Sharp-interface nematic-isotropic phase transitions without flow

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Abstract

We derive a supplemental evolution equation for an interface between the nematic and isotropic phases of a liquid crystal when flow is neglected. Our approach is based on the notion of configurational force. As an application, we study the behavior a spherical isotropic drop surrounded by a radially-oriented nematic phase: our supplemental evolution equation then reduces to a simple ordinary differential equation admitting a closed form solution. In addition to describing many features of isotropic-to-nematic phase transitions, this simplified model yields insight concerning the occurrence and stability of isotropic cores for hedgehog defects in liquid crystals.

1 Introduction

When quenched from a high-temperature isotropic phase to a low-temperature nematic phase, a liquid crystal undergoes a first-order phase transition (de Gennes 1971). Such transitions proceed via the nucleation, growth, and coalescence of droplets (Ostner, Chan & Kahlweit 1973). Experiments involving free- and directional-growth show that nematic-isotropic phase interfaces exhibit a host of interesting morphological instabilities, instabilities that are manifested by the formation of dendrites (Armitage & Price 1978) and periodic cellular patterns (Oswald, Bechoeffer & Libchaber 1987) resembling those occuring in crystal growth (Langer 1980).

Here, we take a first step toward developing a sharp-interface theory for the description of such phenomena. Our goal is a generalization of the Ericksen–Leslie theory (Ericksen 1961; Leslie 1968) for uniaxial nematics which

- allows for phase transitions,
- models an nematic-isotropic interfaces as a sharp surface across which bulk fields may suffer discontinuities,
- accounts for localized interactions between phases by endowing the interface with excess properties.

Our work is a first step because, for clarity, we neglect effects associated with flow and with heat and mass transport. Hence, what we present is in essence a generalization of the classical curvature elasticity theory (Oseen 1933; Zöcher 1933; Frank 1958).

As we neglect flow and both thermal and compositional influences, the free-energy (density) of the isotropic phase is a constant that, without loss in generality, we set equal to zero. This allows us to restrict attention to the nematic phase and the nematic-isotropic interface.

Our discussion begins with a concise overview of the theory for the nematic phase. In addition to a director momentum balance, that theory is based an isothermal statement of the second law that is used to restrict constitutive equations.

To deal with the nematic-isotropic interface, we rely on recent developments in the theory of configurational forces (Gurtin 1995, 2000; Gurtin & Struthers 1990). Although configurational forces are superfluous away from the interface, the interfacial limits of the bulk configurational stress and configurational momentum are of essential importance.

Prior to considering the interface, we therefore reformulate the theory for the nematic phase in a manner that accounts for the role of configurational forces. Using control volumes that migrate within the nematic phase this yields representations for the configurational stress and momentum in bulk, representations obtained without recourse to constitutive assumptions and, hence, more broadly valid than would be counterparts derived on the basis of variational arguments (Maugin & Trimarco 1995).

Our treatment of the interface is analogous to that taken in our reformulation of the bulk theory. Aside from the director momentum balance, we impose a configurational momentum balance and an isothermal version of the second law that accounts for power expended by both the director and configurational forces. As in the theory for the nematic phase, the interfacial dissipation inequality is used to obtain restrictions on constitutive equations. With those restrictions, we arrive at the general system of evolution equations for the interface. Those equations, which enforce the director momentum balance and the normal component of the configurational momentum balance, supplement the bulk director momentum balance arising from the standard theory.

Precisely, denote by $\mathbf{n}$ the director, let $\mathbf{G} = \mathsf{grad}\,\mathbf{n}$, and let $\hat{\Psi}(\mathbf{n}, \mathbf{G})$ denote the bulk free energy. The evolution equation in the nematic phase in the absence of flow is classical:

$$\sigma(\ddot{\mathbf{n}} + |\dot{\mathbf{n}}|^2\mathbf{n}) + \gamma\dot{\mathbf{n}} = \mathsf{div}\left(\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\right) + \left(\mathbf{G}\colon\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\right)\mathbf{n} - \frac{\partial\hat{\Psi}}{\partial\mathbf{n}}, \tag{1.1}$$

with $\sigma > 0$ the director mass density and $\gamma \geq 0$ a viscosity associated with changes in director-orientation. The conditions at a *stationary* nematic-isotropic interface are also classical, and involve an interfacial free energy (density) ψ to describe weak anchoring (Rapini & Papoular 1969) and a dissipative contribution (Derzhanski & Petrov 1979): denoting by $\mathbf{m}$ the unit interfacial normal directed away from the nematic phase and by $\mathring{\mathbf{n}}$ the normal-time derivative of $\mathbf{n}$, our generalization of the Derzhanski–Petrov condition to an evolving interface has $\psi = \hat{\psi}(\mathbf{n}, \mathbf{m})$ and takes the form

$$\beta_1\mathring{\mathbf{n}} + \sigma V\dot{\mathbf{n}} = -\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\mathbf{m} - \frac{\partial\hat{\psi}}{\partial\mathbf{n}}, \tag{1.2}$$

with $\beta_1 \geq 0$ a dissipative coefficient.

The configurational balance provides the evolution equation for the phase interface. Denoting by V the normal velocity of the interface, by K its total curvature (twice the mean curvature) and by div_s the surface divergence, we obtain the evolution equation

$$\beta_1\mathbf{G}\mathbf{m}\cdot\mathring{\mathbf{n}} + \mathsf{div}_s(\beta_2\mathring{\mathbf{m}}) + \beta_3 V = \psi K - \mathsf{div}_s\left(\frac{\partial\hat{\psi}}{\partial\mathbf{m}}\right) - \mathbf{G}\mathbf{m}\cdot\frac{\partial\hat{\psi}}{\partial\mathbf{n}} - (\Psi - \tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2). \tag{1.3}$$

with $\beta_2 \geq 0$ and $\beta_3 \geq 0$ additional dissipative coefficients. To our knowledge this equation has never been proposed in the literature. However, our developments complement recent work (Poniewierski 2000; Rey 2000*a*, *b*, *c*, 2001; Cheong & Rey 2002) concerning the rheology of a *material* interface between a nematic liquid crystal and an isotropic fluid.

We specialize (1.3) to two simple applications. In the first we develop approximate equations for a perturbed planar interface $\mathcal{S}_0$ such that

$$\mathbf{m} = \mathbf{e} + \epsilon \mathbf{m}_1 + o(\epsilon), \qquad V = V_0 + \epsilon V_1 + o(\epsilon), \qquad \mathbf{n} = \mathbf{e} + \epsilon \mathbf{n}_1 + o(\epsilon), \tag{1.4}$$

with $\mathbf{e}$ a fixed unit vector and ϵ a small parameter. The simplest such equations arise for $\hat{\psi}(\mathbf{n}, \mathbf{m}) = \psi_0$ and $\Psi = \Psi_0 + \epsilon \Psi_1 + o(\epsilon)$, with ψ_0, Ψ_0 and Ψ_1 given constants. Then, with β_2 constant and inertia neglected, (1.3) is approximated, at the zeroth and first order in ϵ, by

$$\beta_3 V_0 = -\Psi_0, \qquad -\beta_2 \mathring{K}_1 + \beta_3 V_1 = \psi_0 K_1 - \Psi_1, \tag{1.5}$$

the second of which, for $\beta_2 = 0$, is the classical *curvature-flow equation* (cf., e.g., Gurtin 2000).

