

Continuum Theory for Liquid Crystals

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1 Continuum Theory for Liquid Crystals

1.1 Introduction

The continuum theories for liquid crystals that are in use today largely stem from the original work of Oseen [88, 89] and Zocher [115, 116], and the general classifications of liquid crystal phases described by Friedel [44], in the 1920s and 1930s. Friedel proposed a classification scheme for liquid crystals that consists of three broad categories called *nematic*, *cholesteric* and *smectic*. This classification has been widely adopted and is now in general usage. In 1958, Frank [41] gave a direct formulation of the energy function needed for the continuum theory and this rejuvenated interest in the subject in the 1960s when Ericksen [34] developed a static theory for nematic liquid crystals which consequently led to balance laws for dynamical behaviour [33]. This work encouraged Leslie [60, 61] to formulate constitutive equations for dynamics and thereby complete what has turned out to be an extremely successful and comprehensive dynamic theory for nematic liquid crystals. The continuum theory, and crucial continuum descriptions, will be reviewed below. More recently, there has been a renewal of interest in biaxial nematics and smectic liquid crystals and continuum theories that extend the notions developed by Ericksen and Leslie to these phases of liquid crystals will also be mentioned in this Chapter.

There are various detailed accounts, and examples of applications, of the continuum theory for liquid crystals that are readily available. These can be found in the books by Barbero and Evangelista [10], Blinov [15], Chandrasekhar [22], de Gennes and Prost [48], Pasechnik, Chigrinov and Shmeliova [92], Stewart [104] and Virga [107], and also in the review articles by Ericksen [36], Jenkins [54], Leslie [62] and Stephen and Straley [103]. A convenient summary of the continuum equations for nematic, biaxial nematic and smectic C liquid crystals can be found in the article by Atkin, Sluckin and Stewart [5].

1.2 Equilibrium Theory for Nematics

1.2.1 Notation

It will be assumed throughout that the reader has some familiarity with standard vector notation and index (or suffix) notation for Cartesian tensors; there are many readily available introductions such as those by, for example, Aris [4], Leigh [59], Goodbody [50] and Spencer [102]. The liquid crystal literature makes extensive use of both direct vector notation and index notation.

For example, a vector \mathbf{a} can be expressed in terms of its components a_i relative to a set of basis vectors \mathbf{e}_i , $i = 1, 2, 3$. The Einstein summation convention enables \mathbf{a} to be written as

$$\mathbf{a} = a_i \mathbf{e}_i, \tag{1}$$

where it is understood that the repeated index i is summed from, in this example, 1 to 3. The summation convention obeys the following rule: whenever an index appears twice, and only twice, in the same term, a summation is implied over all the contributions obtained by letting that particular index assume all its possible values, unless an explicit statement is made to the contrary. Thus the scalar product of the vectors \mathbf{a} and \mathbf{b} is

simply

$$\mathbf{a} \cdot \mathbf{b} = a_i b_i. \quad (2)$$

The summation convention can also be applied to matrices. For example, if $A = [a_{ij}]$ and $B = [b_{ij}]$ are $n \times n$ matrices, then their product $AB \equiv C = [c_{ij}]$ is the matrix with components

$$c_{ij} = a_{ik} b_{kj}, \quad (3)$$

with a summation over the index k from 1 to n being implied. The dyadic product of the vectors \mathbf{a} and \mathbf{b} is denoted $\mathbf{a} \otimes \mathbf{b}$ and it can be considered as a matrix with components given by $[\mathbf{a} \otimes \mathbf{b}]_{ij} = a_i b_j$.

Two quantities that are widely used are the Kronecker delta δ_{ij} and the alternator ϵ_{ijk} , defined when i, j and k can each take any of the values 1, 2 or 3. These are defined by, respectively,

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases} \quad (4)$$

and

$$\epsilon_{ijk} = \begin{cases} 1 & \text{if } i, j \text{ and } k \text{ are unequal and in cyclic order,} \\ -1 & \text{if } i, j \text{ and } k \text{ are unequal and in non-cyclic order,} \\ 0 & \text{if any two of } i, j \text{ or } k \text{ are equal.} \end{cases} \quad (5)$$

The vector product of two vectors \mathbf{a} and \mathbf{b} is defined by

$$\mathbf{a} \times \mathbf{b} = \mathbf{e}_i \epsilon_{ijk} a_j b_k. \quad (6)$$

The partial derivative with respect to the i^{th} variable is denoted by a comma followed by the variable. For instance, $p_{,i}$ represents the partial derivative of the quantity p with respect to the i^{th} variable. Similarly, $a_{i,j}$ is the partial derivative of the i^{th} component of the vector \mathbf{a} with respect to the j^{th} variable. The gradient of a scalar field p is defined by

$$\nabla p = \mathbf{e}_i p_{,i}, \quad (7)$$

while the divergence of a vector \mathbf{a} is given by

$$\nabla \cdot \mathbf{a} = a_{i,i}, \quad (8)$$

and its curl is defined by

$$\nabla \times \mathbf{a} = \mathbf{e}_i \epsilon_{ijk} a_{k,j}. \quad (9)$$

In this Chapter, the gradient of the vector \mathbf{a} will be defined by [59]

$$\nabla \mathbf{a} = a_{i,j} \mathbf{e}_i \otimes \mathbf{e}_j. \quad (10)$$

We can consider $\nabla \mathbf{a}$ as a matrix with components given by $[\nabla \mathbf{a}]_{ij} = a_{i,j}$. The divergence of a second order tensor with components T_{ij} will be defined here by

$$T_{ij,j}. \quad (11)$$

There is also an alternative definition in the literature for the divergence of a second order tensor which happens to involve the transpose of T_{ij} ; however, the above definition is in accordance with the convention adopted by Truesdell and Noll [106], Leigh [59] and Leslie [62].

1.2.2 Nematics

The Austrian botanist Reinitzer is generally acknowledged as the discoverer of liquid crystals and he reported his findings in 1888 [96] (an English translation of this article is now available [97]). It transpired that Reinitzer had actually observed ‘two melting points’ when heating up cholesteryl benzoate, now known to be a cholesteric liquid crystal, also called a chiral nematic liquid crystal. In 1907, Vorländer [108] discovered that an essential prerequisite for the observations of Reinitzer was the presence of rod-like molecules. Vorländer’s discovery was, and remains, crucial for the theoretical modelling of liquid crystals because it allows many of the basic molecular structure of liquid crystals to be described via a rod-like model. It therefore proves convenient to introduce a unit vector \mathbf{n} , called the director, to describe the local direction of the average molecular alignment, as shown in Fig. 1, where short bold lines show schematically the rod-like structure of what are called nematic liquid crystals. The absence of polarity in nematics

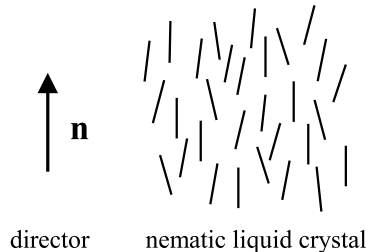


Figure 1: A schematic representation of a nematic liquid crystal phase where the short bold lines represent the molecules. A unit vector \mathbf{n} , called the director, describes the average direction of the molecular alignment.

means that \mathbf{n} and $-\mathbf{n}$ are indistinguishable, in the sense that the sign of \mathbf{n} has no physical significance.

The continuum theory of nematic liquid crystals employs the director \mathbf{n} to describe the mean molecular alignment at a point \mathbf{x} in a given sample volume V . Hence

$$\mathbf{n} = \mathbf{n}(\mathbf{x}), \quad \mathbf{n} \cdot \mathbf{n} = 1. \quad (12)$$

This alignment exhibits elasticity and it is therefore supposed that there is a free energy density, also called the free energy integrand, associated with distortions of the director of the form

$$w = w(\mathbf{n}, \nabla \mathbf{n}), \quad (13)$$

with the total elastic energy being

$$W = \int_V w(\mathbf{n}, \nabla \mathbf{n}) dV. \quad (14)$$

It will be assumed here that the liquid crystal is incompressible, that is, the mass density remains constant. A liquid crystal sample exhibiting a completely relaxed configuration in the absence of forces, fields and boundary conditions, is said to be in a natural orientation. The free energy is defined to within the addition of an arbitrary constant and therefore this constant is chosen such that $w = 0$ for any natural orientation, in which case we suppose that any other state or configuration induced upon the sample

produces an energy that is greater than or equal to that for a completely relaxed natural orientation. It is therefore supposed that

$$w(\mathbf{n}, \nabla \mathbf{n}) \geq 0. \quad (15)$$

Nematic liquid crystals generally lack polarity and so the vectors \mathbf{n} and $-\mathbf{n}$ are physically indistinguishable. It is then natural to require

$$w(\mathbf{n}, \nabla \mathbf{n}) = w(-\mathbf{n}, -\nabla \mathbf{n}). \quad (16)$$

The free energy must also be the same when described in any two frames of reference, that is, it must be frame-indifferent. This means that the energy density must be invariant to arbitrary superposed rigid body rotations and consequently it is required that

$$w(\mathbf{n}, \nabla \mathbf{n}) = w(Q\mathbf{n}, Q\nabla \mathbf{n}Q^T), \quad (17)$$

where Q is any proper orthogonal matrix ($\det Q = 1$), Q^T being its transpose. This condition suffices for chiral nematics, but needs to be extended to apply to any orthogonal matrix Q with $\det Q = \pm 1$ for nematics (see [104] for further details).

Both Oseen [88] and Frank [41] considered an integrand that was quadratic in the gradients of \mathbf{n} . The aforementioned symmetry constraints lead to [41]

$$w = \frac{1}{2}K_1(\nabla \cdot \mathbf{n})^2 + \frac{1}{2}K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{1}{2}K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 + \frac{1}{2}(K_2 + K_4)\nabla \cdot [(\mathbf{n} \cdot \nabla)\mathbf{n} - (\nabla \cdot \mathbf{n})\mathbf{n}], \quad (18)$$

where the constants K_i are known as the Frank elastic constants; K_1 , K_2 and K_3 are often called the splay, twist and bend elastic constants, respectively. The combination $K_2 + K_4$ is called the saddle-splay constant and is often omitted in many calculations because, being a divergence, it may be expressed as a surface energy using the usual divergence theorem. The energy density in equation (18) is generally known as the Frank–Oseen energy for nematic liquid crystals. The non-negativity requirement $w \geq 0$ arising from equation (15) leads to the inequalities

$$\begin{aligned} K_1 &\geq 0, & K_2 &\geq 0, & K_3 &\geq 0, \\ K_2 &\geq |K_4|, & 2K_1 &\geq K_2 + K_4 & \geq 0. \end{aligned} \quad (19)$$

These are often referred to as Ericksen’s inequalities [35]. The elastic constants generally have a magnitude of around 5×10^{-12} N [48, 103, 104]; tabulated data for many nematic liquid crystals can be found in [31].

There is an important identity due to Ericksen [37] that is used for the simplification of the continuum equations; we record it here for reference and note that it can be extended to smectic liquid crystal theory [72, 105] (discussed below). It can be written as

$$\epsilon_{ijk} \left(n_j \frac{\partial w}{\partial n_k} + n_{j,p} \frac{\partial w}{\partial n_{k,p}} + n_{p,j} \frac{\partial w}{\partial n_{p,k}} \right) = 0. \quad (20)$$

Sometimes, for example, when the relative values of the elastic constants are unknown or when the resulting equilibrium equations are complicated, the one-constant approximation

$$K \equiv K_1 = K_2 = K_3, \quad K_4 = 0, \quad (21)$$

is made. (Some authors, in the one-constant approximation, equate the splay, twist and bend constants and assume that $K_2 + K_4 = 0$ rather than $K_4 = 0$. In the case of strong anchoring this alternative approximation leads to equilibrium equations that are identical to those obtained using (21); of course, the total energy will be different because there will be alternative surface contributions to the energy (cf. the example in [104, p.118].) The energy density w in (18) can then be simplified, via various vector identities [104], so that it can be written as

$$w_F = \frac{1}{2}K \|\nabla \mathbf{n}\|^2 = \frac{1}{2}K n_{i,j} n_{i,j}. \quad (22)$$

This means that, in Cartesian coordinates, the energy density is simply the sum of the squares of the components of $\nabla \mathbf{n}$.

