance of power reduces to that contemplated by BEATTY's theory of general interactions presented in Section 2.1.6 only when the motion of  $\mathbf{n}$  relative to the flow is artificially suppressed. An equivalent way of saying this is that BEATTY's theory is subsumed under ERICKSEN-LESLIE's.

## 3.2 Variable Degree of Orientation

We have seen in Section 1.3 that the MAIER-SAUPE mean field theory predicts uniaxial equilibrium states of the form

$$\mathbf{Q} = S \left( \mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right), \quad (3.122)$$

with a temperature-dependent scalar order parameter  $S$  that is given by

$$S = \langle P_2(\mathbf{n} \cdot \mathbf{u}) \rangle,$$

where the brackets  $\langle \dots \rangle$  indicate a local orientational average over the molecules and  $P_2$  is the second Legendre polynomial in  $\mathbf{n} \cdot \mathbf{u}$ , the cosine of the angle between the molecular figure symmetry axis  $\mathbf{u}$  and the nematic director  $\mathbf{n}$ .  $S$  can take values between  $-\frac{1}{2}$  and 1. It can be expected and it is usually observed that the alignment is well approximated by the form (3.122) also away from equilibrium as long as distortions do not get too large. A theory for uniaxial nematics with variable order can naturally be obtained as a special case of a theory for the alignment tensor as treated in Chapter 4. Here, following mainly ERICKSEN [99], we directly derive such a theory by treating  $S$  and  $\mathbf{n}$  as independent variables and extending the uniaxial director theory with constant scalar order presented in the preceding section. In this way, the new theory arises as an extension of the old one, and the differences between the two theories present themselves in a most transparent fashion.

The formal development of the theory is precisely the same as before, but now the ingredients of the power and dissipation can also depend on the variable scalar order parameter  $S$  and its spatial and time derivatives. D'ALEMBERT's principle and the principle of reduced minimum dissipation hold in the very same form. However, because  $\mathbf{n}$  and  $S$  are treated as independent variables, a new independent generalized velocity  $\dot{S}$  is present, and apart from the equations governing flow and director evolution, a third equation for the evolution of  $S$  arises.

### 3.2.1 Nondissipative Dynamics

Conceptually, our development here parallels rather closely that of Section 3.1, and so we can afford to be more concise, almost schematic.

#### External Agents

The external power expended on a uniaxial nematic with variable order is an extension of (3.7) that accounts for possible external actions on  $S$ ,

$$\mathcal{W}^{(a)}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} (\mathbf{b} \cdot \mathbf{v} + \mathbf{k}_n \cdot \dot{\mathbf{n}} + L\dot{S}) dV + \int_{\partial^* \mathcal{P}_t} (\mathbf{t} \cdot \mathbf{v} + \mathbf{c}_n \cdot \dot{\mathbf{n}} + K\dot{S}) dA,$$

where  $L$  and  $K$  are generalized body and contact force densities acting on the order parameter  $S$ .

#### Power of the Constraints

The constraints on the velocity field and the unit director are the same as before. Although  $S$  is by its definition constrained<sup>38</sup> to be between  $-\frac{1}{2}$  and 1, we treat it as a free variable, and so we have, as before,

$$\mathcal{W}^{(c)}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} (\gamma \mathbf{n} \cdot \dot{\mathbf{n}} - \nabla p \cdot \mathbf{v}) dV + \int_{\partial^* \mathcal{P}_t} p \mathbf{v} \cdot \mathbf{v} dA.$$

#### Kinetic Energy

While the kinetic energy in principle contains a contribution related to  $\dot{S}$ , this is generally negligible for the same reasons cited before, namely, that molecular inertia is small. Thus we use as before

$$\mathcal{K}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \rho \dot{\mathbf{v}} \cdot \mathbf{v} dV.$$

#### Free Energy

The free energy density is now a function  $W = W(S, \nabla S, \mathbf{n}, \nabla \mathbf{n})$ , and it will in general contain not only elastic terms, but also a LANDAU-DE GENNES potential in  $S$ , which is illustrated in detail in Section 4.1.1. In analogy to (3.22),  $W$  has to satisfy the invariance requirement

$$W(\mathbf{n}, \nabla \mathbf{n}) = W(S, \mathbf{R} \nabla S, \mathbf{R} \mathbf{n}, \mathbf{R} \nabla \mathbf{n} \mathbf{R}^T) \quad (3.123)$$

<sup>38</sup> The unilateral bounds to which  $S$  is subject are different from the other constraints considered so far: they are to be valid on the solutions to the equations of the theory and may be favored by the action of some internal potential, such as the one considered in Section 4.1.1.

for any proper orthogonal transformation  $\mathbf{R}$ .

We again have

$$\dot{\mathcal{F}}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \dot{W} dV,$$

where now

$$\dot{W} = \frac{\partial W}{\partial \mathbf{n}} \cdot \dot{\mathbf{n}} + \frac{\partial W}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^\cdot + \frac{\partial W}{\partial S} \dot{S} + \frac{\partial W}{\partial \nabla S} \cdot (\nabla S)^\cdot.$$