As a second application, we discuss the growth and equilibrium of a spherical isotropic drop in a nematic ocean in which the director is radially oriented. The evolution equation (1.3) then reduces to the ordinary differential equation

$$\beta \dot{R} = \Psi_0 - \frac{2\sigma}{R} + \frac{\kappa}{R^2} \tag{1.6}$$

for the radius R of the isotropic drop. The moduli $\sigma > 0$ and $\kappa > 0$ are related to surface energy and bulk elasticity, while Ψ_0 is a measure of the bulk energy difference between the phases, and possibly depends on temperature. The solutions of (1.6) have different behavior according to the size and sign of the nematic-isotropic energy difference Ψ_0. When $\Psi_0 \leq 0$, so that the energy of the nematic phase is lower than that of the isotropic phase, (1.6) has a stable equilibrium R_*. Hence, an isotropic drop in a nematic ocean is stable at the characteristic radius R_*, a fact that might explain the presence of an isotropic core for hedgehog defects: our theory indeed allows for an estimate of the core radius. When $0 < \Psi_0 < \sigma^2/\kappa$, so that the nematic phase has the higher energy, (1.6) still has a stable equilibrium R_*^-, but also has an unstable equilibrium $R_*^+ > R_*^-$: in this regime the surface tension σ is sufficiently large compared to Ψ_0, so that small isotropic droplets persist in the nematic phase. However, if the radius of the drop is large enough, the drop grows and the nematic phase eventually becomes isotropic. This result is consistent with observations showing that, for the phase transformation proceed beyond a certain stage, isotropic nuclei must coalesce. Finally, when $\Psi_0 \geq \sigma^2/\kappa$, so that the energy difference between the nematic and isotropic phase is sufficiently large, (1.6) has no equilibrium points and the isotropic phase grows at the expense of the nematic phase.

2 Theory for the nematic phase

Throughout this section $\mathcal{P}$ denotes an arbitrary (fixed) region lying within the nematic phase.

Our developments can be viewed as a specialization of the Ericksen–Leslie theory (Ericksen 1961; Leslie 1968) that neglects flow and thermal transport.

2.1 Kinematics

We write $\mathbf{n}(\mathbf{x},t)$ for the director field, assumed consistent with the constraint

$$|\mathbf{n}| = 1. \tag{2.1}$$

Using grad to denote the gradient operator, we write

$$\mathbf{G} = \mathsf{grad}\,\mathbf{n} \tag{2.2}$$

for the *director gradient*; then, by (2.1),

$$\mathbf{G}^\top\mathbf{n} = \mathbf{0}. \tag{2.3}$$

We use a superposed dot to denote time-differentiation, so that,

$$\dot{\mathbf{n}}\cdot\mathbf{n} = 0. \tag{2.4}$$

2.2 Balance of director momentum

We write σ for the (constant) *director mass density* (i.e., the peculiar mass density of the mesogens),

$$\mathbf{r} = \sigma\dot{\mathbf{n}} \tag{2.5}$$

for the *director momentum* (*density*), $\mathbf{S}$ for the *director stress*, and $\mathbf{g}$ for the *director body force* (*density*). Balance of director momentum requires that, for any $\mathcal{P}$,

$$\dot{\int_{\mathcal{P}}} \mathbf{r}\,\mathrm{d}v = \int_{\partial\mathcal{P}} \mathbf{S}\mathbf{m}_{\partial\mathcal{P}}\,\mathrm{d}a + \int_{\mathcal{P}} \mathbf{g}\,\mathrm{d}v, \tag{2.6}$$

or, equivalently, that the field equation

$$\dot{\mathbf{r}} = \mathsf{div}\,\mathbf{S} + \mathbf{g} \tag{2.7}$$

hold throughout the nematic phase.

A direct calculation allows us to decompose (2.7) into components,

$$\left.\begin{aligned} \dot{\mathbf{r}} - (\mathbf{r}\cdot\dot{\mathbf{n}})\mathbf{n} &= \mathsf{div}\,(\mathbf{S} - \mathbf{n}\otimes\mathbf{S}^\top\mathbf{n}) + \mathbf{G}\mathbf{S}^\top\mathbf{n} + (\mathbf{G}\,\vdots\,\mathbf{S})\mathbf{n} + \mathbf{g} - (\mathbf{g}\cdot\mathbf{n})\mathbf{n},\\ \dot{\mathbf{r}}\cdot\mathbf{n} &= \mathsf{div}\,(\mathbf{S}^\top\mathbf{n}) - \mathbf{G}\,\vdots\,\mathbf{S} + \mathbf{g}\cdot\mathbf{n}, \end{aligned}\right\} \tag{2.8}$$

perpendicular and parallel to the director.

2.3 Energy imbalance

We restrict attention to isothermal processes, in which case the first and second laws of thermodynamics reduce to an imbalance of energy asserting that, for any $\mathcal{P}$, the net (free plus kinetic) energy of $\mathcal{P}$ change at a rate that is not greater than the power expended on $\mathcal{P}$. Writing Ψ for the *free-energy* (*density*), so that $\Psi + \frac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}$ represents the net energy per unit volume, and noting that $\int_{\partial\mathcal{P}} \mathbf{S}\mathbf{m}_{\partial\mathcal{P}}\cdot\dot{\mathbf{n}}\,\mathrm{d}a$ represents the power expended on $\mathcal{P}$ by material exterior to $\mathcal{P}$, the energy imbalance requires that

$$\dot{\int_{\mathcal{P}}} (\Psi + \tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}})\,\mathrm{d}v \le \int_{\partial\mathcal{P}} \mathbf{S}\mathbf{m}_{\partial\mathcal{P}}\cdot\dot{\mathbf{n}}\,\mathrm{d}a. \tag{2.9}$$

Using the balance of director momentum, (2.7), we may write (2.9) equivalently as

$$\int_{\mathcal{P}} (\dot{\Psi} - \mathbf{S}\colon\dot{\mathbf{G}} + \mathbf{g}\cdot\dot{\mathbf{n}})\,\mathrm{d}v \leq 0. \tag{2.10}$$

The requirement that (2.10) hold for all $\mathcal{P}$ is therefore equivalent to the requirement that the dissipation inequality

$$\dot{\Psi} - \mathbf{S}\colon\dot{\mathbf{G}} + \mathbf{g}\cdot\dot{\mathbf{n}} \leq 0 \tag{2.11}$$

hold throughout the nematic phase.

2.4 Constitutive equations

We take Ψ to be given constitutively as a function

$$\Psi = \hat{\Psi}(\mathbf{n}, \mathbf{G}). \tag{2.12}$$

Then (2.11) takes the form

$$\left\{\frac{\partial\hat{\Psi}(\mathbf{n},\mathbf{G})}{\partial\mathbf{G}} - \mathbf{S}\right\}\colon\dot{\mathbf{G}} + \left\{\frac{\partial\hat{\Psi}(\mathbf{n},\mathbf{G})}{\partial\mathbf{n}} + \mathbf{g}\right\}\cdot\dot{\mathbf{n}} \leq 0. \tag{2.13}$$

Constitutive equations for $\mathbf{S}$ and $\mathbf{g}$ that ensure satisfaction of the dissipation inequality (2.11) are given by

$$\left.\begin{aligned} \mathbf{S} &= \mathbf{n}\otimes\boldsymbol{\alpha} + \frac{\partial\hat{\Psi}(\mathbf{n},\mathbf{G})}{\partial\mathbf{G}}, \\ \mathbf{g} &= \lambda\mathbf{n} - \mathbf{G}\boldsymbol{\alpha} - \frac{\partial\hat{\Psi}(\mathbf{n},\mathbf{G})}{\partial\mathbf{n}} - \gamma(\mathbf{n},\mathbf{G})\dot{\mathbf{n}}, \end{aligned}\right\} \tag{2.14}$$

with $\gamma \geq 0$ and with $\boldsymbol{\alpha}$ and λ constitutively indeterminate fields that arise in response to the constraint (2.1),[1] where differentiation is performed on the manifold defined by (2.1), so that $(\partial\hat{\Psi}/\partial\mathbf{G})^{\top}\mathbf{n} = \mathbf{0}$ and $(\partial\hat{\Psi}/\partial\mathbf{n})\cdot\mathbf{n} = 0$.

2.5 Basic partial differential equation in the nematic phase

If we combine the balance $(2.8)_1$ and the constitutive equations (2.14), we arrive at the partial differential equation that governs the evolution of the director in the nematic phase:

$$\sigma\big(\ddot{\mathbf{n}} - |\dot{\mathbf{n}}|^2\mathbf{n}\big) + \gamma\dot{\mathbf{n}} = \mathsf{div}\left(\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\right) + \left(\mathbf{G}\colon\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\right)\mathbf{n} - \frac{\partial\hat{\Psi}}{\partial\mathbf{n}}. \tag{2.15}$$

We refer to (2.15) as the (constitutively augemented) director momentum balance in bulk.

[1] We avoid a detailed discussion of constraints and associated multiplier fields. A modern geometrical treatment of constraints in a material with nematic microstructure is given by Anderson, Carlson & Fried (1999).