1.2.3 Equilibrium equations

Ericksen [34] formulated the equilibrium theory for both nematic and cholesteric liquid crystals via a principle of virtual work. A detailed summary of this process can be found in [104]. The variation of the total energy is postulated to satisfy the principle of virtual work, given by

$$\delta \int_V w(\mathbf{n}, \nabla \mathbf{n}) dV = \int_V (\mathbf{F} \cdot \delta \mathbf{x} + \mathbf{G} \cdot \Delta \mathbf{n}) dV + \int_S (\mathbf{t} \cdot \delta \mathbf{x} + \mathbf{s} \cdot \Delta \mathbf{n}) dS, \quad (23)$$

where V is the volume of the liquid crystal sample, S is its boundary surface, w is the energy density and the virtual displacements are denoted by $\delta \mathbf{x}$. The quantity $\Delta \mathbf{n}$ is defined by

$$\Delta \mathbf{n} = \delta \mathbf{n} + (\delta \mathbf{x} \cdot \nabla) \mathbf{n}, \quad (24)$$

which can be interpreted as the variational equivalent of the material derivative of \mathbf{n} . The body force per unit volume is denoted by \mathbf{F} , \mathbf{t} is the surface force per unit area, and \mathbf{G} and \mathbf{s} are generalised body and surface forces, respectively. The virtual displacements and the variations in the director are not arbitrary, but are subject to the constraints

$$\nabla \cdot (\delta \mathbf{x}) = 0, \quad \mathbf{n} \cdot \delta \mathbf{n} = 0, \quad \mathbf{n} \cdot \Delta \mathbf{n} = 0. \quad (25)$$

The first constraint in (25) is due to the assumption of incompressibility when the mass density $\rho(\mathbf{x})$ is constant. This follows from the requirement that the variations must satisfy

$$\delta \rho + \nabla \cdot (\rho \delta \mathbf{x}) = 0, \quad (26)$$

reflecting the conservation of mass property due to incompressibility, which clearly reduces to the first constraint when ρ is constant. The latter two constraints in (25) follow from applying the rules for variations to the original constraint (12) which forces $n_i n_{i,j} = 0$ and using the definition of $\Delta \mathbf{n}$ in equation (24).

By the consideration of an arbitrary, infinitesimal, rigid displacement $\delta \mathbf{x} = \mathbf{a}$, with \mathbf{a} a constant vector, and for which $\Delta \mathbf{n} = \mathbf{0}$, it can be shown using (23) that

$$\int_V \mathbf{F} dV + \int_S \mathbf{t} dS = \mathbf{0}, \quad (27)$$

which obviously expresses the fact that the resultant force at equilibrium is zero. Similarly, consideration of an arbitrary (constant) infinitesimal, rigid rotation $\boldsymbol{\omega}$ for which

$$\delta \mathbf{x} = \boldsymbol{\omega} \times \mathbf{x}, \quad \Delta \mathbf{n} = \boldsymbol{\omega} \times \mathbf{n}, \quad (28)$$

leads to, after an application of Ericksen's identity (20) applied to a calculation that involves (23), the balance of moments being expressed as

$$\int_V (\mathbf{x} \times \mathbf{F} + \mathbf{n} \times \mathbf{G}) dV + \int_S (\mathbf{x} \times \mathbf{t} + \mathbf{n} \times \mathbf{s}) dS = \mathbf{0}. \quad (29)$$

This is a statement that the balance of moments at equilibrium is zero. From this relationship it is seen that the generalised body and surface forces are related to the body moment \mathbf{K} and couple stress vector \mathbf{l} defined by, respectively,

$$\mathbf{K} = \mathbf{n} \times \mathbf{G}, \quad \mathbf{l} = \mathbf{n} \times \mathbf{s}. \quad (30)$$

The left-hand side of the virtual work hypothesis (23) can be written, using the first constraint in (25), as

$$\delta \int_V w dV = \int_V (\delta w + (\delta \mathbf{x} \cdot \nabla) w) dV. \quad (31)$$

The right-hand side of (31) can be rearranged so that it is in a similar form to that expressed on the right-hand side of (23). This then makes it possible to obtain expressions for the surface force \mathbf{t} and generalised surface force \mathbf{s} . Firstly, it is noted that if $\boldsymbol{\nu}$ is the outward unit normal to the surface S , then, by the standard tetrahedral argument [106], it can be shown that

$$t_i = t_{ij} \nu_j, \quad (32)$$

$$s_i = s_{ij} \nu_j + \beta n_i, \quad (33)$$

where t_{ij} are the components of the stress tensor and s_{ij} are the components of what Ericksen [34] calls the torque stress. The scalar β is arbitrary and is due to the third constraint in (25). Calculations reveal that the stress tensor and the torque stress are given by

$$t_{ij} = -p \delta_{ij} - \frac{\partial w}{\partial n_{k,j}} n_{k,i}, \quad (34)$$

$$s_{ij} = \frac{\partial w}{\partial n_{i,j}}, \quad (35)$$

with p being an arbitrary pressure arising from the assumed incompressibility. A consequent assessment of the volume integrals gives the equilibrium equations. In component form they are

$$t_{ij,j} + F_i = 0, \quad (36)$$

$$\left(\frac{\partial w}{\partial n_{i,j}} \right)_{,j} - \frac{\partial w}{\partial n_i} + G_i + \lambda n_i = 0, \quad (37)$$

where λ is a scalar Lagrange multiplier that arises from the unit vector constraint in (12). Equation (36) clearly represents the point form of the balance of forces in equation (27), while (37) can be shown to be the point form of the balance of moments given by (29). As shown in the next section, it is generally only necessary to solve equation (37) because (36) may be neglected in many equilibrium problems.

1.2.4 Body forces and moments

A major simplification of the equilibrium equations (36) and (37) is possible if we consider the body forces \mathbf{F} and \mathbf{G} to be specified functions of \mathbf{x} and \mathbf{n} of the forms

$$F_i = \frac{\partial \Psi}{\partial x_i}, \quad G_i = \frac{\partial \Psi}{\partial n_i}, \quad (38)$$

where $\Psi(\mathbf{n}, \mathbf{x})$ is some scalar energy density function, as has been considered by Ericksen [34]. After careful manipulation of the derivatives in the equilibrium equations [34, 104], the balance of forces given by equation (36) reduces to

$$(\Psi - p - w)_{,i} = 0, \quad (39)$$

once the general rule for partial derivatives [34, 104]

$$w_{,i} \equiv \frac{\partial w}{\partial x_i} + \frac{\partial w}{\partial n_j} n_{j,i} + \frac{\partial w}{\partial n_{j,k}} n_{j,ki}, \quad (40)$$

has been applied. This yields an expression for the pressure p , namely,

$$p + w - \Psi = p_0, \quad (41)$$

where p_0 is an arbitrary constant. This ultimate identification of the pressure has the important consequence that if \mathbf{F} and \mathbf{G} obey the relations in (38), then to determine equilibrium configurations in nematic liquid crystals one has to solve only equation (37). In this case we can always neglect equation (36), unless there is a desire to compute forces. Notice that when this is the situation (clearly so if $\Psi \equiv 0$) then equation (37) in conjunction with the constraint in equation (12) results in four equations in four unknowns, namely, the three components of \mathbf{n} and the Lagrange multiplier λ .

In ordinary circumstances, as remarked by Ericksen [34], gravitational or electromagnetic fields are expected to produce the forces \mathbf{F} and \mathbf{G} . For example, in the case of an external gravitational field in the absence of electromagnetic fields

$$F_i = -\frac{\partial \Psi_g}{\partial x_i}, \quad G_i = 0, \quad \Psi_g = \Psi_g(\mathbf{x}), \quad (42)$$

where ψ_g is the gravitational potential.

However, in many practical applications of interest when the effect of gravity is neglected, an external body force \mathbf{F} and external body moment \mathbf{K} can arise from the presence of a magnetic field \mathbf{H} . It is possible to introduce the magnetic potential ψ_m as

$$\Psi_m(\mathbf{n}, \mathbf{x}) = \frac{1}{2} \mathbf{M} \cdot \mathbf{H}, \quad (43)$$

where the magnetisation \mathbf{M} can be written as [34, 104]

$$\mathbf{M} = \chi_{m_\perp} \mathbf{H} + \chi_a (\mathbf{n} \cdot \mathbf{H}) \mathbf{n}, \quad \chi_a = \chi_{m_\parallel} - \chi_{m_\perp}, \quad (44)$$

where the coefficients χ_{m_\parallel} and χ_{m_\perp} denote the diamagnetic (negative) susceptibilities when the magnetic field and the director are parallel and perpendicular, respectively.

The magnetic anisotropy is defined by χ_a , which is generally positive but may be negative [104]; in general, χ_a is relatively small and consequently the influence of the liquid crystal upon the magnetic field can be mostly ignored, but not vice-versa. The magnetic potential can then be formulated as

$$\Psi_m = \frac{1}{2}\chi_a(\mathbf{n} \cdot \mathbf{H})^2, \quad (45)$$

when constant contributions to the potential that are independent of the orientation of \mathbf{n} are ignored. In this situation we have

$$F_i = \frac{\partial \Psi_m}{\partial x_i}, \quad G_i = \frac{\partial \Psi_m}{\partial n_i}, \quad (46)$$

with $\partial/\partial x_i$ denoting the usual notion of partial derivative of Ψ_m with respect to x_i when \mathbf{n} and \mathbf{x} are treated as independent variables. The resulting body force \mathbf{F} and body moment \mathbf{K} due to an external magnetic field may then take the forms [34]

$$\mathbf{F} = \mathbf{M} \cdot (\nabla \mathbf{H}), \quad \mathbf{K} = \mathbf{n} \times \mathbf{G}, \quad \text{where} \quad \mathbf{G} = \chi_a \mathbf{H}(\mathbf{n} \cdot \mathbf{H}). \quad (47)$$

It follows from equations (42) and (46) that in general we can incorporate the effects of gravity and magnetic fields by considering

$$F_i = \frac{\partial \Psi}{\partial x_i}, \quad G_i = \frac{\partial \Psi}{\partial n_i}, \quad \Psi = -\rho \Psi_g + \Psi_m, \quad (48)$$

when the density ρ is constant. Further, since $\Psi = \Psi(\mathbf{n}, \mathbf{x})$, it is seen that, using the general definition for partial derivatives in (40),

$$F_i + G_j n_{j,i} = \frac{\partial \Psi}{\partial x_i} + \frac{\partial \Psi}{\partial n_j} n_{j,i} = \Psi_{,i}, \quad (49)$$

which then allows the pressure to be identified as stated in equation (41).

There are analogous expressions and results for an electric field \mathbf{E} . We can define the electric displacement \mathbf{D} by

$$\mathbf{D} = \epsilon_{\perp} \mathbf{E} + \epsilon_a (\mathbf{n} \cdot \mathbf{E}) \mathbf{n}, \quad \epsilon_a = \epsilon_{\parallel} - \epsilon_{\perp}, \quad (50)$$

and set

$$\Psi_e = \frac{1}{2} \mathbf{D} \cdot \mathbf{E}, \quad \mathbf{F} = \mathbf{D} \cdot (\nabla \mathbf{E}), \quad \mathbf{G} = \epsilon_a \mathbf{E}(\mathbf{n} \cdot \mathbf{E}), \quad (51)$$

where the coefficients ϵ_{\parallel} and ϵ_{\perp} denote the dielectric permittivities when the electric field and the director are parallel and perpendicular, respectively, and ϵ_a is defined as the dielectric anisotropy. The expression for Ψ_e that is analogous to that in equation (45) for magnetic fields is

$$\Psi_e = \frac{1}{2} \epsilon_a (\mathbf{n} \cdot \mathbf{E})^2, \quad (52)$$

when constant contributions to the potential that are independent of the orientation of the director are ignored. If either of the fields \mathbf{H} or \mathbf{E} is assumed to be uniform and independent of \mathbf{x} then the body force \mathbf{F} associated with the corresponding field is zero. It should be mentioned here that one important difference between the effects of magnetic and electric fields upon liquid crystals is that an electric field can give rise to

significant dielectric permittivities, as pointed out by Deuling [30]; in such circumstances an allowance must be made for the influence of the liquid crystal upon the applied field by employing an appropriate reduced version of Maxwell's equations [30, 104].