Computations analogous to those performed to arrive at (3.16) show that the material time derivative of the gradient of  $S$  can be written as

$$(\nabla S)^\cdot = \nabla \dot{S} - (\nabla \mathbf{v})^\top \nabla S.$$

With this, after an integration by parts we find that

$$\begin{aligned} \dot{\mathcal{F}}(\mathcal{P}_t, \chi) = & \int_{\mathcal{P}_t} \left\{ \operatorname{div} \left[ (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} + \nabla S \otimes \frac{\partial W}{\partial \nabla S} \right] \cdot \mathbf{v} \right. \\ & + \left( \frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \cdot \dot{\mathbf{n}} + \left( \frac{\partial W}{\partial S} - \operatorname{div} \frac{\partial W}{\partial \nabla S} \right) \cdot \dot{S} \Big\} dV \\ & + \int_{\partial^* \mathcal{P}_t} \left\{ \left[ -(\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} - \nabla S \otimes \frac{\partial W}{\partial \nabla S} \mathbf{v} \right] \cdot \mathbf{v} \right. \\ & \left. + \left( \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \right) \cdot \dot{\mathbf{n}} + \left( \frac{\partial W}{\partial \nabla S} \cdot \mathbf{v} \right) \dot{S} \right\} dA. \end{aligned}$$

### Variation of the Working

Requiring the variation  $\delta \mathcal{W}$  of the total power to vanish shows that the equations for the director remain the same as before, while the balance of linear momentum and the associated traction condition hold with the stress tensor

$$\mathbf{T} = -p \mathbf{I} - (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} - \nabla S \otimes \frac{\partial W}{\partial \nabla S}.$$

In addition, requiring the generalized forces multiplying the variations  $\delta \dot{S}$  to vanish shows that the equation

$$\frac{\partial W}{\partial S} - \operatorname{div} \frac{\partial W}{\partial \nabla S} = L \quad (3.124)$$

must hold in  $\mathcal{P}_t$  and that

$$\frac{\partial W}{\partial \nabla S} \cdot \mathbf{v} = K$$

on  $\partial^* \mathcal{P}_t$ .



### 3.2.2 Dissipative Dynamics

Since  $S$  is an indifferent scalar, its material time derivative  $\dot{S}$  is frame-indifferent by (2.80), and we can construct the dissipation function as  $R = R(\mathbf{n}, S; \mathbf{D}, \dot{\mathbf{n}}, \dot{S})$ , which is a quadratic form in  $(\mathbf{D}, \dot{\mathbf{n}}, \dot{S})$ , where both  $\mathbf{n}$  and  $S$  are regarded as parameters. The most general shape this can take that complies with the nematic symmetry (3.4) is

$$\begin{aligned} R(\mathbf{n}, S; \mathbf{D}, \dot{\mathbf{n}}, \dot{S}) = & \beta_1 \dot{S} \mathbf{n} \cdot \mathbf{D} \mathbf{n} + \frac{1}{2} \beta_2 \dot{S}^2 + \frac{1}{2} \gamma_1 \dot{\mathbf{n}}^2 + \gamma_2 \dot{\mathbf{n}} \cdot \mathbf{D} \mathbf{n} \\ & + \frac{1}{2} \gamma_3 (\mathbf{D} \mathbf{n})^2 + \frac{1}{2} \gamma_4 (\mathbf{n} \cdot \mathbf{D} \mathbf{n})^2 + \frac{1}{2} \gamma_5 \text{tr} \mathbf{D}^2, \end{aligned} \quad (3.125)$$

where only two new viscosity coefficients  $\beta_1$  and  $\beta_2$  are needed to account for the dissipation due to changes in  $S$ . However, the viscosity coefficients are no longer constants, but all  $\beta$ 's and  $\gamma$ 's are functions of  $S$  subject to the requirement that  $R$  in (3.125) be positive semidefinite. Reasoning as to arrive at (3.57) above, we easily prove that the positive semidefiniteness of  $R$  is equivalent to the following list of inequalities:

$$\begin{aligned} \gamma_1 &\geq 0, \\ \gamma_5 &\geq 0, \\ \gamma_1(\gamma_3 + 2\gamma_5) - \gamma_2^2 &\geq 0, \\ \beta_2 &\geq 0, \\ \beta_2(2\gamma_4 + 2\gamma_3 + 3\gamma_5) - \beta_1^2 &\geq 0, \end{aligned}$$

which were also obtained by ERICKSEN [99] by a different method.

It then follows that the equations of motion still hold in the form (3.24) and (3.25), where the stress instead of being given by (3.44) is now

$$\begin{aligned} \mathbf{T} = & -p \mathbf{I} - (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} + \frac{1}{2} \left( \mathbf{n} \otimes \frac{\partial R}{\partial \dot{\mathbf{n}}} - \frac{\partial R}{\partial \dot{\mathbf{n}}} \otimes \mathbf{n} \right) + \frac{\partial R}{\partial \mathbf{D}} \\ & - \nabla S \otimes \frac{\partial W}{\partial \nabla S} + \beta_1 \dot{S} \overline{\mathbf{n} \otimes \mathbf{n}}. \end{aligned}$$

Furthermore, the additional equation (3.124) becomes

$$\frac{\partial W}{\partial S} - \text{div} \frac{\partial W}{\partial \nabla S} + \frac{\partial R}{\partial \dot{S}} = L,$$

which with (3.125) is

$$\frac{\partial W}{\partial S} - \text{div} \frac{\partial W}{\partial \nabla S} + \beta_1 \mathbf{n} \cdot \mathbf{D} \mathbf{n} + \beta_2 \dot{S} = L.$$

Apart from the microinertia, which we have neglected here, the evolution equations that we find are the same as ERICKSEN's [99], where again the extra PARODI-type relation he derived is automatically satisfied.