3 Configurational forces and configurational momentum in the nematic phase

The goal of this study is a complete theory of nematic-isotropic transitions in which the interface is allowed to move relative to the material. In variational treatments of related *equilibrium* problems, independent kinematical quantities may be independently varied, and each such variation yields a corresponding Euler–Lagrange balance. In dynamics with general forms of dissipation there is no encompassing variational principle, but experience has demonstrated the need for an additional balance associated with the kinematics of the interface. Here, guided by variational treatments in which such a balance is a consequence of the assumption of equilibrium, we follow Gurtin & Struthers (1990) and Gurtin (1995, 2000) and introduce, as primitive objects, configurational forces and momentum together with an independent *balance of configurational momentum*. Roughly speaking, configurational forces are related to the integrity of the material structure and expend power in the transfer of material and in the evolution of the interface.

In this part we discuss configurational forces in bulk. Within that context such forces are extraneous to the solution of actual boundary-value problems. But in general situations knowledge of the structure of configurational forces in bulk away from the interface is central to the understanding of their localized behavior at the interface.

3.1 Balance of configurational momentum

We consider a configurational momentum balance involving three fields: a *configurational momentum* (*density*) $\mathbf{q}$, a *configurational stress* $\mathbf{C}$, and a *configurational body force* (*density*) $\mathbf{f}$. Balance of configurational momentum then requires that, for any $\mathcal{P}$,

$$\overset{\cdot}{\int_{\mathcal{P}} \mathbf{q}\,\mathrm{d}v} = \int_{\partial\mathcal{P}} \mathbf{C}\mathbf{m}_{\partial\mathcal{P}}\,\mathrm{d}a + \int_{\mathcal{P}} \mathbf{f}\,\mathrm{d}v, \tag{3.1}$$

or, equivalently, that the field equation

$$\dot{\mathbf{q}} = \mathsf{div}\,\mathbf{C} + \mathbf{f} \tag{3.2}$$

hold throughout the liquid.

3.2 Migrating control volumes. Observed and relative velocities

To characterize the manner in which configurational forces perform work, a means of capturing the kinematics associated with the transfer of material is needed. Following Gurtin (1995, 2000), we accomplish this with the aid of *control volumes* $\mathcal{R}(t)$ that *migrate relative to the liquid* and thereby result in the transfer of material to — and the removal of material from — $\mathcal{R}(t)$ at $\partial\mathcal{R}(t)$. Here *it is essential that fixed regions $\mathcal{P}$ not be confused with control volumes $\mathcal{R}(t)$ that migrate relative to the material*. The use of migrating control volumes allows us to determine representations for the configurational stresses and momenta in bulk.

Let $\mathcal{R} = \mathcal{R}(t)$ be a *migrating control volume* with $V_{\partial\mathcal{R}}(\mathbf{x},t)$ the (scalar) *normal velocity* of $\partial\mathcal{R}(t)$ in the direction of the outward unit normal $\mathbf{m}_{\partial\mathcal{R}}(\mathbf{x},t)$. To describe power expenditures associated with the migration of $\mathcal{R}(t)$, we introduce a field $\mathbf{v}_{\partial\mathcal{R}}(\mathbf{x},t)$ defined over $\partial\mathcal{R}(t)$ for all t. Compatibility then requires that $\mathbf{v}_{\partial\mathcal{R}}$ have $V_{\partial\mathcal{R}}$ as its normal component,

$$\mathbf{v}_{\partial\mathcal{R}}\cdot\mathbf{m}_{\partial\mathcal{R}} = V_{\partial\mathcal{R}}, \tag{3.3}$$

but $\mathbf{v}_{\partial\mathcal{R}}$ *is otherwise arbitrary.* We refer to any such field $\mathbf{v}_{\partial\mathcal{R}}$ as a *velocity field for* $\partial\mathcal{R}$.

Nonnormal velocity fields, while not intrinsic, are important. For example, given an arbitrary time-dependent parametrization $\mathbf{x} = \hat{\mathbf{x}}(\xi_1, \xi_2, t)$ of $\partial\mathcal{R}$, the field defined by $\mathbf{v}_{\partial\mathcal{R}} = \partial\hat{\mathbf{x}}/\partial t$ (holding (ξ_1, ξ_2) fixed) generally represents a nonnormal velocity field for $\partial\mathcal{R}$. But while it is important that we allow for the use of non-normal velocity fields, *it is essential that the theory itself not depend on the particular velocity field used to describe a given migrating control volume.* As we shall see, this observation has important consequences.

We refer to the normal velocity $V_{\partial\mathcal{R}}$ and any choice of the velocity field $\mathbf{v}_{\partial\mathcal{R}}$ for $\partial\mathcal{R}$ as *migrational velocities* for $\partial\mathcal{R}$.

Given a migrating control volume $\mathcal{R}$, the field

$$\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}} \tag{3.4}$$

represents the *rate of change of the director following the migration of* $\partial\mathcal{R}$.

Useful in what follows is the following transport identity: given a smooth field $\Phi(\mathbf{x}, t)$ and a migrating control volume $\mathcal{R} = \mathcal{R}(t)$,

$$\overset{\cdot}{\int_{\mathcal{R}} \Phi \, \mathrm{d}v} = \int_{\mathcal{R}} \dot{\Phi} \, \mathrm{d}v + \int_{\partial\mathcal{R}} \Phi V_{\partial\mathcal{R}} \, \mathrm{d}a. \tag{3.5}$$

3.3 Expended power

3.3.1 Power expended by tractions

The conventional form for the power expended by material exterior to a fixed region $\mathcal{P}$ is $\int_{\partial\mathcal{P}} \mathbf{S}\mathbf{m}_{\partial\mathcal{P}} \cdot \dot{\mathbf{n}} \, \mathrm{d}a$. Consider, instead, a migrating control volume $\mathcal{R} = \mathcal{R}(t)$. The migration of $\mathcal{R}$ involves a transfer of material across $\partial\mathcal{R}$ and we expect that this transfer should be accompanied by a power expenditure over and above the conventional expenditure. Configurational forces are introduced to account for power expenditures associated with material transfer. Specifically, we view the configurational traction $\mathbf{C}\mathbf{m}_{\partial\mathcal{R}}$ distributed over $\partial\mathcal{R}$ as a force, per unit area, associated with the transfer of material across $\partial\mathcal{R}$. Since any velocity field $\mathbf{v}_{\partial\mathcal{R}}$ for $\partial\mathcal{R}$ represents the velocity with which material is transferred across $\partial\mathcal{R}$, we take $\mathbf{v}_{\partial\mathcal{R}}$ to be an appropriate power-conjugate velocity for $\mathbf{C}\mathbf{m}_{\partial\mathcal{R}}$, and hence assume that the migration of $\mathcal{R}$ is accompanied by the power expenditure $\int_{\partial\mathcal{R}} \mathbf{C}\mathbf{m}_{\partial\mathcal{R}} \cdot \mathbf{v}_{\partial\mathcal{R}} \, \mathrm{d}a$.

We assume that the velocity power-conjugate to the director traction $\mathbf{S}\mathbf{m}_{\partial\mathcal{R}}$ is not given by $\dot{\mathbf{n}}$, but rather by $\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}$, the rate of change of the director following the migration of $\partial\mathcal{R}$ (cf. (3.4)); granted this, $\int_{\partial\mathcal{R}} \mathbf{S}\mathbf{m}_{\partial\mathcal{R}} \cdot (\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}) \, \mathrm{d}a$ represents the power expended on $\partial\mathcal{R}$ by the director traction.