We close this section with the remark that the magnetic and electric energy densities are often simply obtained as $w_m = -\Psi_m$ and $w_e = -\Psi_e$ and that in many instances in static equilibrium it is immaterial whether these fields are incorporated via an energy density formulation or potential formulation. However, in dynamics, as will be seen below, the use of a potential formulation is generally more convenient.

1.2.5 Reformulation of the equilibrium equations

It is very common in liquid crystal theory to use a representation for the director that automatically ensures \mathbf{n} is a unit vector, for example,

$$\mathbf{n} = (\cos \theta \cos \phi, \cos \theta \sin \phi, \sin \theta), \quad -\frac{\pi}{2} \leq \theta \leq \frac{\pi}{2}, \quad 0 \leq \phi < 2\pi, \quad (53)$$

where \mathbf{n} can be interpreted as a point on the unit sphere. This type of representation enables a reformulation which simplifies the equilibrium equations. For example, following Ericksen [37], suppose in general that

$$\mathbf{n} = \mathbf{f}(\theta, \phi), \quad \mathbf{f} \cdot \mathbf{f} = 1. \quad (54)$$

The constraint that \mathbf{f} is a unit vector leads to

$$n_i \frac{\partial f_i}{\partial \theta} = 0, \quad n_i \frac{\partial f_i}{\partial \phi} = 0. \quad (55)$$

The notation \mathbf{n} for the director in the original description is retained and we adopt the notation \mathbf{f} to describe the director when using θ and ϕ . It must also be the case that

$$\frac{\partial \mathbf{f}}{\partial \theta} \times \frac{\partial \mathbf{f}}{\partial \phi} \neq \mathbf{0}, \quad (56)$$

to ensure that the tangent vectors in the resulting unit sphere description do not coincide, so that θ and ϕ can act as local coordinate directions. As Ericksen [37] points out, any such characterisation is somewhere singular, and so some exceptional directions will fail to be represented. Some care must therefore be exercised when using equations that rely upon the conditions (54) to (56) for their derivation.

In an obvious notation, the bulk energy density and any of the aforementioned potentials, generically denoted by Φ , can be reformulated, respectively, as

$$w = w(\mathbf{n}, \nabla \mathbf{n}) = \hat{w}(\theta, \phi, \nabla \theta, \nabla \phi), \quad \Psi(\mathbf{n}, \mathbf{x}) = \hat{\Psi}(\theta, \phi, \mathbf{x}). \quad (57)$$

It is possible to show that [104]

$$\left(\frac{\partial \hat{w}}{\partial \theta_{,i}} \right)_{,i} - \frac{\partial \hat{w}}{\partial \theta} = \left[\left(\frac{\partial w}{\partial n_{k,i}} \right)_{,i} - \frac{\partial w}{\partial n_k} \right] \frac{\partial f_k}{\partial \theta}, \quad (58)$$

$$\left(\frac{\partial \hat{w}}{\partial \phi_{,i}} \right)_{,i} - \frac{\partial \hat{w}}{\partial \phi} = \left[\left(\frac{\partial w}{\partial n_{k,i}} \right)_{,i} - \frac{\partial w}{\partial n_k} \right] \frac{\partial f_k}{\partial \phi}. \quad (59)$$

If we additionally suppose that the body forces \mathbf{F} and \mathbf{G} are specified functions of \mathbf{x} and \mathbf{n} so that the relations in (38) hold, then, in particular, we have

$$G_i = \frac{\partial \Psi}{\partial n_i}, \quad \Psi = \Psi(\mathbf{n}, \mathbf{x}). \quad (60)$$

and it is then seen that

$$\frac{\partial \widehat{\Psi}}{\partial \theta} = \frac{\partial \Psi}{\partial n_k} \frac{\partial f_k}{\partial \theta} = G_k \frac{\partial f_k}{\partial \theta}, \quad \frac{\partial \widehat{\Psi}}{\partial \phi} = \frac{\partial \Psi}{\partial n_k} \frac{\partial f_k}{\partial \phi} = G_k \frac{\partial f_k}{\partial \phi}. \quad (61)$$

These results can be employed with those in equations (58) and (59) to show that the three equilibrium equations that occur in (37) can be multiplied appropriately by $\frac{\partial f_i}{\partial \theta}$ and $\frac{\partial f_i}{\partial \phi}$ to reduce them to an equivalent simpler reduced set of two equations

$$\left(\frac{\partial \widehat{w}}{\partial \theta_{,i}} \right)_{,i} - \frac{\partial \widehat{w}}{\partial \theta} + \frac{\partial \widehat{\Psi}}{\partial \theta} = 0, \quad \left(\frac{\partial \widehat{w}}{\partial \phi_{,i}} \right)_{,i} - \frac{\partial \widehat{w}}{\partial \phi} + \frac{\partial \widehat{\Psi}}{\partial \phi} = 0, \quad (62)$$

with the Lagrange multiplier λ automatically being eliminated because of condition (55). These reformulated equations are more tractable but necessarily hold only whenever $\frac{\partial f_i}{\partial \theta} \neq 0$, $\frac{\partial f_i}{\partial \phi} \neq 0$ and the condition (56) holds, which highlights the previously mentioned concern over the validity of this formulation when special directions of the director may require more careful treatment.

In some circumstances the total energy density may also depend on the spatial variable \mathbf{x} , as may be the case for the magnetic or electric energies discussed above. This situation is a special case of that generally encountered when curvilinear coordinates are introduced. Let θ_1 and θ_2 denote the two orientation angles for the director and let $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)$ denote the curvilinear spatial coordinates so that [37, 63]

$$\mathbf{x} = \mathbf{x}(\boldsymbol{\xi}), \quad \mathbf{n} = \mathbf{f}(\theta_1, \theta_2, \boldsymbol{\xi}), \quad (63)$$

and set

$$\widetilde{w}(\theta_1, \theta_2, \nabla \theta_1, \nabla \theta_2, \boldsymbol{\xi}) = wJ, \quad (64)$$

where J denotes the usual Jacobian

$$J = \left| \frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}} \right|. \quad (65)$$

The total energy W can then be reformulated as

$$W = \int_{\Omega} w \, dx_1 dx_2 dx_3 = \int_{\widetilde{\Omega}} \widetilde{w} \, d\xi_1 d\xi_2 d\xi_3, \quad (66)$$

with $\widetilde{\Omega}$ being the transformed spatial domain. Obviously, if $\boldsymbol{\xi} = \mathbf{x}$ then $J \equiv 1$ so that the case when the energy is also dependent upon \mathbf{x} is included in this discussion. Calculations similar to those mentioned above show that the equilibrium equations become

$$\left(\frac{\partial \widetilde{w}}{\partial \theta_{\alpha,i}} \right)_{,i} - \frac{\partial \widetilde{w}}{\partial \theta_{\alpha}} + \frac{\partial \widetilde{\Psi}}{\partial \theta_{\alpha}} = 0, \quad \alpha = 1, 2, \quad (67)$$

where, adopting the earlier supposition that \mathbf{G} satisfies (60), we have set

$$\tilde{\Psi}(\theta_1, \theta_2, \boldsymbol{\xi}) = J\Psi(\mathbf{n}, \mathbf{x}), \quad (68)$$

and a comma now denotes partial differentiation with respect to ξ_i , with the same comments after equation (62) also being applicable here.

It is evident that equations (62) and (67) are the appropriate Euler–Lagrange equations for an energy integral of the form

$$W = \int_V (w - \Psi) dV. \quad (69)$$

1.2.6 Boundary conditions

The boundary conditions for the director alignment at a liquid crystal–solid interface can essentially be of two types, either strong or weak anchoring [48, 104]. Strong anchoring occurs when the director orientation is prescribed at the boundary by a suitable treatment of the solid surface; this alignment is always supposed fixed. Frequently, the director has a fixed direction in the plane of the surface (planar) or perpendicular (homeotropic) to it; it need not always be so, and there are examples of strong anchoring, called conical anchoring, where the director at a surface makes a non-zero fixed angle with the tangent plane of the surface. (cf. [48, p.160] and [104]). On the other hand, weak anchoring, first proposed by Rapini and Papoular [95], supposes that a weak anchoring energy is available at the liquid crystal–solid interface, and presumes a balance between the moment (or torque) in the liquid crystal due to the Frank–Oseen energy density and that arising from this interfacial energy. Such a weak anchoring energy, which we will denote by w_s , can be employed to determine how the angle between the director and the solid, or other interface, may vary under the influence of applied fields, for example.

The simplest assumption is that w_s has a dependence upon the director \mathbf{n} relative to some proposed preferred direction at the interface, say \mathbf{n}_p ; equivalently, and quite commonly, we can equally consider w_s to depend upon \mathbf{n} and $\boldsymbol{\nu}$ where $\boldsymbol{\nu}$ is the outward unit normal at the interface. One version of a weak anchoring energy that proves convenient (and is equivalent to that introduced by Rapini and Papoular) can be written as [104, 107]

$$w_s = \frac{1}{2}\tau_0(1 + \omega(\mathbf{n} \cdot \boldsymbol{\nu})^2), \quad (70)$$

where $\tau_0 > 0$ and $\omega > -1$. For $-1 < \omega < 0$ the weak anchoring surface energy w_s will favour a director alignment parallel to $\boldsymbol{\nu}$ so that the energy is reduced and the favoured orientation of \mathbf{n} will be homeotropic. When $\omega > 0$, w_s will favour an orientation orthogonal to $\boldsymbol{\nu}$, indicating that a homogeneous alignment tangential to the boundary or interface will be favoured. These comments are equally valid in an analogous fashion when $\boldsymbol{\nu}$ is replaced by a preferred interfacial director alignment \mathbf{n}_p . Rapini and Papoular [95] estimated $\tau_0\omega \sim 10^{-3} \text{ J m}^{-2}$ as a general value; for the nematic liquid crystal 5CB, Yokoyama and van Sprang [110] experimentally calculated $\tau_0\omega$ to be around $4 \times 10^{-5} \text{ J m}^{-2}$. Reviews of various techniques for measuring the anchoring strength have been written by Yokoyama [109] and Blinov, Kabayenkov and Sonin [16].