### 3.2.3 Rotational Momentum and Couple Stress

The invariance property (3.123) of the free energy here leads us to the equation

$$\left[ \nabla S \otimes \frac{\partial W}{\partial \nabla S} + \frac{\partial W}{\partial \mathbf{n}} \otimes \mathbf{n} + \frac{\partial W}{\partial \nabla \mathbf{n}} (\nabla \mathbf{n})^\top + \left( \frac{\partial W}{\partial \nabla \mathbf{n}} \right)^\top (\nabla \mathbf{n}) \right] \in \text{Sym}(\mathcal{V}),$$

in analogy to (3.21). Performing exactly the same computations as in Section 3.1.3 for the standard director theory then shows that the balance of rotational momentum holds with body couple and couple stress that are formally precisely the same as in (3.72) and (3.73). No use is made in this derivation of the balance equation (3.124) for  $S$ , and the external actions on  $S$  do not contribute to the body couple. This shows that while once again the classical balance equation of rotational momentum is valid, other than in the case of the standard ERICKSEN–LESLIE theory, the continuum theory for a director with variable scalar order parameter cannot simply be reduced to the balance of rotational momentum.

## 3.3 Biaxial Nematics

As we have seen in Chapter 1, the average orientation of an ensemble of biaxial molecules can be represented by two order tensors  $\mathbf{Q}$  and  $\mathbf{B}$ , defined in (1.66) in terms of their microscopic counterparts  $\mathbf{q}$  and  $\mathbf{b}$ . If the simplifying assumption is made that these tensors share a common eigenframe  $(\mathbf{n}, \mathbf{m}, \mathbf{l})$ , they can be written in the form

$$\mathbf{Q} = S \left( \mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) + T (\mathbf{m} \otimes \mathbf{m} - \mathbf{l} \otimes \mathbf{l}), \quad (3.126a)$$

$$\mathbf{B} = S' \left( \mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) + T' (\mathbf{m} \otimes \mathbf{m} - \mathbf{l} \otimes \mathbf{l}) \quad (3.126b)$$

with four scalar order parameters  $S$ ,  $T$ ,  $S'$ , and  $T'$ .

It is easy to confuse the microscopic origin of biaxiality and its macroscopic manifestation. Even experienced researchers have made the simplification of identifying the microscopic molecular axes with the macroscopic directors, for example in [43]. However, this is sensible and permissible only in special cases, such as for a perfectly oriented sample. In such a sample, the four order parameters have the values  $T = S' = 0$  and  $S = T' = 1$ , and so  $\mathbf{Q}$  and  $\mathbf{B}$  take the form

$$\mathbf{Q} = \mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \quad \text{and} \quad \mathbf{B} = \mathbf{m} \otimes \mathbf{m} - \mathbf{l} \otimes \mathbf{l}.$$

In this case, all the long molecular axes are aligned along the common direction  $\mathbf{n}$  and all short molecular axes are aligned along  $\mathbf{m}$ . However, the more general case (3.126) can also be used to motivate a director theory. If all four order parameters are assumed to be constant, the orientation of the biaxial nematic can indeed be

described by the triad of unit vectors  $(\mathbf{n}, \mathbf{m}, \mathbf{l})$ , where now no assumption is made about individual molecules.

The first theories for biaxial nematics were formulated in terms of three perpendicular directors [287, 165, 123]. While this approach has a certain appeal because of its symmetry with respect to the three directors, it ultimately leads to unnecessarily complicated equations. It also fails to account for the fact that the symmetry in the three directors is superficial: there is usually a dominant director that is the only one that survives in the transition from a biaxial to a uniaxial nematic phase.

A more transparent approach was presented in [186]: there the theory is phrased in terms of two unit vectors, the usual director  $\mathbf{n}$  and a single secondary director  $\mathbf{m}$  perpendicular to it.<sup>39</sup> In line with their interpretation as eigenvectors of  $\epsilon$ , both directors have to obey the nematic symmetry, that is, one requires that both  $\mathbf{n} \sim -\mathbf{n}$  and  $\mathbf{m} \sim -\mathbf{m}$ . In practice, this implies that scalar quantities like the elastic free energy have to be even expressions independently in both  $\mathbf{n}$  and  $\mathbf{m}$ . The resulting equations for both directors are analogous to the one for the single director in the uniaxial case, and also many of the stress components are analogous to those found in the uniaxial case. We follow this approach and derive equations for two directors.

### Two-Director Description of the Biaxial Phase

We want to phrase a continuum theory for a biaxial liquid crystal, assuming that the degree of orientational order is constant throughout. This means that we need to employ two orthogonal unit vectors, the directors  $\mathbf{n}$  and  $\mathbf{m}$ . They satisfy the constraints

$$\mathbf{n} \cdot \mathbf{n} \equiv \mathbf{m} \cdot \mathbf{m} \equiv 1, \text{ and } \mathbf{n} \cdot \mathbf{m} \equiv 0. \quad (3.127)$$

We assume biaxial nematic symmetry of the material, that is,

$$\mathbf{n} \sim -\mathbf{n} \quad \text{and} \quad \mathbf{m} \sim -\mathbf{m}. \quad (3.128)$$

#### 3.3.1 Nondissipative Dynamics

Here our development parallels that in Section 3.2.1: an extra order descriptor is added to  $\mathbf{n}$ , but instead of being the scalar  $S$  it is the other director  $\mathbf{m}$ .