Material is added to $\mathcal{R}$ only along its boundary $\partial\mathcal{R}$; there is no transfer of material to the interior of $\mathcal{R}$. For that reason, the configurational body force $\mathbf{f}$ expends no power. The total power expended on $\mathcal{R}$ by tractions over $\partial\mathcal{R}$ is therefore given by

$$W(\mathcal{R}) = \int_{\partial\mathcal{R}} \left(\mathbf{S}\mathbf{m}_{\partial\mathcal{R}} \cdot (\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}) + \mathbf{C}\mathbf{m}_{\partial\mathcal{R}} \cdot \mathbf{v}_{\partial\mathcal{R}} \right) \mathrm{d}a. \tag{3.6}$$

3.3.2 Momentum forces and their associated power expenditures

The momentum balance (3.1), written for a migrating control volume $\mathcal{R}$, takes the form

$$\left.\begin{aligned}\overset{\cdot}{\overline{\int_{\mathcal{R}} \mathbf{r}\,\mathrm{d}v}} &= \int_{\partial\mathcal{R}} \mathbf{Sm}_{\partial\mathcal{R}}\,\mathrm{d}a + \int_{\mathcal{R}} \mathbf{g}\,\mathrm{d}v + \int_{\partial\mathcal{R}} \mathbf{r}V_{\partial\mathcal{R}}\,\mathrm{d}a,\\ \overset{\cdot}{\overline{\int_{\mathcal{R}} \mathbf{q}\,\mathrm{d}v}} &= \int_{\partial\mathcal{R}} \mathbf{Cm}_{\partial\mathcal{R}}\,\mathrm{d}a + \int_{\mathcal{R}} \mathbf{f}\,\mathrm{d}v + \int_{\partial\mathcal{R}} \mathbf{q}V_{\partial\mathcal{R}}\,\mathrm{d}a.\end{aligned}\right\} \tag{3.7}$$

To verify, say, the first of these expressions, we simply integrate (2.7) over $\mathcal{R}$ and use the transport identity (3.5).

In the balances (3.7), the vector fields

$$\mathbf{k} = V_{\partial\mathcal{R}}\mathbf{r} \qquad \text{and} \qquad \mathbf{j} = V_{\partial\mathcal{R}}\mathbf{q} \tag{3.8}$$

represent flows of director and configurational momentum, respectively, across $\partial\mathcal{R}$ induced by its migration. When there is no migration, so that $V_{\partial\mathcal{R}} = 0$, these momentum flows vanish.

We may view $\mathbf{k}$ *and* $\mathbf{j}$ *as tractions*, for then each of the momentum balances in (3.7) asserts that

$$\frac{\mathrm{d}}{\mathrm{d}t}\big\{\text{momentum of } \mathcal{R}(t)\big\} = \big\{\text{net force on } \mathcal{R}(t)\big\}. \tag{3.9}$$

This view is essential to a discussion of configurational forces, as $\mathbf{k}$ and $\mathbf{j}$ represent *tractions associated with the transfer of material across* $\partial\mathcal{R}$.[2]

Considering the momentum flows as tractions allows us to associate with each such flow a power expenditure. Let $\mathcal{R}$ be a migrating control volume. The traction $\mathbf{j}$ is configurational, as it corresponds to the configurational momentum $\mathbf{q}$, and, as with the traction $\mathbf{Cm}_{\partial\mathcal{R}}$, we take $\mathbf{v}_{\partial\mathcal{R}}$ as the velocity power-conjugate to $\mathbf{j}$. On the other hand, $\mathbf{k}$ is a traction associated with director momentum and, as with $\mathbf{Sm}_{\partial\mathcal{R}}$, we take $\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}$ as the respective power-conjugates of $\mathbf{j}$ and $\mathbf{k}$. The power expended by the momentum flows therefore has the form

$$M(\mathcal{R}) = \int_{\partial\mathcal{R}} \big(\mathbf{k}\cdot(\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}) + \mathbf{j}\cdot\mathbf{v}_{\partial\mathcal{R}}\big)\,\mathrm{d}a. \tag{3.10}$$

3.3.3 Invariance of the total power under changes in velocity field

Given a migrating control volume $\mathcal{R}$,

$$\overbrace{\int_{\partial\mathcal{R}} \big\{\mathbf{Sm}_{\partial\mathcal{R}}\cdot(\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}) + \mathbf{Cm}_{\partial\mathcal{R}}\cdot\mathbf{v}_{\partial\mathcal{R}}\big\}\,\mathrm{d}a}^{W(\mathcal{R})} + \overbrace{\int_{\partial\mathcal{R}} \big\{\mathbf{k}\cdot(\dot{\mathbf{n}} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}) + \mathbf{j}\cdot\mathbf{v}_{\partial\mathcal{R}}\big\}\,\mathrm{d}a}^{M(\mathcal{R})} \tag{3.11}$$

represents the *total power expended on* $\mathcal{R}$. We require that, given any migrating control volume $\mathcal{R}$, (3.11) be independent of the observed velocity field $\mathbf{v}_{\partial\mathcal{R}}$ chosen to characterize the migration of $\mathcal{R}$. More precisely, we require that (3.11) be invariant under all transformations of the form

$$\mathbf{v}_{\partial\mathcal{R}} \mapsto \mathbf{v}_{\partial\mathcal{R}} + \mathbf{t}, \tag{3.12}$$

[2] This treatment of momentum within the context of configurational forces is based on but differs conceptually from the treatment of Cermelli & Fried (2002).

with $\mathbf{t}\cdot\mathbf{m}=0$. A necessary and sufficient condition that (3.11) be invariant under all transformations (3.12) is then that $\int_{\partial\mathcal{R}}\big\{(\mathbf{G}^\top\mathbf{S}+\mathbf{C})\mathbf{m}_{\partial\mathcal{R}}+V_{\partial\mathcal{R}}(\mathbf{G}^\top\mathbf{r}+\mathbf{q})\big\}\cdot\mathbf{t}\,\mathrm{d}a=0$, where we have used (3.8). Thus, since $\mathcal{R}$ and $\mathbf{t}$ (tangential to $\partial\mathcal{R}$) may be arbitrarily chosen, it follows that

$$\big\{(\mathbf{G}^\top\mathbf{S}+\mathbf{C})\mathbf{m}+V(\mathbf{G}^\top\mathbf{r}+\mathbf{q})\big\}\cdot\mathbf{t}=0 \tag{3.13}$$

for any scalar V, any unit vector $\mathbf{m}$, and any vector $\mathbf{t}$ orthogonal to $\mathbf{m}$. Since V is arbitrary, we may use (2.5) to obtain the relation,

$$\mathbf{q}=-\mathbf{G}^\top\mathbf{r}=-\sigma\mathbf{G}^\top\dot{\mathbf{n}}. \tag{3.14}$$

Hence, the configurational momentum is completely determined by the director momentum.

Next, by (3.13),

$$\mathbf{t}\cdot\underbrace{\big(\mathbf{G}^\top\mathbf{S}+\mathbf{C}\big)}_{\mathbf{A}}\mathbf{m}=0$$

for all $\mathbf{t}$ and $\mathbf{m}$ with $\mathbf{t}$ orthogonal to $\mathbf{m}$. Hence, for each $\mathbf{m}$, $\mathbf{A}\mathbf{m}$ must lie in the direction of $\mathbf{m}$, which is possible if and only if $\mathbf{A}$ has the form $\mathbf{A}=\Phi\mathbf{1}$, with Φ a scalar field. Invariance therefore yields the *pre-Eshelby* relation

$$\mathbf{C}=\Phi\mathbf{1}-\mathbf{G}^\top\mathbf{S} \tag{3.15}$$

for the configurational stress.