The total energy for a sample of liquid crystal occupying the region V having boundary S is given by

$$W = \int_V w d\Omega + \int_S w_s dS, \quad (71)$$

which will generally lead to two sets of coupled equilibrium equations, one set arising solely from the equilibrium equations for the bulk energy (namely, those stated in equation (37)) and the other arising from both the bulk and surface energies. This second set of equations stems from the equilibrium boundary condition which is given by

$$\frac{\partial w}{\partial n_{i,j}} \nu_j + \frac{\partial w_s}{\partial n_i} = \gamma n_i \quad \text{on } S, \quad (72)$$

where γ is an arbitrary scalar function; this requirement was first mentioned by Jenkins and Barratt [55]. The weak boundary condition (72) can also be reformulated using the orientation angles $\theta_1 = \theta$ and $\theta_2 = \phi$ introduced in equation (53). The result, in an obvious nomenclature, is [104]

$$\frac{\partial \hat{w}}{\partial \theta_{\alpha,j}} \nu_j + \frac{\partial \hat{w}_s}{\partial \theta_\alpha} = 0, \quad \alpha = 1, 2. \quad (73)$$

We mention a particularly prevalent special case. Consider a liquid crystal sample confined between parallel planar boundary plates placed a distance d apart at $z = \pm d/2$ and suppose that $\phi \equiv 0$ and $\theta = \theta(z)$ in equation (53). Then $\boldsymbol{\nu} = (0, 0, \pm 1)$ in accordance with $z = \pm d/2$ and equation (73) then reduces to the two conditions

$$\frac{\partial \hat{w}}{\partial \theta'} - \frac{\partial \hat{w}_s}{\partial \theta} = 0 \quad \text{at } z = -\frac{d}{2}, \quad \frac{\partial \hat{w}}{\partial \theta'} + \frac{\partial \hat{w}_s}{\partial \theta} = 0 \quad \text{at } z = \frac{d}{2}, \quad (74)$$

where a prime denotes the derivative with respect to z . Of course, if one surface, at $z = -d/2$ for example, has strong anchoring or a weak anchoring energy that differs from that at the other surface at $z = d/2$, then the corresponding condition at $z = -d/2$ in equation (74) either does not arise, as in the case for strong anchoring, or is adapted to incorporate the appropriate form for \hat{w}_s at $z = -d/2$. If no anchoring conditions, strong or weak, are prescribed then the requirements in (74) are seen to be the usual natural boundary conditions that arise from the calculus of variations [104, 107].

It has become apparent, nevertheless, that weak anchoring can be more complex because surface anchoring in nematics can be bistable, as reported by Jerome, Pieranski and Boix [56] and Monkade, Boix and Durand [84]. Nobili and Durand [86] have suggested that more a complex form for the surface energy must be considered and have reported measurements from a more sophisticated model, as have Sergan and Durand [100] who have also described further measurements. A more extensive discussion on the modelling of weak anchoring that incorporates the combinations of director ‘tilt and twist’ at the boundary can be found in the articles by Zhao, Wu and Iwamoto [113, 114].

1.2.7 Extensions to nematic equilibrium theory

The energy for nematics given in equation (18) has its analogue for chiral nematics, also called cholesterics, given by

$$w_{ch} = \frac{1}{2}K_1(\nabla \cdot \mathbf{n})^2 + \frac{1}{2}K_2(\mathbf{n} \cdot \nabla \times \mathbf{n} + q)^2 + \frac{1}{2}K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 + \frac{1}{2}(K_2 + K_4)\nabla \cdot [(\mathbf{n} \cdot \nabla)\mathbf{n} - (\nabla \cdot \mathbf{n})\mathbf{n}], \quad (75)$$

where q is related to the natural pitch p of the characteristic helical configurations that occur in cholesterics through the relation $p = 2\pi/q$ (see [48, 104] for further general details). Depending on the material, the pitch p can range in magnitude from 200 nm upwards with typical values being around 600 nm [48] and so it is frequently much larger than the molecular dimensions. The continuum theory as outlined above for nematics has its clear analogue when w is replaced by w_{ch} . Mention should also be made of the results for a weak anchoring surface energy model that has been developed for cholesterics by Belyakov *et al.* [11–13] as an alternative to the Rapini–Papoular form for weak anchoring.

The Frank–Oseen energy can be used to identify basic defects in nematic liquid crystals and these were classified by Frank [41] in 1958. In 1991 Ericksen [38] proposed an extension to the Frank–Oseen theory in order to improve the modelling of defects. Ericksen’s model incorporates the order parameter and proposes an energy density of the form

$$w = w(s, \mathbf{n}, \nabla s, \nabla \mathbf{n}), \quad (76)$$

where s is a scalar function that represents the degree of order or alignment. In this theory, the scalar s is permitted to vanish at point or line defects in such a way that the energy remains finite, which then avoids the infinite energies that can occur when modelling defects with the Frank–Oseen version of the energy. A relevant account, and developments of, this approach may be found in the book by Virga [107].

1.3 Dynamic Theory for Nematics

The earliest attempt at a dynamic theory for nematic liquid crystals was made by Anzelius [3] in 1931, although the first widely accepted dynamic theory was formulated much later by Ericksen [33] in 1961 using balance laws from the classical theory of continuum mechanics based upon a generalisation of the equilibrium theory discussed above. This dynamic theory was completed in 1968 by Leslie [61], who derived constitutive equations and proposed expressions for the various dynamic contributions, after he considered constitutive equations for anisotropic fluids in 1966 [60]. A more concise derivation of the dynamic theory for nematics was later published by Leslie [64] in 1992; details can also be found in [104].

As in the equilibrium case discussed above, it will be assumed that the nematic is incompressible. For a volume V of nematic bounded by the surface S the three conservation laws for mass, linear momentum and angular momentum are, respectively,

$$\frac{D}{Dt} \int_V \rho dV = 0, \quad (77)$$

$$\frac{D}{Dt} \int_V \rho \mathbf{v} dV = \int_V \rho \mathbf{F} dV + \int_S \mathbf{t} dS, \quad (78)$$

$$\frac{D}{Dt} \int_V \rho(\mathbf{x} \times \mathbf{v}) dV = \int_V \rho(\mathbf{x} \times \mathbf{F} + \mathbf{K}) dV + \int_S (\mathbf{x} \times \mathbf{t} + \mathbf{l}) dS, \quad (79)$$

where ρ denotes the density, \mathbf{x} is the position vector, \mathbf{v} is the velocity, \mathbf{F} is the external body force per unit mass, \mathbf{t} is the surface force per unit area, \mathbf{K} is the external body moment per unit mass, \mathbf{l} is the surface moment per unit area (also called the couple

stress vector) and D/Dt , also denoted by a superposed dot, represents the usual material time derivative defined by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}. \quad (80)$$

No ‘director inertial term’ has been incorporated since it is generally considered to be negligible in nematic liquid crystal flow problems. There is a general convention in the liquid crystal literature that \mathbf{F} appears in static theory while $\rho\mathbf{F}$ appears in dynamic theory: this means that in statics \mathbf{F} represents the external body force per unit volume while it represents the external body force per unit mass in dynamics. An analogous statement applies to the external body moment \mathbf{K} .

If $\boldsymbol{\nu}$ denotes the outward unit normal to the surface S , then, similar to the situation in equation (32), the surface force t_i and surface moment l_i are expressible in terms of the stress tensor t_{ij} and couple stress tensor l_{ij} , respectively, through the relations

$$t_i = t_{ij}\nu_j, \quad l_i = l_{ij}\nu_j. \quad (81)$$

The mass conservation law (77) can be shown to reduce to the usual incompressibility condition

$$\nabla \cdot \mathbf{v} = 0, \quad (82)$$

and the density ρ can then be considered as being homogeneously constant throughout any given volume V . After detailed manipulations that involve transport theorems, the balance of linear momentum (78) and balance of angular momentum (79) reduce to, in point form,

$$\rho\dot{v}_i = \rho F_i + t_{ij,j}, \quad (83)$$

and

$$\rho K_i + \epsilon_{ijk}t_{kj} + l_{ij,j} = 0, \quad (84)$$

respectively.

It is relevant at this point to mention some key concepts related to different angular velocities that occur in anisotropic fluids that are absent from classical isotropic continuum theories. The Eulerian description of the instantaneous motion of a fluid with microstructure employs two independent vector fields. The first is the usual velocity $\mathbf{v}(\mathbf{x}, t)$ and the second is an axial vector $\mathbf{w}(\mathbf{x}, t)$ which, in the case of nematic liquid crystals, represents the local angular velocity of the director \mathbf{n} at position \mathbf{x} and time t . More details on this terminology, in the context of polar fluids, can be found in the review by Cowin [26]. This is in contrast to the classical isotropic continuum theories where the only independent field is the velocity \mathbf{v} of the fluid because the angular velocity in such traditional theories equals one half of the curl of the velocity. We denote this particular classical angular velocity by $\widehat{\boldsymbol{\omega}}$, defined by

$$\widehat{\boldsymbol{\omega}} = \frac{1}{2}\nabla \times \mathbf{v}, \quad (85)$$

and refer to it as the regional angular velocity, to distinguish it from other angular velocities. It is a measure of the average rotation of the fluid over a neighbourhood of the director. The angular velocity of the director relative to the regional angular velocity in which the director is embedded is denoted by $\boldsymbol{\omega}$ and is defined by [26, 104]

$$\boldsymbol{\omega} = \mathbf{w} - \widehat{\boldsymbol{\omega}} = \mathbf{w} - \frac{1}{2}\nabla \times \mathbf{v}. \quad (86)$$

The quantity $\boldsymbol{\omega}$ is called the relative angular velocity and is introduced to measure the difference between the local angular velocity \mathbf{w} of the liquid crystal director and the regional angular velocity $\widehat{\mathbf{w}}$ of the fluid in the neighbourhood of the director.

It proves convenient to introduce The rate of strain tensor \mathbf{A} and vorticity tensor \mathbf{W} in the usual way by

$$\mathbf{A} = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad \mathbf{W} = \frac{1}{2} (\nabla \mathbf{v} - (\nabla \mathbf{v})^T), \quad (87)$$

where the index T denotes the transpose. The vorticity tensor is also sometimes called the spin tensor or angular velocity tensor. Following Leslie [64], the vector \mathbf{N} is introduced and defined by

$$\mathbf{N} = \boldsymbol{\omega} \times \mathbf{n}. \quad (88)$$

It can be shown [104] that this definition is equivalent to

$$\mathbf{N} = \dot{\mathbf{n}} - \mathbf{W}\mathbf{n}, \quad (89)$$

this being the form discussed originally by Ericksen and Leslie. In the terminology used by Truesdell and Noll [106], \mathbf{N} is called the co-rotational time flux of the director \mathbf{n} ; it is, nevertheless, important to recognise the interpretation of \mathbf{N} in the context of relative angular velocities as indicated by equations (86) and (88), in which case it is clear that \mathbf{N} provides a measure of the rotation of \mathbf{n} relative to the fluid.

At this level of description, Leslie [64] introduced a rate of work hypothesis. This assumed that the rate at which forces and moments do work on a volume of nematic will be absorbed into changes in the nematic energy w or the kinetic energy, or will be lost by means of viscous dissipation. The rate of work postulate is taken to be

$$\int_V \rho (\mathbf{F} \cdot \mathbf{v} + \mathbf{K} \cdot \mathbf{w}) dV + \int_S (\mathbf{t} \cdot \mathbf{v} + \mathbf{l} \cdot \mathbf{w}) dS = \frac{D}{Dt} \int_V (\frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + w) dV + \int_V \mathcal{D} dV, \quad (90)$$

where \mathcal{D} is the rate of viscous dissipation per unit volume, also called the dissipation function; \mathcal{D} is always assumed positive. It is known that the material derivative of \mathbf{n} satisfies the relation

$$\dot{\mathbf{n}} = \mathbf{w} \times \mathbf{n}, \quad (91)$$

a well-known consequence of \mathbf{n} being a unit vector. With the aid of the relations in (81) and simplification through the expressions (83) and (84), the rate of work hypothesis in (90) can be expressed in point form as

$$t_{ij} v_{i,j} + l_{ij} w_{i,j} - w_i \epsilon_{ijk} t_{kj} = \dot{w} + \mathcal{D}, \quad (92)$$

a result that can then be exploited to obtain expressions for the stress and couple stress.