#### External Agents

In the case of a biaxial nematic, external agents can expend power against both directors. Even though the directors themselves are not free to move independently, forces acting on them can in principle be completely independent. One could, for example, imagine molecules with two different axes of symmetry where each of the axes is susceptible to a different type of interaction with external fields. The macroscopic

<sup>39</sup> If desired, the third director  $\mathbf{l}$  can always be recovered via the vector product  $\mathbf{l} = \mathbf{n} \times \mathbf{m}$ , but there is no need for  $\mathbf{l}$  to enter explicitly the dynamical equations.

directors as averages of the molecular axes' orientations would in turn be susceptible to different external influences. The power of the external agents is thus given in the general form

$$\begin{aligned} \mathcal{W}^{(a)}(\mathcal{P}_t, \chi) &= \int_{\mathcal{P}_t} (\mathbf{b} \cdot \mathbf{v} + \mathbf{k}_n \cdot \dot{\mathbf{n}} + \mathbf{k}_m \cdot \dot{\mathbf{m}}) dV \\ &+ \int_{\partial^* \mathcal{P}_t} (\mathbf{t} \cdot \mathbf{v} + \mathbf{c}_n \cdot \dot{\mathbf{n}} + \mathbf{c}_m \cdot \dot{\mathbf{m}}) dA \end{aligned} \quad (3.129)$$

with the body force  $\mathbf{b}$  and traction  $\mathbf{t}$ , and generalized volume and surface forces  $\mathbf{k}_n$  and  $\mathbf{c}_n$  acting on  $\mathbf{n}$  and  $\mathbf{k}_m$  and  $\mathbf{c}_m$  acting on  $\mathbf{m}$ .

### Power of the Constraints

The power of the constraints has four parts. As usual, a pressure  $p$  serves as LAGRANGE multiplier for the incompressibility constraint. Three further terms arise from the directors' constraints (3.127): they keep the directors at unit length and perpendicular to each other. We introduce three further LAGRANGE multiplier fields  $\gamma$ ,  $\tau$ , and  $\kappa$  that ensure that the power of the constraints, obtained by differentiating (3.127) with respect to time, vanishes. We obtain

$$\begin{aligned} \mathcal{W}^{(c)}(\mathcal{P}_t, \chi) &= \int_{\mathcal{P}_t} [\gamma \mathbf{n} \cdot \dot{\mathbf{n}} + \tau \mathbf{m} \cdot \dot{\mathbf{m}} + \kappa (\mathbf{m} \cdot \dot{\mathbf{n}} + \mathbf{n} \cdot \dot{\mathbf{m}}) + p \operatorname{div} \mathbf{v}] dV \\ &= \int_{\mathcal{P}_t} [\gamma \mathbf{n} \cdot \dot{\mathbf{n}} + \tau \mathbf{m} \cdot \dot{\mathbf{m}} + \kappa (\mathbf{m} \cdot \dot{\mathbf{n}} + \mathbf{n} \cdot \dot{\mathbf{m}}) - \nabla p \cdot \mathbf{v}] dV \\ &+ \int_{\partial^* \mathcal{P}_t} p \mathbf{v} \cdot \mathbf{v} dA. \end{aligned}$$

### Kinetic Energy

While the kinetic energy in principle contains contributions related to  $\dot{\mathbf{n}}$  and  $\dot{\mathbf{m}}$ , these can usually be considered negligible because of the small molecular inertia. Thus we use as before

$$\mathcal{K}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} \varrho \dot{\mathbf{v}} \cdot \mathbf{v} dV.$$

### Free Energy Density

We assume that the elastic free energy density is a function of the two directors and their first gradients,  $W = W(\mathbf{n}, \nabla \mathbf{n}, \mathbf{m}, \nabla \mathbf{m})$ . For such a function  $W$  to be compatible with the biaxial nematic symmetry (3.128), it has to satisfy

$$W(\mathbf{n}, \nabla \mathbf{n}, \mathbf{m}, \nabla \mathbf{m}) = W(-\mathbf{n}, -\nabla \mathbf{n}, \mathbf{m}, \nabla \mathbf{m}) = W(\mathbf{n}, \nabla \mathbf{n}, -\mathbf{m}, -\nabla \mathbf{m}).$$

Furthermore, in analogy to (3.12),  $W$  has to satisfy the invariance requirement

$$W(\mathbf{n}, \nabla \mathbf{n}, \mathbf{m}, \nabla \mathbf{m}) = W(\mathbf{R}\mathbf{n}, \mathbf{R}\nabla \mathbf{n}\mathbf{R}^\top, \mathbf{R}\mathbf{m}, \mathbf{R}\nabla \mathbf{m}\mathbf{R}^\top),$$

where  $\mathbf{R}$  is an arbitrary orthogonal transformation, or, in the case of a chiral biaxial nematic, a proper orthogonal transformation. The general form of  $W$  is derived in [122], an equivalent expression also including surface terms is given in the appendix of [318].

The total free energy  $\mathcal{F}$  then results as usual from the integral

$$\mathcal{F}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} W(\mathbf{n}, \nabla \mathbf{n}, \mathbf{m}, \nabla \mathbf{m}) dV.$$

Using exactly the same steps that led us to (3.17), we can cast its time rate  $\dot{\mathcal{F}}$  in the form

$$\begin{aligned} \dot{\mathcal{F}}(\mathcal{P}_t, \chi) = & \int_{\mathcal{P}_t} \left\{ \operatorname{div} \left[ (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} + (\nabla \mathbf{m})^\top \frac{\partial W}{\partial \nabla \mathbf{m}} \right] \cdot \mathbf{v} \right. \\ & + \left( \frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} \right) \cdot \dot{\mathbf{n}} + \left( \frac{\partial W}{\partial \mathbf{m}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{m}} \right) \cdot \dot{\mathbf{m}} \Big\} dV \\ & + \int_{\partial^* \mathcal{P}_t} \left\{ \left[ -(\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} + -(\nabla \mathbf{m})^\top \frac{\partial W}{\partial \nabla \mathbf{m}} \mathbf{v} \right] \cdot \mathbf{v} \right. \\ & + \left( \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \right) \cdot \dot{\mathbf{n}} + \left( \frac{\partial W}{\partial \nabla \mathbf{m}} \mathbf{v} \right) \cdot \dot{\mathbf{m}} \Big\} dA. \end{aligned}$$