Next, in view of (3.8), (3.14), and (3.15), if we take the velocity $\mathbf{v}_{\partial\mathcal{R}}$ in its intrinsic form $V_{\partial\mathcal{R}}\mathbf{m}_{\partial\mathcal{R}}$, then the total power expended on $\mathcal{R}$ becomes

$$W(\mathcal{R})+M(\mathcal{R})=\int_{\partial\mathcal{R}}\big(\mathbf{S}\mathbf{m}_{\partial\mathcal{R}}\cdot\dot{\mathbf{n}}+(\Phi+\mathbf{r}\cdot\dot{\mathbf{n}})V_{\partial\mathcal{R}}\big)\,\mathrm{d}a. \tag{3.16}$$

3.4 Energy imbalance

We now generalize the energy imbalance (2.9) to account for power expenditures associated with the addition of material. Specifically, we consider an imbalance that, for migrating control volumes $\mathcal{R}$, has the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\big\{\text{total energy of }\mathcal{R}(t)\big\}\le\big\{\text{total power expended on }\mathcal{R}(t)\big\} \tag{3.17}$$

and, thus, accounts for power expended by configurational and momentum forces, but not explicitly for flows (relative to the material) of free and kinetic energy into $\mathcal{R}$ across $\partial\mathcal{R}$. Precisely, this imbalance takes the form

$$\overset{\cdot}{\int_{\mathcal{R}}\big(\Psi+\tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}\big)\,\mathrm{d}v}\le W(\mathcal{R})+M(\mathcal{R}). \tag{3.18}$$

By (3.5),

$$\overset{\cdot}{\int_{\mathcal{R}}\big(\Psi+\tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}\big)\,\mathrm{d}v}=\int_{\mathcal{R}}\overset{\cdot}{\big(\Psi+\tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}\big)}\,\mathrm{d}v+\int_{\partial\mathcal{R}}\big(\Psi+\tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}\big)V_{\partial\mathcal{R}}\,\mathrm{d}a$$

and therefore, by (3.16), the energy imbalance (3.17) for $\mathcal{R}$ becomes

$$\int_{\mathcal{R}} \dot{\overline{\big(\Psi + \tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}\big)}}\, \mathrm{d}v \leq \int_{\partial\mathcal{R}} \mathbf{S}\mathbf{m}_{\partial\mathcal{R}}\cdot\dot{\mathbf{n}}\, \mathrm{d}a + \int_{\partial\mathcal{R}} \big(\Phi - \Psi + \tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}\big) V_{\partial\mathcal{R}}\, \mathrm{d}a. \tag{3.19}$$

In view of (a) of the Variation Lemma given in the Appendix, this inequality can hold for all migrating control volumes $\mathcal{R}$ only if the coefficient of $V_{\partial\mathcal{R}}$ vanishes: $\Phi = \Psi - \frac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}}$. Thus, by (3.15), we have the *Eshelby relation*

$$\mathbf{C} = (\Psi - \tfrac{1}{2}\mathbf{r}\cdot\dot{\mathbf{n}})\mathbf{1} - \mathbf{G}^{\top}\mathbf{S}. \tag{3.20}$$

We emphasize that our derivation of (3.20) is independent of constitutive assumptions. Hence, the validity of that representation goes beyond that of comparable expressions derived on the basis of particular constitutive theories. Finally, by (2.3), (2.5), and (2.14), (3.20) becomes (Eshelby 1980; Maugin & Trimarco 1995)

$$\mathbf{C} = \big(\Psi - \tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2\big)\mathbf{1} - \mathbf{G}^{\top}\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}. \tag{3.21}$$

In view of (3.20), the ultimate term in (3.19) vanishes. In addition, if $\mathcal{R} = \mathcal{P}$ is fixed then (3.19) reduces to the more conventional imbalance (2.9).

4 Theory for the interface

4.1 Kinematics

We suppose that the isotropic and nematic phases are separated by a surface $\mathcal{S} = \mathcal{S}(t)$ oriented by a *unit normal field* $\mathbf{m}(\mathbf{x}, t)$ directed from the region occupied by the nematic phase into the region occupied by the isotropic phase.

We write $V(\mathbf{x}, t)$ for the (scalar) *normal velocity* of $\mathcal{S}$. To describe power expenditures associated with the motion of $\mathcal{S}$, we introduce a field $\mathbf{v}(\mathbf{x}, t)$ defined over $\mathcal{S}(t)$ for all t. Compatibility then requires that $\mathbf{v}$ have V as its normal component,

$$\mathbf{v}\cdot\mathbf{m} = V, \tag{4.1}$$

but $\mathbf{v}$ *is otherwise arbitrary*. We refer to any such field $\mathbf{v}$ as a *velocity field for* $\mathcal{S}$.

We require that the theory be independent of the choice of velocity field $\mathbf{v}$ for $\mathcal{S}$. At some point we shall specialize our results to a velocity field $\mathbf{v}$ that is normal,

$$\mathbf{v} = V\mathbf{m}, \tag{4.2}$$

but for now $\mathbf{v}$ need only satisfy (4.1).

4.1.1 Superficial fields

We refer to scalar and vector fields defined on $\mathcal{S}$ for all time as *superficial* fields. A superficial vector field $\mathbf{f}(\mathbf{x}, t)$ is *tangential* if $\mathbf{f}\cdot\mathbf{m} = 0$. We refer to a tensor field $\mathbf{F}(\mathbf{x}, t)$ defined on $\mathcal{S}$ for all time as *superficial* if $\mathbf{F}\mathbf{m} = \mathbf{0}$; such a field $\mathbf{F}$ is *fully tangential* if $\mathbf{F}^{\top}\mathbf{m} = \mathbf{0}$. An example of a fully tangential tensor field is the *projection*

$$\mathbf{P} = \mathbf{1} - \mathbf{m}\otimes\mathbf{m}. \tag{4.3}$$

Each superficial tensor field $\mathbf{F}$ admits a decomposition of the form

$$\mathbf{F} = \mathbf{F}_{\tan} + \mathbf{m}\otimes\mathbf{f}, \qquad \begin{cases} \mathbf{F}_{\tan} = \mathbf{P}\mathbf{F}\mathbf{P}, \\ \mathbf{f} = \mathbf{F}^{\top}\mathbf{m}, \end{cases} \tag{4.4}$$

with $\mathbf{F}_{\tan}$ fully tangential and $\mathbf{f}$ tangential. Thus, for $\mathbf{F}$ fully tangential, $\mathbf{F} = \mathbf{F}_{\tan}$.

The *superfical gradient* $\mathsf{grad}_{\mathcal{S}}$ is defined by the chain rule; that is, for $\varphi(\mathbf{x},t)$ a superficial scalar field, $\mathbf{f}(\mathbf{x},t)$ a superficial vector field, and $\mathbf{z}(\lambda)$ an *arbitrary* curve on $\mathcal{S}$,

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\varphi(\mathbf{z}(\lambda),t) = \big[\mathsf{grad}_{\mathcal{S}}\varphi(\mathbf{z}(\lambda),t)\big]\cdot\mathbf{z}'(\lambda),$$

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathbf{f}(\mathbf{z}(\lambda),t) = \big[\mathsf{grad}_{\mathcal{S}}\mathbf{f}(\mathbf{z}(\lambda),t)\big]\mathbf{z}'(\lambda).$$

Since $d\mathbf{z}/d\lambda$ is tangent to $\mathcal{S}$, this defines $\mathsf{grad}_{\mathcal{S}}\varphi$ and $\mathsf{grad}_{\mathcal{S}}\mathbf{f}$ only on vectors tangent to $\mathcal{S}$, but in accord with the requirement that $\mathbf{F}\mathbf{m} = \mathbf{0}$ for any superficial tensor field $\mathbf{F}$, we extend $\mathsf{grad}_{\mathcal{S}}\varphi$ and $\mathsf{grad}_{\mathcal{S}}\mathbf{f}$ by requiring that $(\mathsf{grad}_{\mathcal{S}}\varphi)\cdot\mathbf{m} = 0$ and $(\mathsf{grad}_{\mathcal{S}}\mathbf{f})\mathbf{m} = \mathbf{0}$. Thus $\mathsf{grad}_{\mathcal{S}}\varphi$ is a tangential vector field, while $\mathsf{grad}_{\mathcal{S}}\mathbf{f}$ is a superficial tensor field. The *superficial divergence* of $\mathbf{f}$ is then defined by

$$\mathsf{div}_{\mathcal{S}}\mathbf{f} = \mathsf{tr}\,(\mathsf{grad}_{\mathcal{S}}\mathbf{f}), \tag{4.5}$$

while the surface divergence $\mathsf{div}_{\mathcal{S}}\mathbf{F}$ of a superficial tensor field $\mathbf{F}$ is the superficial vector field defined through the identity

$$\mathbf{c}\cdot\mathsf{div}_{\mathcal{S}}\mathbf{F} = \mathsf{div}_{\mathcal{S}}(\mathbf{F}^{\top}\mathbf{c}) \tag{4.6}$$

for all *constant* vectors $\mathbf{c}$.