It is possible to express the material derivative of w in terms of velocity gradients and the angular velocity and its gradients. After much intricate calculation [64, 104] and an application of the Ericksen identity (20), this leads to the conclusion that the stress tensor t_{ij} and couple stress tensor l_{ij} can take the forms [64]

$$t_{ij} = -p \delta_{ij} - \frac{\partial w}{\partial n_{p,j}} n_{p,i} + \tilde{t}_{ij}, \quad (93)$$

$$l_{ij} = \epsilon_{ipq} n_p \frac{\partial w}{\partial n_{q,j}} + \tilde{l}_{ij}, \quad (94)$$

where p is an arbitrary pressure arising from the assumed incompressibility and \tilde{t}_{ij} and \tilde{l}_{ij} denote possible dynamic contributions. In the terminology of Leslie [65, 67], \tilde{t}_{ij} is called the viscous stress. The expressions in (93) and (94) allows the result in (92) to reduce to

$$\tilde{t}_{ij}v_{i,j} + \tilde{l}_{ij}w_{i,j} - w_i\epsilon_{ijk}\tilde{t}_{kj} = \mathcal{D} \geq 0, \quad (95)$$

given that \mathcal{D} is positive. This inequality is of crucial importance in the constitutive theory and imposes restrictions upon the forms of the dynamic terms.

1.3.1 The viscous stress in nematics

The simplest forms for the viscous parts of the stress and couples stress that are consistent with experimental experience assume that \tilde{t}_{ij} and \tilde{l}_{ij} depend only on \mathbf{A} , \mathbf{n} and \mathbf{w} , but not on the gradients of \mathbf{w} . It then follows directly from the inequality in (95) that

$$\tilde{l}_{ij} \equiv 0, \quad (96)$$

and hence the viscous dissipation inequality in (95) reduces to

$$\tilde{t}_{ij}v_{i,j} - w_i\epsilon_{ijk}\tilde{t}_{kj} = \mathcal{D} \geq 0, \quad (97)$$

which further restricts the contributions to the viscous stress \tilde{t}_{ij} . It can be shown that \mathbf{A} , \mathbf{n} and \mathbf{N} are material frame-indifferent and that the aforementioned dependence of \tilde{t}_{ij} upon \mathbf{A} , \mathbf{n} and \mathbf{w} can be replaced by dependence upon \mathbf{A} , \mathbf{n} and \mathbf{N} . The required material frame-indifference of \tilde{t}_{ij} , combined with nematic symmetries and an assumed linear dependence upon \mathbf{A} and \mathbf{N} , leads to the identification of the viscous stress in its most widely adopted and well known form given by [64, 104]

$$\begin{aligned} \tilde{t}_{ij} = & \alpha_1 n_k A_{kp} n_p n_i n_j + \alpha_2 N_i n_j + \alpha_3 n_i N_j + \alpha_4 A_{ij} \\ & + \alpha_5 n_j A_{ik} n_k + \alpha_6 n_i A_{jk} n_k. \end{aligned} \quad (98)$$

The coefficients $\alpha_1, \alpha_2, \dots, \alpha_6$, are called the Leslie viscosity coefficients, or simply the Leslie viscosities. They are dynamic viscosities. For notational and physical reasons, it is convenient to define the viscosities

$$\gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_6 - \alpha_5. \quad (99)$$

The coefficient γ_1 is called the rotational viscosity (or twist viscosity) while γ_2 is referred to as the torsion coefficient. Moreover, inserting the expression (98) into the inequality (97) forces restrictions in the relative signs of the Leslie viscosities and it is then possible to deduce that [60, 104]

$$\gamma_1 = \alpha_3 - \alpha_2 \geq 0, \quad (100)$$

$$\alpha_4 \geq 0, \quad (101)$$

$$2\alpha_4 + \alpha_5 + \alpha_6 \geq 0, \quad (102)$$

$$2\alpha_1 + 3\alpha_4 + 2\alpha_5 + 2\alpha_6 \geq 0, \quad (103)$$

$$4\gamma_1(2\alpha_4 + \alpha_5 + \alpha_6) \geq (\alpha_2 + \alpha_3 + \gamma_2)^2. \quad (104)$$

Parodi [91] proposed, via Onsager relations, that the viscosity coefficients should be further restricted by the relation

$$\gamma_2 \equiv \alpha_6 - \alpha_5 = \alpha_2 + \alpha_3, \quad (105)$$

a result that was subsequently obtained by Currie [27] by a stability argument. This reduces the number of independent viscosities to five rather than six and often leads to some simplification of the theory. It is a generally accepted relation in the theory. When the Parodi relation (105) holds, the viscous dissipation function, defined by the left-hand side of the equality in (97), can be written down explicitly to arrive at

$$\begin{aligned} \mathcal{D} = & \alpha_1(n_i A_{ij} n_j)^2 + 2\gamma_2 N_i A_{ij} n_j + \alpha_4 A_{ij} A_{ij} \\ & + (\alpha_5 + \alpha_6) n_i A_{ij} A_{jk} n_k + \gamma_1 N_i N_i \geq 0. \end{aligned} \quad (106)$$

In many cases it is simpler to deduce particular viscosity inequalities by calculating the dissipation inequality for \mathcal{D} explicitly from (106) rather than from the inequalities in (100) to (104).

1.3.2 The dynamic equations for nematics

It is possible to combine the results in equations (30), (81), (93), (94), (96) and use the Ericksen identity (20) to derive from equations (83) and (84), respectively, the final forms for the balances of linear and angular momentum. They are given by

$$\rho \dot{v}_i = \rho F_i - (p + w)_{,i} + \tilde{g}_j n_{j,i} + G_j n_{j,i} + \tilde{t}_{ij,j}, \quad (107)$$

$$\left(\frac{\partial w}{\partial n_{i,j}} \right)_{,j} - \frac{\partial w}{\partial n_i} + \tilde{g}_i + G_i = \lambda n_i, \quad (108)$$

where

$$\tilde{g}_i = -\gamma_1 N_i - \gamma_2 A_{ip} n_p. \quad (109)$$

The scalar function λ is a Lagrange multiplier which can usually be eliminated or evaluated by taking the scalar product of equation (108) with \mathbf{n} . These equations, in conjunction with the constraint from (12) that \mathbf{n} is a unit vector and the incompressibility condition (82) that arises from the conservation of mass, provide a complete set of dynamic equations for nematic liquid crystals.

The number of unknowns in the dynamic theory equals the number of available equations. The unknowns are the velocity $\mathbf{v}(\mathbf{x}, t)$, the director $\mathbf{n}(\mathbf{x}, t)$, the pressure $p(\mathbf{x}, t)$ and the Lagrange multiplier λ . Therefore the total number of unknown quantities is clearly eight: there are three arising from the components of \mathbf{v} , three from \mathbf{n} , one from p and one from λ . The director constraint (12) and the incompressibility condition (82) provide two equations while the balances of linear and angular momentum in equations (107) and (108) provide six equations. There are therefore eight equations to be satisfied, and this matches the number of unknowns.

We remark that if the body force and moment satisfy the relations

$$\rho F_i = \frac{\partial \Psi}{\partial x_i}, \quad G_i = \frac{\partial \Psi}{\partial n_i}, \quad \Psi = -\rho \Psi_g + \Psi_m, \quad (110)$$

when ρ is constant (cf. the notation used for the equilibrium case above in Section 1.2.4) then equation (107) reduces to the simpler form

$$\rho \dot{v}_i = -\tilde{p}_{,i} + \tilde{g}_j n_{j,i} + \tilde{t}_{ij,j}, \quad (111)$$

with

$$\tilde{p} = p + w - \Psi, \quad \Psi = -\rho \Psi_g + \Psi_m, \quad (112)$$

where p is an arbitrary pressure. This follows from an identity analogous to that in equation (49) with \mathbf{F} replaced by $\rho \mathbf{F}$.

The boundary conditions for dynamic theory, which may include weak or strong anchoring boundary conditions on the director, are usually supplemented by the classical no-slip boundary conditions on the velocity \mathbf{v} ; for example, at a solid interface at rest it is assumed that $\mathbf{v} = \mathbf{0}$ on the boundary.

1.3.3 Reformulation of the dynamic equations

The Ericksen–Leslie equations summarised above can be reformulated in a manner similar to the reformulation of the equilibrium equations in Section 1.2.5. Many of the technical details can be found in detail in [104]. Firstly, we note that Ericksen [37] pointed out that when the Parodi relation (105) applies then the vector \tilde{g}_i and the viscous stress \tilde{t}_{ij} in equations (109) and (98) can be obtained directly from the dissipation function \mathcal{D} (which we can accept for our purposes as being defined by equation (106)), through the properties

$$\tilde{g}_i = -\frac{1}{2} \frac{\partial \mathcal{D}}{\partial \dot{n}_i}, \quad \tilde{t}_{ij} = \frac{1}{2} \frac{\partial \mathcal{D}}{\partial v_{i,j}}. \quad (113)$$

We can again adopt the notation from equations (53), (54) and (57) and further introduce a rescaled dissipation function $\widehat{\mathcal{D}}$ defined by

$$\widehat{\mathcal{D}}(\nabla \mathbf{v}, \theta, \phi, \dot{\theta}, \dot{\phi}) = \frac{1}{2} \mathcal{D}(\mathbf{A}, \mathbf{n}, \mathbf{N}). \quad (114)$$

In addition to the aforementioned reformulations we record here that

$$n_{i,j} = \frac{\partial f_i}{\partial \theta_\beta} \theta_{\beta,j}, \quad \left(\frac{\partial f_k}{\partial \theta_\alpha} \right)_{,i} = \frac{\partial n_{k,i}}{\partial \theta_\alpha}, \quad (115)$$

$$\dot{n}_k = \frac{\partial f_k}{\partial \theta} \dot{\theta} + \frac{\partial f_k}{\partial \phi} \dot{\phi}, \quad (116)$$

so that, in particular, by the first result in (113),

$$\frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\theta}} = \frac{1}{2} \frac{\partial \mathcal{D}}{\partial \dot{n}_k} \frac{\partial \dot{n}_k}{\partial \dot{\theta}} = -\tilde{g}_k \frac{\partial f_k}{\partial \theta}, \quad \frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\phi}} = \frac{1}{2} \frac{\partial \mathcal{D}}{\partial \dot{n}_k} \frac{\partial \dot{n}_k}{\partial \dot{\phi}} = -\tilde{g}_k \frac{\partial f_k}{\partial \phi}, \quad (117)$$

$$\tilde{g}_j n_{j,i} = \tilde{g}_j \frac{\partial f_j}{\partial \theta} \theta_{,i} + \tilde{g}_j \frac{\partial f_j}{\partial \phi} \phi_{,i} = -\frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\theta}} \theta_{,i} - \frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\phi}} \phi_{,i}. \quad (118)$$

Further, using the expression for G_i in equation (110),

$$\frac{\partial \widehat{\Psi}}{\partial \theta} = \frac{\partial \Psi}{\partial n_i} \frac{\partial f_i}{\partial \theta} = G_i \frac{\partial f_i}{\partial \theta}, \quad \text{and} \quad \frac{\partial \widehat{\Psi}}{\partial \phi} = \frac{\partial \Psi}{\partial n_i} \frac{\partial f_i}{\partial \phi} = G_i \frac{\partial f_i}{\partial \phi}. \quad (119)$$

Combining the results from (58), (59), (117) and (119) and employing calculations similar in style to those required to obtain the expressions in (62), we see that

$$\left(\frac{\partial \widehat{w}}{\partial \theta_{,i}}\right)_{,i} - \frac{\partial \widehat{w}}{\partial \theta} - \frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\theta}} + \frac{\partial \widehat{\Psi}}{\partial \theta} = \left[\left(\frac{\partial w}{\partial n_{k,i}}\right)_{,i} - \frac{\partial w}{\partial n_k} + \tilde{g}_k + G_k \right] \frac{\partial f_k}{\partial \theta}, \quad (120)$$

accompanied by an analogous result in terms of ϕ also. Therefore by equations (55) and (108) the balance of angular momentum reduces to the two equations

$$\left(\frac{\partial \widehat{w}}{\partial \theta_{,i}}\right)_{,i} - \frac{\partial \widehat{w}}{\partial \theta} - \frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\theta}} + \frac{\partial \widehat{\Psi}}{\partial \theta} = 0, \quad (121)$$

$$\left(\frac{\partial \widehat{w}}{\partial \phi_{,i}}\right)_{,i} - \frac{\partial \widehat{w}}{\partial \phi} - \frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\phi}} + \frac{\partial \widehat{\Psi}}{\partial \phi} = 0, \quad (122)$$

while with the aid of the relations (113), (114) and (118) the balance of linear momentum (107) becomes

$$\rho \dot{v}_i = -\tilde{p}_{,i} + \left(\frac{\partial \widehat{\mathcal{D}}}{\partial v_{i,j}}\right)_{,j} - \frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\theta}} \theta_{,i} - \frac{\partial \widehat{\mathcal{D}}}{\partial \dot{\phi}} \phi_{,i}, \quad i = 1, 2, 3, \quad (123)$$

where

$$\tilde{p} = p + \widehat{w} - \widehat{\Psi}. \quad (124)$$

These alternative forms given in (121), (122) and (123) for the main balance equations provide a complete set of dynamic equations that can be deployed more easily and rapidly, remembering, of course, that under the assumption of incompressibility the constraint $\nabla \cdot \mathbf{v} = 0$ must also hold.