### Variation of the Working

The variation of the total power  $\mathcal{W}$  now takes the form

$$\begin{aligned} \delta \mathcal{W} = & \int_{\mathcal{P}_t} \left\{ \left[ \mathbf{b} - \nabla p - \rho \dot{\mathbf{v}} - \operatorname{div} \left( (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} + (\nabla \mathbf{m})^\top \frac{\partial W}{\partial \nabla \mathbf{m}} \right) \right] \cdot \delta \mathbf{v} \right. \\ & + \left[ \mathbf{k}_n + \gamma \mathbf{n} + \kappa \mathbf{m} - \frac{\partial W}{\partial \mathbf{n}} + \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} \right] \cdot \delta \dot{\mathbf{n}} \\ & + \left[ \mathbf{k}_m + \tau \mathbf{m} + \kappa \mathbf{n} - \frac{\partial W}{\partial \mathbf{m}} + \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{m}} \right] \cdot \delta \dot{\mathbf{m}} \Big\} dV \\ & + \int_{\partial^* \mathcal{P}_t} \left\{ \left[ \mathbf{t} + \left( p \mathbf{I} + (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} + (\nabla \mathbf{m})^\top \frac{\partial W}{\partial \nabla \mathbf{m}} \right) \mathbf{v} \right] \cdot \delta \mathbf{v} \right. \\ & + \left[ \mathbf{c}_n - \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v} \right] \cdot \delta \dot{\mathbf{n}} + \left[ \mathbf{c}_m - \frac{\partial W}{\partial \nabla \mathbf{m}} \mathbf{v} \right] \cdot \delta \dot{\mathbf{m}} \Big\} dA. \end{aligned}$$

The equations resulting from the requirement that this variation be identically zero are

$$\rho \dot{\mathbf{v}} = \mathbf{b} + \operatorname{div} \mathbf{T},$$

$$\frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \mathbf{k}_n = \gamma \mathbf{n} + \kappa \mathbf{m},$$

and

$$\frac{\partial W}{\partial \mathbf{m}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{m}} - \mathbf{k}_m = \tau \mathbf{m} + \kappa \mathbf{n}$$

in  $\mathcal{P}_t$  and

$$\begin{aligned} \mathbf{t} &= \mathbf{T} \mathbf{v}, \\ \mathbf{c}_n &= \frac{\partial W}{\partial \nabla \mathbf{n}} \mathbf{v}, \end{aligned}$$

and

$$\mathbf{c}_m = \frac{\partial W}{\partial \nabla \mathbf{m}} \mathbf{v},$$

on  $\partial^* \mathcal{P}_t$ . Here, the stress tensor is

$$\mathbf{T} = -p \mathbf{I} - (\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} - (\nabla \mathbf{m})^\top \frac{\partial W}{\partial \nabla \mathbf{m}}.$$

The part of the stress that is analogous to the ERICKSEN stress (3.31) is

$$\mathbf{T}_E = -(\nabla \mathbf{n})^\top \frac{\partial W}{\partial \nabla \mathbf{n}} - (\nabla \mathbf{m})^\top \frac{\partial W}{\partial \nabla \mathbf{m}}.$$

### 3.3.2 Dissipative Dynamics

According to our principle, the dissipation function depends on the stretching  $\mathbf{D}$ , the directors  $\mathbf{n}$  and  $\mathbf{m}$ , and indifferent time derivatives of the directors. We choose the corotational time derivatives

$$\dot{\mathbf{n}} = \dot{\mathbf{n}} - \mathbf{W} \mathbf{n} \quad \text{and} \quad \dot{\mathbf{m}} = \dot{\mathbf{m}} - \mathbf{W} \mathbf{m}.$$

The dissipation function needs to be a quadratic form in  $(\mathbf{D}, \dot{\mathbf{n}}, \dot{\mathbf{m}})$ ; it is found by considering all scalar invariants in these three rates and the two directors. The biaxial nematic symmetry (3.128) requires that this function be even independently in both  $(\mathbf{n}, \dot{\mathbf{n}})$  and  $(\mathbf{m}, \dot{\mathbf{m}})$ . The relevant invariants can be constructed, for example, from the table in [357]. However, the integrity basis given there is minimal only if all the vectors and tensors entering it are unrestrained and independent of one another, so care has to be taken to remove redundant terms.

We write the dissipation function as

$$\begin{aligned} R(\mathbf{n}, \mathbf{m}; \mathbf{D}, \dot{\mathbf{n}}, \dot{\mathbf{m}}) &= \frac{1}{2} \gamma_1 \dot{\mathbf{n}}^2 + \gamma_2 \dot{\mathbf{n}} \cdot \mathbf{D} \mathbf{n} + \frac{1}{2} \gamma_3 (\mathbf{D} \mathbf{n})^2 + \frac{1}{2} \gamma_4 (\mathbf{n} \cdot \mathbf{D} \mathbf{n})^2 + \frac{1}{2} \gamma_5 \operatorname{tr} \mathbf{D}^2 \\ &\quad + \frac{1}{2} \mu_1 \dot{\mathbf{m}}^2 + \mu_2 \dot{\mathbf{m}} \cdot \mathbf{D} \mathbf{m} + \frac{1}{2} \mu_3 (\mathbf{D} \mathbf{m})^2 + \frac{1}{2} \mu_4 (\mathbf{m} \cdot \mathbf{D} \mathbf{m})^2 \\ &\quad + \frac{1}{4} \lambda_1 [(\dot{\mathbf{n}} \cdot \mathbf{m})^2 + (\dot{\mathbf{m}} \cdot \mathbf{n})^2] + \frac{1}{2} \lambda_2 (\dot{\mathbf{n}} \cdot \mathbf{m} - \dot{\mathbf{m}} \cdot \mathbf{n}) (\mathbf{n} \cdot \mathbf{D} \mathbf{m}) \\ &\quad + \frac{1}{2} \lambda_3 (\mathbf{n} \cdot \mathbf{D} \mathbf{m})^2, \end{aligned} \tag{3.130}$$