We write

$$\mathbf{K} = -\mathsf{grad}_{\mathcal{S}}\mathbf{m} \tag{4.7}$$

for the *curvature tensor* and

$$K = \mathsf{tr}\,\mathbf{K} = -\mathsf{div}_{\mathcal{S}}\mathbf{m} \tag{4.8}$$

for the *total curvature* (i.e., twice the mean curvature). As is well known, $\mathbf{K}$ is *fully tangential* and *symmetric*. An important identity based on (4.3) and these definitions is

$$\mathsf{div}_{\mathcal{S}}\mathbf{P} = K\mathbf{m}. \tag{4.9}$$

Let $\mathcal{A}$ denote an arbitrary subsurface of $\mathcal{S}$, and let $\mathbf{m}_{\partial\mathcal{A}}$ denote the *outward unit normal* to the boundary curve $\partial\mathcal{A}$ of $\mathcal{A}$, so that $\mathbf{m}_{\partial\mathcal{A}}$ is *tangent* to the surface $\mathcal{S}$ and *normal* to the curve $\partial\mathcal{A}$. The superficial divergence theorem, for $\mathbf{f}$ a tangential vector field and $\mathbf{F}$ a superficial tensor field, can then be stated as follows:

$$\int_{\partial\mathcal{A}} \mathbf{f}\cdot\mathbf{m}_{\partial\mathcal{A}}\,\mathrm{d}s = \int_{\mathcal{A}} \mathsf{div}_{\mathcal{S}}\mathbf{f}\,\mathrm{d}a, \qquad \int_{\partial\mathcal{A}} \mathbf{F}\mathbf{m}_{\partial\mathcal{A}}\,\mathrm{d}s = \int_{\mathcal{A}} \mathsf{div}_{\mathcal{S}}\mathbf{F}\,\mathrm{d}a. \tag{4.10}$$

4.1.2 Migrating pillboxes. Superficial time differentiation

We assume throughout that all fields defined in the nematic phase are *smooth up to the interface*.

Consider an arbitrary migrating subsurface $\mathcal{A} = \mathcal{A}(t)$ of $\mathcal{S} = \mathcal{S}(t)$. The *superficial pillbox* determined by $\mathcal{A}$ is a control volume of infinitesimal thickness consisting of (Fig. 1):

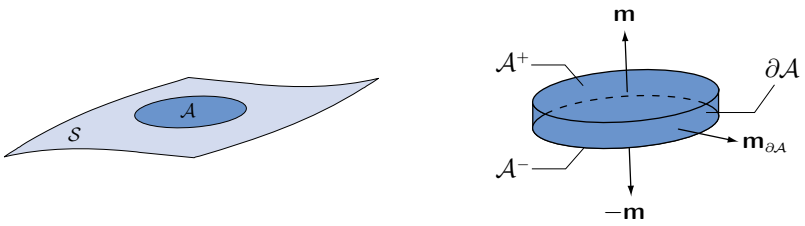

Figure 1: Schematic of a migrating subsurface $\mathcal{A}$ of the interface $\mathcal{S}$ showing an enlarged view of the associated superficial pillbox.

- a surface $\mathcal{A}^+$, with unit normal $\mathbf{m}$, that lies in the isotropic phase;
- a surface $\mathcal{A}^-$, with unit normal $-\mathbf{m}$, that lies in the nematic phase;
- a lateral bounding surface $\partial\mathcal{A}$ with outward unit normal $\mathbf{m}_{\partial\mathcal{A}}$.

Intrinsic velocities for the evolution of $\partial\mathcal{A}(t)$ are its scalar velocity $V_{\partial\mathcal{A}}(\mathbf{x},t)$ in the direction of $\mathbf{m}_{\partial\mathcal{A}}(\mathbf{x},t)$ and the normal migration velocity $V(\mathbf{x},t)$. To describe power expenditures associated with the migration of $\mathcal{A}(\mathbf{x},t)$, we introduce a field $\mathbf{v}_{\partial\mathcal{A}}(\mathbf{x},t)$ defined over $\partial\mathcal{A}(t)$ for all t. Compatibility then requires that

$$\mathbf{v}_{\partial\mathcal{A}}\cdot\mathbf{m}=V \qquad \text{and} \qquad \mathbf{v}_{\partial\mathcal{A}}\cdot\mathbf{m}_{\partial\mathcal{A}}=V_{\partial\mathcal{A}}. \tag{4.11}$$

Otherwise, however, $\mathbf{v}_{\partial\mathcal{A}}$ is arbitrary. We refer to any such field $\mathbf{v}_{\partial\mathcal{A}}$ and to $V_{\partial\mathcal{A}}$ as *migrational velocities* for $\partial\mathcal{A}$.

Let $\mathbf{v}$ be a velocity field for $\mathcal{S}$. For φ a superficial field, the *time-derivative* $\mathring{\varphi}$ *of* φ *following the motion of* $\mathcal{S}$ *as described by* $\mathbf{v}$ is defined as follows: given any time t_0 and any point $\mathbf{x}_0$ on $\mathcal{S}(t_0)$, let $\mathbf{z}(t)$ denote the unique solution of

$$\frac{\mathrm{d}\mathbf{z}(t)}{\mathrm{d}t}=\mathbf{v}(\mathbf{z}(t),t), \qquad \mathbf{z}(t_0)=\mathbf{x}_0; \tag{4.12}$$

then

$$\mathring{\varphi}(\mathbf{x}_0,t_0)=\left.\frac{\mathrm{d}\varphi(\mathbf{z}(t),t)}{\mathrm{d}t}\right|_{t=t_0}. \tag{4.13}$$

For a parametrization of $\mathcal{S}$ with $\mathbf{v}$ normal, so that

$$\mathbf{v}=V\mathbf{m}, \tag{4.14}$$

$\mathring{\varphi}$ is the time derivative of φ following the normal trajectories of $\mathcal{S}$. With a slight abuse of notation, we shall use the same notation for the normal time derivative and the time derivative involving an arbitrary velocity field $\mathbf{v}$, the meaning being clear from the context.

The normal time-rate $\mathring{\mathbf{m}}$ of the interfacial orientation $\mathbf{m}$ and the surface-gradient of the normal migrational velocity V are related by the classical identity

$$\mathsf{grad}_{\mathcal{S}}V=-\mathring{\mathbf{m}}. \tag{4.15}$$

Important to what follows is the *superficial transport theorem* (cf. Gurtin, Struthers & Williams 1989): for $\varphi(\mathbf{x},t)$ a smooth superficial scalar field and $\mathring{\varphi}$ its normal time-derivative,

$$\overset{\cdot}{\int_{\mathcal{A}}}\varphi\,\mathrm{d}a=\int_{\mathcal{A}}\left(\mathring{\varphi}-\varphi KV\right)\mathrm{d}a+\int_{\partial\mathcal{A}}\varphi V_{\partial\mathcal{A}}\,\mathrm{d}s. \tag{4.16}$$

4.2 Balance of director momentum

In addition to the stress $\mathbf{S}$ and the body force $\mathbf{g}$ associated with the director in bulk, we account for a *superficial body force* associated with the *director* through a field $\mathbf{g}$. The director forces on a migrating superficial pillbox $\mathcal{A}$ then consist of the internal force $\int_{\mathcal{A}} \mathbf{g}\,\mathrm{d}a$ and the force $-\int_{\mathcal{A}} \mathbf{S}\mathbf{m}\,\mathrm{d}a$ exerted on $\mathcal{A}$ by the bulk material in the nematic phase. Also acting on $\mathcal{A}$ from the nematic phase is the director momentum flow $-\int_{\mathcal{A}} \mathbf{r}V\,\mathrm{d}a$.

We neglect superficial distributions of director momentum. The balance of director momentum then requires that, for any migrating superficial pillbox $\mathcal{A}$,

$$\int_{\mathcal{A}} (\mathbf{g} - \mathbf{S}\mathbf{m} - \mathbf{r}V)\,\mathrm{d}a = \mathbf{0} \tag{4.17}$$

or, equivalently, that the field equation

$$\mathbf{g} = \mathbf{S}\mathbf{m} + V\mathbf{r} \tag{4.18}$$

hold on the interface $\mathcal{S}$.

In view of (2.5), the interfacial director momentum balance decomposes into components

$$(\mathbf{1} - \mathbf{n}\otimes\mathbf{n})(\mathbf{g} - \mathbf{S}\mathbf{m}) = V\mathbf{r} \qquad \text{and} \qquad \mathbf{g}\cdot\mathbf{n} = (\mathbf{S}^{\top}\mathbf{n})\cdot\mathbf{m} \tag{4.19}$$

perpendicular and parallel to the director.