1.3.4 Extension to the dynamic theory of biaxial nematics

Many aspects of the dynamic theory for nematics can be extended to the biaxial nematic phase of liquid crystals. The possibility of a biaxial nematic phase was first raised in 1970 by Freiser [42, 43] and the earliest experimental results were obtained by Yu and Saupe [112] in 1980. Other early reports followed on the synthesis of thermotropic biaxial nematics (see, for example, [23, 24, 77, 93]) and a review and discussion of such materials was made by Luckhurst [74]. Saupe [99] appears to have made the first attempt at a biaxial continuum theory, followed by other formulations developed by Liu [73], Kini [57], Govers and Vertogen [51–53], Chauré [25] and Leslie, Laverty and Carlsson [70]. These authors essentially obtained the same continuum theory from different viewpoints, as discussed by Leslie and Carlsson [68], who theoretically examined flow alignment in a biaxial nematic. There has recently been a resurgence of interest in the continuum modelling of biaxial nematic liquid crystals, due largely to emerging experimental results that have appeared in the literature [1, 76, 82, 101, 111]. A series of comments on many of these results has been made by Luckhurst [75]. A brief summary of the biaxial nematic continuum equations can be found in [5].

1.4 Continuum Theory for Smectic Liquid Crystals

This section reviews some basic results from smectic liquid crystals. It is principally concerned with the liquid crystal phase known as smectic C (SmC).

1.4.1 Smectic C liquid crystals

Smectic liquid crystals are layered structures that have a well defined interlayer distance. Smectics are more ordered than nematics and the smectic phase generally occurs at a temperature below that for which the same material will exhibit a nematic phase. Here we shall be considering only the smectic C liquid crystal phase, although it should be mentioned that other smectic phases have also been classified; see de Gennes and Prost [48] for details. A brief survey on the development and classification of various smectic phases has been written by Sackmann [98]. Much of the original continuum theory for smectic phases was initiated by the Orsay Group in the 1970s (see [48]), who were the first to present an energy density for SmC liquid crystals based on small perturbations of planar aligned samples of SmC [87]. Leslie, Stewart and Nakagawa [71] formulated an energy density for SmC that was not restricted to small perturbations, yet is identical to that introduced by the Orsay Group when it is suitably restricted.

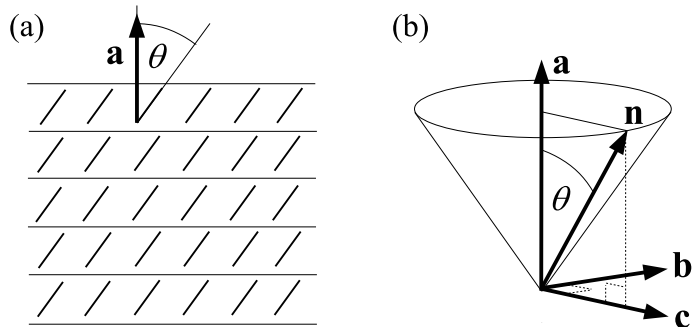


Figure 2: Schematic diagrams of SmC liquid crystals. The molecules are equidistantly spaced in layers as shown. In SmC the director \mathbf{n} makes an angle θ to the local unit layer normal \mathbf{a} .

In isothermal SmC liquid crystals the director \mathbf{n} is tilted at a fixed angle θ relative to the unit layer normal, denoted by \mathbf{a} , as shown in Fig. 2(a) (θ is generally temperature dependent). The normal \mathbf{a} is also referred to as the density wave vector. The director continues to be defined as the average direction of the molecular alignment and \mathbf{n} and $-\mathbf{n}$ remain indistinguishable, as in nematics. In non-chiral SmC liquid crystals the director is often uniformly aligned as shown in the Figure. The smectic interlayer distance may be anything from something close to the full length of the constituent molecules up to about twice their length [48, p.19] (typical values may be in the range $2 \sim 80$ nm). The tilt angle θ is commonly called the smectic cone angle because the director can be oriented around a fictitious cone of semi-vertical angle θ as shown in Fig. 2(b). The vector \mathbf{c} is introduced as the unit orthogonal projection of \mathbf{n} onto the local smectic planes; it further proves convenient to introduce the unit vector \mathbf{b} defined by $\mathbf{b} = \mathbf{a} \times \mathbf{c}$, also shown in Fig. 2(b). It is easily seen from the geometrical arrangement that \mathbf{n} can

be written as

$$\mathbf{n} = \mathbf{a} \cos \theta + \mathbf{c} \sin \theta, \quad (125)$$

which is often useful when making comparisons with the results from nematic theory. The phase known as smectic A (SmA) liquid crystals occurs when $\theta \equiv 0$.

It is clear that \mathbf{a} and \mathbf{c} are mutually orthogonal unit vectors and so they are subject to the constraints

$$\mathbf{a} \cdot \mathbf{a} = 1, \quad \mathbf{c} \cdot \mathbf{c} = 1, \quad \mathbf{a} \cdot \mathbf{c} = 0. \quad (126)$$

Further, in the absence of any singularities or defects in the smectic layers the unit layer normal \mathbf{a} is additionally subject to the constraint

$$\nabla \times \mathbf{a} = \mathbf{0}, \quad (127)$$

a requirement first identified by Oseen [89] for SmA liquid crystals and later exploited by the Orsay Group [87] and de Gennes and Prost [48] for general planar layers of SmC. A general justification of this result can be found in [104]. Notice that the constraint (127) is equivalent to the condition $a_{i,j} = a_{j,i}$ in Cartesian component form.

As in nematic theory, an energy density is presumed to exist and satisfy certain symmetry requirements. The energy density for non-chiral SmC is of the form

$$w = w(\mathbf{a}, \mathbf{c}, \nabla \mathbf{a}, \nabla \mathbf{c}), \quad (128)$$

with the total free energy being given by

$$W = \int_V w(\mathbf{a}, \mathbf{c}, \nabla \mathbf{a}, \nabla \mathbf{c}) dV, \quad (129)$$

where V is the sample volume. Similar to the construction of the nematic energy, the energy density must be invariant to arbitrary superposed rigid body rotations and therefore

$$w(\mathbf{a}, \mathbf{c}, \nabla \mathbf{a}, \nabla \mathbf{c}) = w(Q\mathbf{a}, Q\mathbf{c}, Q\nabla \mathbf{a}Q^T, Q\nabla \mathbf{c}Q^T), \quad (130)$$

where Q is any proper ($\det Q = 1$) orthogonal matrix, Q^T being its transpose. Moreover, for non-chiral SmC the requirement in (130) must additionally hold for any orthogonal matrix Q ($\det Q = \pm 1$). The energy also has to be invariant to the simultaneous changes in sign

$$\mathbf{a} \rightarrow -\mathbf{a} \quad \text{and} \quad \mathbf{c} \rightarrow -\mathbf{c}, \quad (131)$$

this being an invariance that arises from a consideration of the symmetry invariance required when \mathbf{n} is replaced by $-\mathbf{n}$. The resulting energy density w for non-chiral SmC then takes the form stated by Leslie, Stewart, Carlsson and Nakagawa [71]

$$\begin{aligned} w = & \frac{1}{2}K_1(\nabla \cdot \mathbf{a})^2 + \frac{1}{2}K_2(\nabla \cdot \mathbf{c})^2 + \frac{1}{2}K_3(\mathbf{a} \cdot \nabla \times \mathbf{c})^2 + \frac{1}{2}K_4(\mathbf{c} \cdot \nabla \times \mathbf{a})^2 \\ & + \frac{1}{2}K_5(\mathbf{b} \cdot \nabla \times \mathbf{c})^2 + K_6(\nabla \cdot \mathbf{a})(\mathbf{b} \cdot \nabla \times \mathbf{c}) + K_7(\mathbf{a} \cdot \nabla \times \mathbf{c})(\mathbf{c} \cdot \nabla \times \mathbf{a}) \\ & + K_8(\nabla \cdot \mathbf{c})(\mathbf{b} \cdot \nabla \times \mathbf{a}) + K_9(\nabla \cdot \mathbf{a})(\nabla \cdot \mathbf{c}), \end{aligned} \quad (132)$$

where the K_i , $i = 1, 2, \dots, 9$, are elastic constants. As in nematic theory, it is always supposed that

$$w(\mathbf{a}, \mathbf{c}, \nabla \mathbf{a}, \nabla \mathbf{c}) \geq 0. \quad (133)$$

Other equivalent forms for the energy in terms of any two of the vectors \mathbf{a} , \mathbf{b} and \mathbf{c} are available [71] (including alternative Cartesian component forms) and these allow comparisons with results across the literature, particularly the Orsay Group [87], Rapini [94], Dahl and Lagerwall [28] and Nakagawa [85]. One alternative form for w that can be constructed exclusively in terms of the vectors \mathbf{b} and \mathbf{c} is particularly revealing. It is given by [20, 71]

$$\begin{aligned}
w = & \frac{1}{2}A_{12}(\mathbf{b} \cdot \nabla \times \mathbf{c})^2 + \frac{1}{2}A_{21}(\mathbf{c} \cdot \nabla \times \mathbf{b})^2 + A_{11}(\mathbf{b} \cdot \nabla \times \mathbf{c})(\mathbf{c} \cdot \nabla \times \mathbf{b}) \\
& + \frac{1}{2}B_1(\nabla \cdot \mathbf{b})^2 + \frac{1}{2}B_2(\nabla \cdot \mathbf{c})^2 + \frac{1}{2}B_3 \left[\frac{1}{2}(\mathbf{b} \cdot \nabla \times \mathbf{b} + \mathbf{c} \cdot \nabla \times \mathbf{c}) \right]^2 \\
& + B_{13}(\nabla \cdot \mathbf{b}) \left[\frac{1}{2}(\mathbf{b} \cdot \nabla \times \mathbf{b} + \mathbf{c} \cdot \nabla \times \mathbf{c}) \right] \\
& + C_1(\nabla \cdot \mathbf{c})(\mathbf{b} \cdot \nabla \times \mathbf{c}) + C_2(\nabla \cdot \mathbf{c})(\mathbf{c} \cdot \nabla \times \mathbf{b}), \tag{134}
\end{aligned}$$

where the elastic constants are those introduced by the Orsay Group [87], except that for notational convenience we have set $A_{11} = -\frac{1}{2}A_{11}^{Orsay}$ and $C_1 = -C_1^{Orsay}$. This allows a direct physical interpretation of the elastic constants, as detailed in Carlsson *et al.* [20] and [104], and a direct comparison with the original Orsay Group formulation provided we set

$$\begin{aligned}
K_1 = A_{21}, \quad K_2 = B_2, \quad K_3 = B_1, \\
K_4 = B_3, \quad K_5 = 2A_{11} + A_{12} + A_{21} + B_3, \quad K_6 = -(A_{11} + A_{21} + \frac{1}{2}B_3), \\
K_7 = -B_{13}, \quad K_8 = C_1 + C_2 - B_{13}, \quad K_9 = -C_2. \tag{135}
\end{aligned}$$