where the  $\gamma$ 's are the viscosity coefficients already encountered in (3.49) for the single director theory, while the  $\mu$ 's and the  $\lambda$ 's are additional viscosities introduced by the biaxial director theory.<sup>40</sup> The contributions to  $R$  in  $\lambda_1$  and  $\lambda_2$  are written in a symmetric fashion. Only one term is needed for each of these dissipation modes due to the identity  $\dot{\mathbf{n}} \cdot \mathbf{m} = -\dot{\mathbf{m}} \cdot \mathbf{n}$ , which is obtained by differentiating with respect to time  $\mathbf{n} \cdot \mathbf{m} \equiv 0$ . However, because we treat the constraints using LAGRANGE multipliers, the two directors should be considered independent in performing the variation, and hence both terms need to be retained. This also ensures that the two resulting director equations will have the same form; keeping only one of the two ultimately equivalent terms would destroy this formal symmetry.

Furthermore, a term proportional to  $(\mathbf{n} \cdot \mathbf{Dn})(\mathbf{m} \cdot \mathbf{Dm})$  has been omitted because of the identity

$$\text{tr } \mathbf{D}^2 = 2 \{ (\mathbf{Dn})^2 + (\mathbf{Dm})^2 + (\mathbf{m} \cdot \mathbf{Dm})(\mathbf{n} \cdot \mathbf{Dn}) - (\mathbf{m} \cdot \mathbf{Dn})^2 \},$$

which holds for any traceless  $\mathbf{D}$  and orthonormal vectors  $\mathbf{n}$  and  $\mathbf{m}$ . Clearly, other terms could equivalently have been omitted. Our choice is the same as that made in [43].

### Stress Tensor

In analogy to (3.45), the viscous stress takes the general form

$$\begin{aligned} \mathbf{T}_{\text{dis}} &= \frac{\partial R}{\partial \nabla \mathbf{v}} \\ &= \frac{\partial R}{\partial \mathbf{D}} + \frac{1}{2} \left( \mathbf{n} \otimes \frac{\partial R}{\partial \dot{\mathbf{n}}} - \frac{\partial R}{\partial \dot{\mathbf{n}}} \otimes \mathbf{n} + \mathbf{m} \otimes \frac{\partial R}{\partial \dot{\mathbf{m}}} - \frac{\partial R}{\partial \dot{\mathbf{m}}} \otimes \mathbf{m} \right). \end{aligned}$$

With  $\mathcal{R}$  given by (3.130), the symmetric part of the viscous stress is

$$\begin{aligned} \overline{\mathbf{T}}_{\text{dis}} &= \frac{\partial R}{\partial \mathbf{D}} \\ &= \gamma_2 \overline{\mathbf{n} \otimes \dot{\mathbf{n}}} + \gamma_3 \overline{\mathbf{n} \otimes \mathbf{Dn}} + \gamma_4 (\mathbf{n} \cdot \mathbf{Dn}) \overline{\mathbf{n} \otimes \mathbf{n}} \\ &\quad + \mu_2 \overline{\mathbf{m} \otimes \dot{\mathbf{m}}} + \mu_3 \overline{\mathbf{m} \otimes \mathbf{Dm}} + \mu_4 (\mathbf{m} \cdot \mathbf{Dm}) \overline{\mathbf{m} \otimes \mathbf{m}} \\ &\quad + [\lambda_2 (\dot{\mathbf{n}} \cdot \mathbf{m}) + \lambda_3 (\mathbf{n} \cdot \mathbf{Dm})] \overline{\mathbf{n} \otimes \mathbf{m}} + \lambda_4 \mathbf{D}. \end{aligned}$$

Furthermore, with

$$\frac{\partial R}{\partial \dot{\mathbf{n}}} = \gamma_1 \dot{\mathbf{n}} + \gamma_2 \mathbf{Dn} + \frac{1}{2} [\lambda_1 (\dot{\mathbf{n}} \cdot \mathbf{m}) + \lambda_2 (\mathbf{n} \cdot \mathbf{Dm})] \mathbf{m} \quad (3.131)$$

<sup>40</sup> To our knowledge, a complete set of inequalities in all these 12 viscosities that would guarantee positive semidefiniteness of the dissipation function  $R$  in (3.130) as (3.57) guarantees positive semidefiniteness of the dissipation function in (3.49) has not yet been derived; some necessary conditions are mentioned in [43].