By $(2.14)_2$ and the requirement that $(\partial\hat{\Psi}/\partial\mathbf{G})^{\top}\mathbf{n} = \mathbf{0}$, $(4.19)_2$ yields

$$\mathbf{g}\cdot\mathbf{n} = \boldsymbol{\alpha}\cdot\mathbf{m}, \tag{4.20}$$

so that the component of $\mathbf{g}$ parallel to $\mathbf{n}$ is determined by the multiplier field $\boldsymbol{\alpha}$ and the orientation $\mathbf{m}$ of $\mathcal{S}$. Further, by (2.5) and $(2.14)_1$, $(4.19)_1$ can be written as

$$(\mathbf{1} - \mathbf{n}\otimes\mathbf{n})\mathbf{g} = \frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\mathbf{m} + \sigma V\dot{\mathbf{n}}. \tag{4.21}$$

The result (4.21) makes it clear that only the component of $\mathbf{g}$ perpendicular to $\mathbf{n}$ can be given constitutively, while (4.20) shows that the component of $\mathbf{g}$ parallel to $\mathbf{n}$ is determined in terms of $\boldsymbol{\alpha}$.

4.3 Balance of configurational momentum

In addition to the stress tensor $\mathbf{C}$ and the internal body force $\mathbf{f}$ that characterize the configurational forces in bulk, we account for configurational forces on the interface through a superficial tensor field $\mathbf{C}$, the stress, and a superficial vector field $\mathbf{f}$, the internal force. The configurational forces on a migrating superficial pillbox $\mathcal{A}$ then consist of the traction $\int_{\partial\mathcal{A}} \mathbf{C}\boldsymbol{\nu}_{\partial\mathcal{A}}\,\mathrm{d}s$ exerted by the portion of $\mathcal{S}$ exterior to $\mathcal{A}$, the internal force $\int_{\mathcal{A}} \mathbf{f}\,\mathrm{d}a$, and the force $-\int_{\mathcal{A}} \mathbf{C}\mathbf{m}\,\mathrm{d}a$ exerted on $\mathcal{A}$ by the bulk material in the nematic phase. Also acting on $\mathcal{A}$ are the configurational momentum flow from the nematic phase, as given by $-\int_{\mathcal{A}} \mathbf{q}V\,\mathrm{d}a$.

We neglect superficial distributions of configurational momentum. Thus the balance of configurational momentum requires that, for any migrating superficial pillbox $\mathcal{A}$,

$$\int_{\partial\mathcal{A}} \mathbf{C}\boldsymbol{\nu}_{\partial\mathcal{A}}\,\mathrm{d}s + \int_{\mathcal{A}} \big(\mathbf{f} - \mathbf{C}\mathbf{m} - V\mathbf{q}\big)\,\mathrm{d}a = \mathbf{0} \tag{4.22}$$

or, equivalently, that the *configurational momentum balance*

$$\mathsf{div}_{\mathcal{S}}\mathbf{C} + \mathbf{f} = \mathbf{C}\mathbf{m} + V\mathbf{q} \tag{4.23}$$

hold on the interface $\mathcal{S}$.

4.4 Power

4.4.1 Power expended by tractions

To express the power expended by the tractions, we proceed as in §3.3.1 and mimick the reasoning leading to the expression (3.6) for the power expenditure on a control volume migrating through the nematic phase. The configurational traction $\mathbf{C}\mathbf{m}_{\partial\mathcal{A}}$ is distributed over the "lateral" boundary $\partial\mathcal{A}$ of the pillbox. As in our discussion of the bulk phases, we take the migrational velocity $\mathbf{v}_{\partial\mathcal{A}}$ of $\partial\mathcal{A}$ to be the appropriate power-conjugate velocity for $\mathbf{C}\mathbf{m}_{\partial\mathcal{A}}$. In addition, we view the configurational traction $-\mathbf{C}\mathbf{m}$ exerted on $\mathcal{A}$ by the nematic phase as forces, per unit area, associated with the transfer of material across $\mathcal{S}$ that occurs as one phase grows with respect to the other. We therefore take the velocity $\mathbf{v}$ of $\mathcal{S}$ to be an appropriate power-conjugate velocity for $\mathbf{C}\mathbf{m}$. Similarly, consistent with our treatment of the power expendend by the director traction on a migrating control volume, we use as a power-conjugate velocity for $-\mathbf{S}\mathbf{m}$ the velocity $\mathring{\mathbf{n}}$ following the motion of $\mathcal{S}$ as described by $\mathbf{v}$. The (net) external power expended on $\mathcal{A}$ therefore has the form

$$w(\mathcal{A}) = \int_{\partial\mathcal{A}} \mathbf{C}\mathbf{m}_{\partial\mathcal{A}}\cdot\mathbf{v}_{\partial\mathcal{A}}\,\mathrm{d}s - \int_{\mathcal{A}} \big(\mathbf{S}\mathbf{m}\cdot\mathring{\mathbf{n}} + \mathbf{C}\mathbf{m}\cdot\mathbf{v}\big)\,\mathrm{d}a. \tag{4.24}$$

4.4.2 Momentum forces and their associated power expenditure

Proceeding as in §3, we view the flows $\mathbf{k} = \mathbf{r}V$ and $\mathbf{j} = \mathbf{q}V$ of director and configurational momentum as tractions and associate with each of these a power expenditure. As appropriate power-conjugates for $\mathbf{k}$ and $\mathbf{j}$, we choose $\mathring{\mathbf{n}}$, and $\mathbf{v}$, respectively. Thus the net power expended on $\mathcal{A}$ by the momentum flows is

$$m(\mathcal{A}) = -\int_{\mathcal{A}} \big(\mathbf{k}\cdot\mathring{\mathbf{n}} + \mathbf{j}\cdot\mathbf{v}\big)\,\mathrm{d}a. \tag{4.25}$$

4.4.3 Invariance of the total power under changes in velocity field

Given a migrating pillbox $\mathcal{A}$, the sum

$$w(\mathcal{A}) + m(\mathcal{A}) = \int_{\partial\mathcal{A}} \mathbf{C}\mathbf{m}_{\partial\mathcal{A}}\cdot\mathbf{v}_{\partial\mathcal{A}}\,\mathrm{d}s - \int_{\mathcal{A}} \big((\mathbf{S}\mathbf{m}+\mathbf{k})\cdot\mathring{\mathbf{n}} + (\mathbf{C}\mathbf{m}+\mathbf{j})\cdot\mathbf{v}\big)\,\mathrm{d}a \tag{4.26}$$

represents the total power expended on $\mathcal{A}$. As in our treatment of the power acting on a migrating control volume (cf. §3), we require that (4.26) be invariant under all transformations of the form

$$\mathbf{v}_{\partial\mathcal{A}} \mapsto \mathbf{v}_{\partial\mathcal{A}} + \mathbf{t}, \qquad \mathbf{t}\cdot\mathbf{m} = \mathbf{t}\cdot\mathbf{m}_{\partial\mathcal{A}} = 0. \tag{4.27}$$

Thus a necessary and sufficient condition that (4.26) be invariant under all transformations of the form (4.27) is that $\int_{\mathcal{A}} \mathbf{C}\mathbf{m}_{\partial\mathcal{A}}\cdot\mathbf{t}\,\mathrm{d}s = 0$. Since $\mathcal{A}$ and $\mathbf{t}$ (tangential to $\partial\mathcal{A}$) may be arbitrarily chosen, it follows that $\mathbf{t}_2\cdot\mathbf{C}\mathbf{t}_1 = 0$ for all $\mathbf{t}_1$ and $\mathbf{t}_2$ orthogonal to $\mathbf{m}$, with $\mathbf{t}_2$ orthogonal to $\mathbf{t}_1$. Thus $\mathbf{C}\mathbf{t}_1$ must lie in the direction of $\mathbf{t}_1$ for each $\mathbf{t}_1$ orthogonal to $\mathbf{m}$, which is possible if and only if the tangential component $\mathbf{C}_{\tan}$ of $\mathbf{C}$ has the form $\mathbf{C}_{\tan} = \varphi\mathbf{P}$, with φ a superficial scalar field. Invariance therefore implies that the fully tangential component $\mathbf{C}_{\tan}$ of interfacial configurational stress $\mathbf{C}$ must be of the form

$$\mathbf{C}_{\tan} = \varphi\mathbf{P}. \tag{4.28}$$

Equivalently, bearing in mind (4.4),

$$\mathbf{C} = \varphi\mathbf{P} + \mathbf{m}\otimes\mathbf{c}, \qquad \mathbf{c} = \mathbf{C}^{\top}\mathbf{m}, \tag{4.29}$$

with $\mathbf{c}$ the *configurational shear* a tangential vector field.