Briefly, the terms associated with the coefficients A_{12} , A_{21} , B_1 , B_2 and B_3 represent five independent deformations of uniformly aligned planar smectic layers with the remaining terms interpreted as coupling terms. The non-negativity of w leads to inequalities in an analogous manner to those for nematics. It can be shown that (cf. [20, 87, 94])

$$A_{12}, A_{21}, B_1, B_2, B_3 \geq 0, \tag{136}$$

$$A_{12}A_{21} - A_{11}^2 \geq 0, \tag{137}$$

$$B_1B_3 - B_{13}^2 \geq 0, \tag{138}$$

$$B_2A_{12} - C_1^2 \geq 0, \tag{139}$$

$$B_2A_{21} - C_2^2 \geq 0. \tag{140}$$

Atkin and Stewart [6] also deduced that

$$A_{12} + A_{21} + 2A_{11} \geq 0 \quad \text{and} \quad A_{12} + A_{21} - 2A_{11} \geq 0, \tag{141}$$

which further implies

$$|A_{11}| \leq \frac{1}{2}(A_{12} + A_{21}). \tag{142}$$

The first inequality in (141) was derived by Carlsson *et al.* [20] for the special case when the smectic tilt angle θ is assumed small. It is very common for the quantities $A_{12} + A_{11}$ and $A_{21} + A_{11}$ to appear in calculations and it is important to recognise that they cannot be negative simultaneously because of the first inequality in (141). Additional analogous inequalities can be derived [6]:

$$B_1 + B_3 \pm 2B_{13} \geq 0 \quad \text{and} \quad |B_{13}| \leq \frac{1}{2}(B_1 + B_3), \tag{143}$$

$$B_2 + A_{12} \pm 2C_1 \geq 0 \quad \text{and} \quad |C_1| \leq \frac{1}{2}(B_2 + A_{12}), \tag{144}$$

$$B_2 + A_{21} \pm 2C_2 \geq 0 \quad \text{and} \quad |C_2| \leq \frac{1}{2}(B_2 + A_{21}). \tag{145}$$

One final set of properties for the elastic constants is worth noting. As the smectic tilt angle θ tends to zero the elastic energy ought to converge to that for the SmA phase, given by [48, 103]

$$w_A = \frac{1}{2}K_1(\nabla \cdot \mathbf{a})^2, \quad (146)$$

where $K_1 \geq 0$ is the usual splay elastic constant of nematic theory. Carlsson *et al.* [20] were able to use the techniques introduced by Dahl and Lagerwall [28] in order to postulate the tilt angle dependence of the SmC elastic constants for small θ . The results showed that

$$\begin{aligned} A_{12} &= K_1 + \bar{A}_{12}\theta^2, & A_{21} &= K_1 + \bar{A}_{21}\theta^2, & A_{11} &= -K_1 + \bar{A}_{11}\theta^2, \\ B_1 &= \bar{B}_1\theta^2, & B_2 &= \bar{B}_2\theta^2, & B_3 &= \bar{B}_3\theta^2, \\ B_{13} &= \bar{B}_{13}\theta^3, & C_1 &= \bar{C}_1\theta, & C_2 &= \bar{C}_2\theta, \end{aligned} \quad (147)$$

where the elastic constants K_1 , \bar{A}_i , \bar{B}_i and \bar{C}_i are assumed to be only weakly temperature dependent (θ is temperature dependent). These approximations are useful when trying to establish what ought to be the dominant elastic constants in particular problems in the SmC phase. Some preliminary measurements of \bar{B}_2 and the combination of elastic constants $\bar{A}_{11} + \bar{A}_{11}$ have been reported by Findon and Gleeson [40]. A more detailed discussion on magnitudes and cone angle dependent estimates for smectic elastic constants can be found in Stewart [104], largely based on the work contained in [20, 28].

It is worth remarking that three surface terms have been identified for the SmC phase, namely [71],

$$S_1 \equiv \nabla \cdot [\mathbf{c}(\nabla \cdot \mathbf{c}) - (\mathbf{c} \cdot \nabla)\mathbf{c}] = (c_i c_{j,j} - c_j c_{i,j})_{,i}, \quad (148)$$

$$S_2 \equiv \nabla \cdot [\mathbf{a}(\nabla \cdot \mathbf{c}) - (\mathbf{a} \cdot \nabla)\mathbf{c}] = (a_i c_{j,j} - a_j c_{i,j})_{,i}, \quad (149)$$

$$S_3 \equiv \nabla \cdot [(\nabla \cdot \mathbf{a})\mathbf{a}] = (a_{i,i})^2 - a_{i,j}a_{i,j}. \quad (150)$$

1.4.2 Equilibrium equations

A principle of virtual work, analogous to that for nematics stated in equation (23), can be adopted. Following the work of Leslie, Stewart and Nakagawa [72] it can be assumed that the variation of the total energy at equilibrium satisfies a principle of virtual work for a given volume V of SmC given by

$$\begin{aligned} \delta \int_V w dV &= \int_V (\mathbf{F} \cdot \delta \mathbf{x} + \mathbf{G}^a \cdot \Delta \mathbf{a} + \mathbf{G}^c \cdot \Delta \mathbf{c}) dV \\ &\quad + \int_S (\mathbf{t} \cdot \delta \mathbf{x} + \mathbf{s}^a \cdot \Delta \mathbf{a} + \mathbf{s}^c \cdot \Delta \mathbf{c}) dS, \end{aligned} \quad (151)$$

where, analogous to the quantity in equation (24),

$$\Delta \mathbf{a} = \delta \mathbf{a} + (\delta \mathbf{x} \cdot \nabla)\mathbf{a}, \quad \Delta \mathbf{c} = \delta \mathbf{c} + (\delta \mathbf{x} \cdot \nabla)\mathbf{c}, \quad (152)$$

with $\delta \mathbf{x}$ being the virtual displacements. In the above, S is the boundary surface, w is the SmC energy density, \mathbf{F} is the external body force per unit volume, \mathbf{G}^a and \mathbf{G}^c are generalised external body forces per unit volume related to \mathbf{a} and \mathbf{c} , respectively, \mathbf{t} is the surface traction per unit area, and \mathbf{s}^a and \mathbf{s}^c are generalised surface tractions per unit

area related to \mathbf{a} and \mathbf{c} , respectively. The virtual displacements $\delta\mathbf{x}$ and the variations in the vectors \mathbf{a} and \mathbf{c} are also subject to the constraints

$$\nabla \cdot (\delta\mathbf{x}) = 0, \quad (153)$$

$$\mathbf{a} \cdot \delta\mathbf{a} = 0, \quad \mathbf{a} \cdot \Delta\mathbf{a} = 0, \quad \mathbf{c} \cdot \delta\mathbf{c} = 0, \quad \mathbf{c} \cdot \Delta\mathbf{c} = 0, \quad (154)$$

$$\mathbf{a} \cdot \delta\mathbf{c} + \mathbf{c} \cdot \delta\mathbf{a} = 0, \quad \mathbf{a} \cdot \Delta\mathbf{c} + \mathbf{c} \cdot \Delta\mathbf{a} = 0. \quad (155)$$

The requirement in (153) is due to the assumption of incompressibility and the others follow from the constraints in equation (126). By carrying out calculations which parallel those required in Section 1.2.3 for nematics in equations (27) and (29), it can be deduced that

$$\int_V \mathbf{F} dV + \int_S \mathbf{t} dS = \mathbf{0}, \quad (156)$$

and

$$\int_V (\mathbf{x} \times \mathbf{F} + \mathbf{a} \times \mathbf{G}^a + \mathbf{c} \times \mathbf{G}^c) dV + \int_S (\mathbf{x} \times \mathbf{t} + \mathbf{a} \times \mathbf{s}^a + \mathbf{c} \times \mathbf{s}^c) dS = \mathbf{0}, \quad (157)$$

which represent, as before, the balance of forces and moments, respectively. It follows from these relationships that the body moment \mathbf{K} and couple stress vector \mathbf{l} can be related to the generalised body and surface forces by, respectively,

$$\mathbf{K} = \mathbf{a} \times \mathbf{G}^a + \mathbf{c} \times \mathbf{G}^c, \quad \mathbf{l} = \mathbf{a} \times \mathbf{s}^a + \mathbf{c} \times \mathbf{s}^c. \quad (158)$$

The generalised body forces \mathbf{G}^a and \mathbf{G}^c can be identified using the formulation of \mathbf{G} for nematics in Section 1.2.4 via the identity (125).

Similar to nematics, the surface forces can be expressed in terms of the corresponding stress tensors and the outward unit normal $\boldsymbol{\nu}$ as

$$t_i = t_{ij}\nu_j, \quad (159)$$

$$s_i^a = \alpha_1 a_i + \alpha_3 c_i + s_{ij}^a \nu_j, \quad (160)$$

$$s_i^c = \alpha_2 c_i + \alpha_3 a_i + s_{ij}^c \nu_j, \quad (161)$$

where the scalar functions α_1 , α_2 and α_3 arise from the constraints in equation (126). Detailed calculations reveal that [72, 104]

$$t_{ij} = -p\delta_{ij} + \beta_p \epsilon_{pjk} a_{k,i} - \frac{\partial w}{\partial a_{k,j}} a_{k,i} - \frac{\partial w}{\partial c_{k,j}} c_{k,i}, \quad (162)$$

$$s_{ij}^a = \epsilon_{ijp} \beta_p + \frac{\partial w}{\partial a_{i,j}}, \quad (163)$$

$$s_{ij}^c = \frac{\partial w}{\partial c_{i,j}}. \quad (164)$$

In the above, the vector $\boldsymbol{\beta}$ is a vector Lagrange multiplier that is due to the vector constraint (127) while p is an arbitrary pressure that arises from incompressibility. The components t_{ij} form the stress tensor and the components s_{ij}^a and s_{ij}^c belong to torque stresses.

Following the method adopted for nematics, the final forms for the equilibrium equations may be stated as [72, 104]

$$t_{ij,j} + F_i = 0, \quad (165)$$

$$\left(\frac{\partial w}{\partial a_{i,j}} \right)_{,j} - \frac{\partial w}{\partial a_i} + G_i^a + \gamma a_i + \mu c_i + \epsilon_{ijk} \beta_{k,j} = 0, \quad (166)$$

$$\left(\frac{\partial w}{\partial c_{i,j}} \right)_{,j} - \frac{\partial w}{\partial c_i} + G_i^c + \tau c_i + \mu a_i = 0. \quad (167)$$

Equation (165) represents a balance of forces, while, similar to the static theory of nematics, equations (166) and (167) are equivalent to a balance of moments. There are four Lagrange multipliers that arise from the four constraints contained in equations (126) and (127): they are the scalar multipliers γ , μ and τ and the vector multiplier $\boldsymbol{\beta}$. The ‘ a -equations’ in (166) are coupled to the ‘ c -equations’ in (167) via the Lagrange multiplier μ . Techniques for obtaining the Lagrange multipliers, particularly $\boldsymbol{\beta}$, can be found in [104].

The details and comments in Section 1.2.4 on body forces, moments and electric and magnetic fields in nematics are equally valid for SmC liquid crystals and follow naturally by suitably inserting the form for \mathbf{n} stated in equation (125). Moreover, it can be shown [104], as for nematics above, that the balance of forces (165) reduces to an expression for the pressure p , namely,

$$p + w - \Psi = p_0, \quad (168)$$

where p_0 is an arbitrary constant and, as for nematics, $\Psi(\mathbf{n}, \mathbf{x})$ is the scalar density function discussed in Section 1.2.4. This has the same consequence as for nematics, in that we can then generally neglect equation (165) so that the essential equilibrium equations reduce to the coupled equations (166) and (167). This then leaves twelve equations from (126), (127), (166) and (167) in the twelve unknowns that are made up from the nine components of \mathbf{a} , \mathbf{c} , and $\boldsymbol{\beta}$ and the three multipliers γ , μ and τ . A reformulation of the equilibrium equations, in the style of that presented above for nematics in Section 1.2.5, has been derived by Leslie [66].