and

$$\frac{\partial R}{\partial \dot{\mathbf{m}}} = \mu_1 \dot{\mathbf{m}} + \mu_2 \mathbf{D}\mathbf{m} - \frac{1}{2} [\lambda_1 (\dot{\mathbf{n}} \cdot \mathbf{m}) + \lambda_2 (\mathbf{n} \cdot \mathbf{D}\mathbf{m})] \mathbf{n} \quad (3.132)$$

we find the skew part of the viscous stress to be

$$\begin{aligned} \text{skw}(\mathbf{T}_{\text{dis}}) &= \text{skw} \left( \mathbf{n} \otimes \frac{\partial R}{\partial \dot{\mathbf{n}}} \right) + \text{skw} \left( \mathbf{m} \otimes \frac{\partial R}{\partial \dot{\mathbf{m}}} \right) \\ &= \gamma_1 \text{skw}(\mathbf{n} \otimes \dot{\mathbf{n}}) + \gamma_2 \text{skw}(\mathbf{n} \otimes \mathbf{D}\mathbf{n}) \\ &\quad + \mu_1 \text{skw}(\mathbf{m} \otimes \dot{\mathbf{m}}) + \mu_2 \text{skw}(\mathbf{m} \otimes \mathbf{D}\mathbf{m}) \\ &\quad + [\lambda_1 (\dot{\mathbf{n}} \cdot \mathbf{m}) + \lambda_2 (\mathbf{n} \cdot \mathbf{D}\mathbf{m})] \text{skw}(\mathbf{n} \otimes \mathbf{m}). \end{aligned}$$

### Director Evolution Equations

The equations for the two directors are formally given by

$$\frac{\partial R}{\partial \dot{\mathbf{n}}} + \frac{\partial W}{\partial \mathbf{n}} - \text{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \mathbf{k}_n = \gamma \mathbf{n} + \kappa \mathbf{m} \quad (3.133)$$

and

$$\frac{\partial R}{\partial \dot{\mathbf{m}}} + \frac{\partial W}{\partial \mathbf{m}} - \text{div} \frac{\partial W}{\partial \nabla \mathbf{m}} - \mathbf{k}_m = \tau \mathbf{m} + \kappa \mathbf{n}. \quad (3.134)$$

Equations (3.133) and (3.134) are basically those obtained in [186]. The only difference is that there the terms with  $\lambda_1$  and  $\lambda_2$  appear only in the equation for  $\mathbf{n}$ . However, this difference is merely formal, because it disappears once the LAGRANGE multipliers have been eliminated.

Formally, the LAGRANGE multipliers can be found by taking the scalar products of equations (3.133) and (3.134) with  $\mathbf{n}$  and  $\mathbf{m}$ . The multipliers can then be inserted to find two scalar equations of motion: they turn out to be the  $\mathbf{l}$ -components of (3.133) and (3.134). A third equation arises from the requirement that the two different expressions obtained for the multiplier  $\kappa$  coincide.

An equivalent, more direct way of finding the equations of motion is by observing that the  $\mathbf{l}$ -components of the left sides of both (3.133) and (3.134) vanish, and that the  $\mathbf{m}$ -component of the left side of (3.133) equals the  $\mathbf{n}$ -component of the left-hand side of (3.134).

Using the abbreviations

$$\begin{aligned} \mathbf{N} &:= \frac{\partial R}{\partial \dot{\mathbf{n}}} + \frac{\partial W}{\partial \mathbf{n}} - \text{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \mathbf{k}_n, \\ \mathbf{M} &:= \frac{\partial R}{\partial \dot{\mathbf{m}}} + \frac{\partial W}{\partial \mathbf{m}} - \text{div} \frac{\partial W}{\partial \nabla \mathbf{m}} - \mathbf{k}_m, \end{aligned}$$

the equations for the director orientation become

$$\mathbf{l} \cdot \mathbf{N} = 0, \quad (3.135a)$$

$$\mathbf{l} \cdot \mathbf{M} = 0, \quad (3.135b)$$

$$\mathbf{m} \cdot \mathbf{N} = \mathbf{n} \cdot \mathbf{M}. \quad (3.135c)$$



As can be seen from (3.131) and (3.132), this is a system of three equations that is implicit in the time derivatives of the directors  $\mathbf{n}$  and  $\mathbf{m}$ . Explicit expressions for the time derivatives can be obtained by observing that

$$\dot{\mathbf{n}} = \alpha \mathbf{l} + \beta \mathbf{m}, \quad (3.136a)$$

$$\dot{\mathbf{m}} = \gamma \mathbf{l} - \beta \mathbf{n}, \quad (3.136b)$$

with some coefficients  $\alpha$ ,  $\beta$ , and  $\gamma$ . This is a consequence of the identities  $\mathbf{n} \cdot \dot{\mathbf{n}} = \mathbf{m} \cdot \dot{\mathbf{m}} = 0$  and  $\mathbf{n} \cdot \dot{\mathbf{m}} = -\mathbf{m} \cdot \dot{\mathbf{n}}$ . Inserting (3.136a) and (3.136b) in (3.135a) to (3.135c) yields a system of three linear equations in the unknowns  $\alpha$ ,  $\beta$ , and  $\gamma$ . Its solution is<sup>41</sup>

$$\begin{aligned} \alpha &= -\frac{\mathbf{l} \cdot \mathbf{A}}{\gamma_1}, \\ \beta &= \frac{\mathbf{n} \cdot \mathbf{B} - \mathbf{m} \cdot \mathbf{A}}{\gamma_1 + \mu_1 + \lambda_1}, \\ \gamma &= -\frac{\mathbf{l} \cdot \mathbf{B}}{\mu_1}. \end{aligned}$$

Here, we have introduced the abbreviations

$$\begin{aligned} \mathbf{A} &:= \frac{\partial W}{\partial \mathbf{n}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{n}} - \mathbf{k}_n + \gamma_2 \mathbf{Dn} + \frac{1}{2} \lambda_2 (\mathbf{n} \cdot \mathbf{Dm}) \mathbf{m}, \\ \mathbf{B} &:= \frac{\partial W}{\partial \mathbf{m}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{m}} - \mathbf{k}_m + \mu_2 \mathbf{Dm} - \frac{1}{2} \lambda_2 (\mathbf{n} \cdot \mathbf{Dm}) \mathbf{n}. \end{aligned}$$