Boundary conditions in the modelling of SmC liquid crystals are very similar to those for nematics and the discussion in Section 1.2.6 remains relevant. There is, as yet, little information on genuinely smectic boundary conditions, although this situation is evidently expected to evolve rapidly in the near future.

1.4.3 Dynamic theory for smectic C

The dynamic theory for SmC can be derived in a similar fashion to that above for nematics and so we refer the reader to [72, 104] for the mathematical details. The dynamic theory introduced in [72] can be summarised as follows. The vectors \mathbf{a} and \mathbf{c} are subject to the constraints

$$\mathbf{a} \cdot \mathbf{a} = 1, \quad \mathbf{c} \cdot \mathbf{c} = 1, \quad \mathbf{a} \cdot \mathbf{c} = 0, \quad \nabla \times \mathbf{a} = \mathbf{0}, \quad (169)$$

and the velocity vector \mathbf{v} must satisfy

$$v_{i,i} = 0. \quad (170)$$

The governing dynamic equations consist of the balance of linear momentum

$$\rho \dot{v}_i = \rho F_i - \tilde{p}_{,i} + G_k^a a_{k,i} + G_k^c c_{k,i} + \tilde{g}_k^a a_{k,i} + \tilde{g}_k^c c_{k,i} + \tilde{t}_{ij,j}, \quad (171)$$

with

$$\tilde{p} = p + w, \quad (172)$$

and the balance of angular momentum, which reduces to the two coupled sets of equations

$$\left(\frac{\partial w}{\partial a_{i,j}} \right)_{,j} - \frac{\partial w}{\partial a_i} + G_i^a + \tilde{g}_i^a + \gamma a_i + \mu c_i + \epsilon_{ijk} \beta_{k,j} = 0, \quad (173)$$

$$\left(\frac{\partial w}{\partial c_{i,j}} \right)_{,j} - \frac{\partial w}{\partial c_i} + G_i^c + \tilde{g}_i^c + \tau c_i + \mu a_i = 0, \quad (174)$$

where the scalar functions γ , μ and τ and the vector function $\boldsymbol{\beta}$ are Lagrange multipliers, as introduced and discussed in Section 1.4.2. In the above equations F_i is the external body force per unit mass, G_i^a and G_i^c are generalised external body forces per unit volume related to \mathbf{a} and \mathbf{c} , respectively, p is the arbitrary pressure and w is the elastic energy density for SmC given by (132). The dynamic contributions \tilde{g}_i^a and \tilde{g}_i^c are given by

$$\begin{aligned} \tilde{g}_i^a = & -2 \left(\lambda_1 D_i^a + \lambda_3 c_i c_p D_p^a + \lambda_4 A_i + \lambda_6 c_i c_p A_p + \tau_2 D_i^c \right. \\ & \left. + \tau_3 c_i a_p D_p^a + \tau_4 c_i c_p D_p^c + \tau_5 C_i \right), \end{aligned} \quad (175)$$

$$\tilde{g}_i^c = -2 \left(\lambda_2 D_i^c + \lambda_5 C_i + \tau_1 D_i^a + \tau_5 A_i \right), \quad (176)$$

while the viscous stress \tilde{t}_{ij} is

$$\tilde{t}_{ij} = \tilde{t}_{ij}^s + \tilde{t}_{ij}^{ss}, \quad (177)$$

where \tilde{t}_{ij}^s and \tilde{t}_{ij}^{ss} are the symmetric and skew-symmetric parts of the viscous stress given by

$$\begin{aligned} \tilde{t}_{ij}^s = & \mu_0 D_{ij} + \mu_1 a_p D_p^a a_i a_j + \mu_2 (D_i^a a_j + D_j^a a_i) + \mu_3 c_p D_p^c c_i c_j \\ & + \mu_4 (D_i^c c_j + D_j^c c_i) + \mu_5 c_p D_p^a (a_i c_j + a_j c_i) \\ & + \lambda_1 (A_i a_j + A_j a_i) + \lambda_2 (C_i c_j + C_j c_i) + \lambda_3 c_p A_p (a_i c_j + a_j c_i) \\ & + \kappa_1 (D_i^a c_j + D_j^a c_i + D_i^c a_j + D_j^c a_i) \\ & + \kappa_2 [a_p D_p^a (a_i c_j + a_j c_i) + 2a_p D_p^c a_i a_j] \\ & + \kappa_3 [c_p D_p^c (a_i c_j + a_j c_i) + 2a_p D_p^c c_i c_j] \\ & + \tau_1 (C_i a_j + C_j a_i) + \tau_2 (A_i c_j + A_j c_i) \\ & + 2\tau_3 c_p A_p a_i a_j + 2\tau_4 c_p A_p c_i c_j, \end{aligned} \quad (178)$$

$$\begin{aligned} \tilde{t}_{ij}^{ss} = & \lambda_1 (D_j^a a_i - D_i^a a_j) + \lambda_2 (D_j^c c_i - D_i^c c_j) + \lambda_3 c_p D_p^a (a_i c_j - a_j c_i) \\ & + \lambda_4 (A_j a_i - A_i a_j) + \lambda_5 (C_j c_i - C_i c_j) + \lambda_6 c_p A_p (a_i c_j - a_j c_i) \\ & + \tau_1 (D_j^a c_i - D_i^a c_j) + \tau_2 (D_j^c a_i - D_i^c a_j) + \tau_3 a_p D_p^a (a_i c_j - a_j c_i) \\ & + \tau_4 c_p D_p^c (a_i c_j - a_j c_i) + \tau_5 (A_j c_i - A_i c_j + C_j a_i - C_i a_j). \end{aligned} \quad (179)$$

In the above expressions

$$D_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i}), \quad W_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i}), \quad (180)$$

$$A_i = \dot{a}_i - W_{ik}a_k, \quad C_i = \dot{c}_i - W_{ik}c_k, \quad (181)$$

$$D_i^a = D_{ij}a_j, \quad D_i^c = D_{ij}c_j, \quad (182)$$

where \mathbf{A} and \mathbf{C} are the smectic analogues of the co-rotational time flux of the director in nematics (cf. equation (89)). There are twenty viscosity coefficients: the twelve viscosities μ_0 to μ_5 and λ_1 to λ_6 are associated with contributions to the dynamic stress which are even in the vector \mathbf{c} or do not contain \mathbf{c} , while the remaining eight viscosities κ_1 to κ_3 and τ_1 to τ_5 are linked to the terms which are odd in the vector \mathbf{c} . A detailed description of properties of these viscosities can be found in [19,104]. Equations (169), (170), (171), (173) and (174) provide sixteen equations in the sixteen unknowns a_i , c_i , v_i , p , β_i , γ , μ and τ .

A list of numerous restrictions to linear combinations of the viscosities, analogous to those for nematics in equations (100) to (104), can be found in [104]. The dependence of the SmC viscosities upon the smectic tilt angle θ has been considered by Carlsson *et al.* [19], based on the method used by Dahl and Lagerwall [28]. Details can be found in [19,104]. It should be remarked that Osipov, Sluckin and Terentjev [90] have given physical reasons for further observing that the viscosities λ_3 , λ_6 , τ_3 and τ_4 , although not identically zero, may be set to zero in very basic problems for the SmC phase because they expect these four viscosities to be much smaller than the remaining sixteen. Galerne, Martinand, Durand and Veyssie [45] have measured some of the smectic viscosities for the SmC liquid crystal DOBCP at 103°C. From these experimental data, Leslie and Gill [69] deduced values for λ_5 and various linear combinations of the viscosities in terms of the theoretical description given above (there are some minor miscalculations in [69] which were later corrected [104]).

1.4.4 Extension to other related smectic theories

A more extensive discussion on an extended energy density for SmC liquid crystals when dilation and variations in the smectic cone angle are allowed has been made by Blake and Virga [14], McKay and Leslie [80] and McKay [79]. Further developments in the continuum theory of the related phase of SmA liquid crystals have been made by Martin, Parodi and Pershan [78], de Gennes [46,47], Ahmadi [2], Capriz [17,18], E [32], Auernhammer *et al.* [7–9], Stewart [105] and De Vita and Stewart [29], with variable methods of approach but with many workers essentially following the principles employed in the classical work of Ericksen and Leslie outlined above for nematics and SmC. It should also be mentioned that Eringen [39] introduced a unified continuum theory for liquid crystal phases that considered nematic, cholesteric and smectic phases in the context of micropolar continua.

Chiral smectic C liquid crystals (SmC*) have a twist axis perpendicular to the usual smectic C layers and are known to be ferroelectric, as first demonstrated in the experiments carried out by Meyer, Liébert, Strzelecki and Keller [83] in 1975 after speculation on the possibility of such ferroelectric liquid crystals by McMillan [81] in 1973. These ferroelectric liquid crystals generally possess a spontaneous polarisation \mathbf{P} which, in terms of the model for SmC introduced above, can be written as a vector parallel to the

vector $\mathbf{b} = \mathbf{a} \times \mathbf{c}$. It turns out that $\mathbf{P} = P_0 \mathbf{b}$ or $\mathbf{P} = -P_0 \mathbf{b}$, where $P_0 = |\mathbf{P}|$, and that the sign of the spontaneous polarisation is material dependent and can be classed as positive or negative; one generally accepted sign convention [48, 58] defines \mathbf{P} as positive if it has the same direction as \mathbf{b} and negative if it has the opposite direction to \mathbf{b} . An energy density for such ferroelectric SmC* liquid crystals, can be constructed, as discussed by Carlsson, Stewart and Leslie [21]. The above expression w for the SmC elastic energy density in (132) or (134) can be extended to that required for the SmC* phase by the introduction of two additional terms. These extra chiral terms may be written as

$$w_1^* = A_{11} \delta (\mathbf{c} \cdot \nabla \times \mathbf{c} - \mathbf{b} \cdot \nabla \times \mathbf{b}) = 2A_{11} \delta \epsilon_{ipk} a_p c_k c_{j,i} a_j, \quad (183)$$

$$w_2^* = \frac{1}{2} B_3 q (\mathbf{c} \cdot \nabla \times \mathbf{c} + \mathbf{b} \cdot \nabla \times \mathbf{b}) = -B_3 q \epsilon_{ipk} a_p c_k c_{i,j} a_j, \quad (184)$$

where A_{11} and B_3 are the elastic constants introduced above and the second equalities in (183) and (184) are consequences of identities found in references [21, 71]. The wave vector q satisfies $q = 2\pi/p$ where p is the inherent helical pitch of the SmC* phase and δ is a constant. The two terms w_1^* and w_2^* also correspond to the terms D_2 and $-D_3$, respectively, discussed by de Gennes and Prost [48, p.378]. The full energy density is then simply $w + w_1^* + w_2^*$. In many instances, it would appear that δ can be set to zero in planar aligned samples of SmC* [21, 104] and it is worth remarking that Gill and Leslie [49] found the term w_1^* to be of no importance in the simple shear flow problems that they investigated. When an electric field is introduced then the electric energy must be supplemented by an additional important electric field contribution due to the spontaneous polarisation that is present in the SmC* phase. This additional energy term is given by

$$w_{pol} = -\mathbf{P} \cdot \mathbf{E}, \quad (185)$$

where, as before, \mathbf{E} is the electric field. Many of the details, such as sign conventions and the physical description and mathematical models of SmC* liquid crystals are beyond the scope of this brief review and can be found in the books by Lagerwall [58], de Gennes and Prost [48] and Stewart [104].

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