Hence, we find that

$$\begin{aligned} \dot{\mathbf{n}} &= -\frac{\mathbf{l} \cdot \mathbf{A}}{\gamma_1} \mathbf{l} + \frac{\mathbf{n} \cdot \mathbf{B} - \mathbf{m} \cdot \mathbf{A}}{\gamma_1 + \mu_1 + \lambda_1} \mathbf{m}, \\ \dot{\mathbf{m}} &= -\frac{\mathbf{l} \cdot \mathbf{B}}{\mu_1} \mathbf{l} + \frac{\mathbf{m} \cdot \mathbf{A} - \mathbf{n} \cdot \mathbf{B}}{\gamma_1 + \mu_1 + \lambda_1} \mathbf{n}. \end{aligned}$$

### 3.3.3 Rotational Momentum

Another form of the power has been used [186], and it is illuminating to compare the two different approaches. Because they ultimately stem from actions on different parts of a molecule, the generalized forces on the two directors are in principle independent. However, if one takes the naïve view that the director triad  $(\mathbf{n}, \mathbf{m}, \mathbf{l})$  behaves as a rigid body, the external power  $\mathcal{W}^{(a)}$  takes the form

$$\mathcal{W}^{(a)}(\mathcal{P}_t, \chi) = \int_{\mathcal{P}_t} (\mathbf{b} \cdot \mathbf{v} + \mathbf{k} \cdot \mathbf{w}_n) dV + \int_{\partial^* \mathcal{P}_t} (\mathbf{t} \cdot \mathbf{v} + \mathbf{c} \cdot \mathbf{w}_n) dA, \quad (3.137)$$

where  $\mathbf{b}$  and  $\mathbf{t}$  are body and surface forces, while  $\mathbf{k}$  and  $\mathbf{c}$  are body and surface moments, and  $\mathbf{w}_n$  is now the local rotational velocity of the director triad in the given frame.

<sup>41</sup> Under the assumption that  $\gamma_1 \neq 0$ ,  $\mu_1 \neq 0$ , and  $\gamma_1 + \mu_1 + \lambda_1 \neq 0$ .

To see that (3.137) is just a special form of the more general power employed in (3.129), we note that if the directors are seen as a rigidly moving whole, then their time derivatives are given as functions of the rotational velocity  $\mathbf{w}_n$  by

$$\dot{\mathbf{n}} = \mathbf{w}_n \times \mathbf{n} \quad \text{and} \quad \dot{\mathbf{m}} = \mathbf{w}_n \times \mathbf{m}. \quad (3.138)$$

An elementary computation, using the orthonormality of the directors  $\mathbf{n}$  and  $\mathbf{m}$  along with (3.138), then shows that  $\mathbf{w}_n$  can in turn be expressed as a function of  $\dot{\mathbf{n}}$  and  $\dot{\mathbf{m}}$  as

$$\mathbf{w}_n = \mathbf{n} \times \dot{\mathbf{n}} + \mathbf{m} \times \dot{\mathbf{m}} + (\dot{\mathbf{n}} \cdot \mathbf{m}) \mathbf{m} \times \mathbf{n}.$$

Taking the scalar product with an arbitrary vector  $\mathbf{l}$  yields

$$\begin{aligned} \mathbf{k} \cdot \mathbf{w}_n &= \dot{\mathbf{n}} \cdot (\mathbf{k} \times \mathbf{n}) + \dot{\mathbf{m}} \cdot (\mathbf{k} \times \mathbf{m}) - (\dot{\mathbf{n}} \cdot \mathbf{m}) [\mathbf{m} \cdot (\mathbf{k} \times \mathbf{n})] \\ &= \dot{\mathbf{n}} \cdot \left( \mathbf{I} - \frac{1}{2} \mathbf{m} \otimes \mathbf{m} \right) (\mathbf{k} \times \mathbf{n}) + \dot{\mathbf{m}} \cdot \left( \mathbf{I} - \frac{1}{2} \mathbf{n} \otimes \mathbf{n} \right) (\mathbf{k} \times \mathbf{m}). \end{aligned} \quad (3.139)$$

To arrive at the second, symmetric, form of the above equation, we have used the identity

$$(\dot{\mathbf{n}} \cdot \mathbf{m}) [\mathbf{m} \cdot (\mathbf{k} \times \mathbf{n})] = (\dot{\mathbf{m}} \cdot \mathbf{n}) [\mathbf{n} \cdot (\mathbf{k} \times \mathbf{m})].$$

Equation (3.139) shows that a torque  $\mathbf{k}$  on the material element can be interpreted in terms of generalized forces on the directors  $\mathbf{n}$  and  $\mathbf{m}$  if we set, for example,

$$\mathbf{k}_n := \left( \mathbf{I} - \frac{1}{2} \mathbf{m} \otimes \mathbf{m} \right) (\mathbf{k} \times \mathbf{n})$$

and

$$\mathbf{k}_m := \left( \mathbf{I} - \frac{1}{2} \mathbf{n} \otimes \mathbf{n} \right) (\mathbf{k} \times \mathbf{m}).$$

Corresponding relations can be used to define  $\mathbf{c}_n$  and  $\mathbf{c}_m$  in terms of the surface moment  $\mathbf{c}$ .



<http://www.springer.com/978-0-387-87814-0>

Dissipative Ordered Fluids  
Theories for Liquid Crystals  
Sonnet, A.M.; Virga, E.G.  
2012, X, 326 p., Hardcover  
ISBN: 978-0-387-87814-0