In view of the configurational momentum-balance (4.23) and the expression (4.29) — which we view as a *superficial pre-Eshelby relation* — it follows, using (4.9), that

$$\big\{\varphi K + \mathsf{div}_{\mathcal{S}}\mathbf{c} + f - \mathbf{m}\cdot(\mathbf{C}\mathbf{m}+\mathbf{q}V)\big\}\mathbf{m} + \mathsf{grad}_{\mathcal{S}}\varphi - \mathbf{K}\mathbf{c} + \mathbf{P}(\mathbf{f}-\mathbf{C}\mathbf{m}-\mathbf{q}V) = \mathbf{0}, \tag{4.30}$$

where we have introduced the *normal configurational force*

$$f = \mathbf{f}\cdot\mathbf{m}. \tag{4.31}$$

Since $\mathsf{grad}_{\mathcal{S}}\varphi$, $\mathbf{K}\mathbf{c}$, and $\mathbf{P}(\mathbf{f}-\mathbf{C}\mathbf{m}-\mathbf{q}V)$ are tangential vector fields on $\mathcal{S}$, it follows that the configurational balance (4.23) decomposes into a normal component

$$\varphi K + \mathsf{div}_{\mathcal{S}}\mathbf{c} + f = \mathbf{m}\cdot(\mathbf{C}\mathbf{m}+\mathbf{q}V) \tag{4.32}$$

and a tangential component $\mathsf{grad}_{\mathcal{S}}\varphi - \mathbf{K}\mathbf{c} + \mathbf{P}\mathbf{f} = \mathbf{P}(\mathbf{C}\mathbf{m}+\mathbf{q}V)$. We restrict attention from now on to velocity fields $\mathbf{v}$ and $\mathbf{v}_{\partial\mathcal{A}}$ in intrinsic form

$$\mathbf{v} = V\mathbf{m}, \qquad \mathbf{v}_{\partial\mathcal{A}} = V\mathbf{m} + V_{\partial\mathcal{A}}\mathbf{m}_{\partial\mathcal{A}}, \tag{4.33}$$

so that a superposed circle denotes the normal time derivative. This restriction, together with (4.29), allows to write the total power (4.26) expended on $\mathcal{A}$ as

$$w(\mathcal{A}) + m(\mathcal{A}) = \int_{\partial\mathcal{A}} \varphi V_{\partial\mathcal{A}}\,\mathrm{d}s + \int_{\partial\mathcal{A}} V\mathbf{c}\cdot\mathbf{m}_{\partial\mathcal{A}}\,\mathrm{d}s - \int_{\mathcal{A}} \big\{(\mathbf{S}\mathbf{m}+\mathbf{k})\cdot\mathring{\mathbf{n}} + (\mathbf{C}\mathbf{m}+\mathbf{j})\cdot\mathbf{v}\big\}\,\mathrm{d}a. \tag{4.34}$$

Using the superficial balances (4.18) and (4.32) of director and configurational momentum, the surface divergence theorem and relations (4.29) and (4.15), (4.34) becomes

$$w(\mathcal{A}) + m(\mathcal{A}) = \int_{\partial\mathcal{A}} \varphi V_{\partial\mathcal{A}}\,\mathrm{d}s - \int_{\mathcal{A}} \big(\varphi K V + \mathbf{c}\cdot\mathring{\mathbf{m}} + fV + \mathbf{g}\cdot\mathring{\mathbf{n}}\big)\,\mathrm{d}a. \tag{4.35}$$

4.5 Imbalance of free energy

Since we neglect superficial distributions of momentum, the first and second laws for the interface reduce to an imbalance of free energy. Writing ψ for the *superficial free energy* (*density*), measured per unit area, so that $\int_{\mathcal{A}}\psi\,\mathrm{d}a$ represents the net free energy of $\mathcal{A}$, the imbalance of free energy requires that, for any migrating interfacial pillbox $\mathcal{A}$,

$$\overset{\cdot}{\int_{\mathcal{A}}} \psi\,\mathrm{d}a \le w(\mathcal{A}) + m(\mathcal{A}), \tag{4.36}$$

with the power $w(\mathcal{A})$ and $m(\mathcal{A})$ as given by (4.24) and (4.25). Thus, by the superficial transport theorem (4.16) and the intrinsic expression (4.35) for $w(\mathcal{A}) + m(\mathcal{A})$,

$$\int_{\mathcal{A}} \big(\mathring{\psi} - (\psi-\varphi)KV\big)\,\mathrm{d}a + \int_{\partial\mathcal{A}} (\psi-\varphi)V_{\partial\mathcal{A}}\,\mathrm{d}s \le -\int_{\mathcal{A}} \big(\mathbf{c}\cdot\mathring{\mathbf{m}} + fV + \mathbf{g}\cdot\mathring{\mathbf{n}}\big)\,\mathrm{d}a. \tag{4.37}$$

This inequality can hold for all migrating pillboxes $\mathcal{A}$ only if the coefficient of $V_{\partial\mathcal{A}}$ in the integral over $\partial\mathcal{A}$ vanishes (cf. (b) of the Variation Lemma given in the Appendix). Thus, by (4.29), we have the *superficial Eshelby relation*

$$\mathbf{C} = \psi\mathbf{P} + \mathbf{m}\otimes\mathbf{c}. \tag{4.38}$$

Consider now the configurational momentum balance (4.23). By (4.32) and (4.38), (4.23) has normal component

$$\psi K + \mathsf{div}_s\mathbf{c} + f = \mathbf{m}\cdot(\mathbf{C}\mathbf{m} + \mathbf{q}V). \tag{4.39}$$

We refer to (4.39) as the *normal configurational force balance*. As opposed to (4.39), the (nonintrinsic) tangential component, $\mathsf{grad}_s\psi - \mathbf{K}\mathbf{c} + \mathbf{P}\mathbf{f} = \mathbf{P}(\mathbf{C}\mathbf{m} + \mathbf{q}V)$, of (4.23) is inconsequential to the theory.

Note, for future use, that, by (3.14) and (3.21), we may write the normal configurational force balance in the form

$$\psi K + \mathsf{div}_s\mathbf{c} + f = \Psi - \tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2 - \mathbf{G}\mathbf{m}\cdot\left(\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\mathbf{m} + \sigma\dot{\mathbf{n}}V\right). \tag{4.40}$$

As another consequence of (4.38) the free-energy imbalance (4.37) reduces to

$$\int_{\mathcal{A}} (\mathring{\psi} + \mathbf{g}\cdot\mathring{\mathbf{n}} + \mathbf{c}\cdot\mathring{\mathbf{m}} + fV)\,\mathrm{d}a \le 0, \tag{4.41}$$

or, equivalently, to the dissipation inequality

$$\mathring{\psi} + \mathbf{g}\cdot\mathring{\mathbf{n}} + \mathbf{c}\cdot\mathring{\mathbf{m}} + fV \le 0. \tag{4.42}$$

4.6 Constitutive equations

We take ψ to be given constitutively as a function

$$\psi = \hat{\psi}(\mathbf{n}, \mathbf{m}). \tag{4.43}$$

Then $\mathring{\psi} = \{\hat{\psi}(\mathbf{n},\mathbf{m})/\partial\mathbf{n}\}\cdot\mathring{\mathbf{n}} + \{\hat{\psi}(\mathbf{n},\mathbf{m})/\mathbf{m}\}\cdot\mathring{\mathbf{m}}$ and the dissipation inequality (4.42) takes the form

$$\left(\frac{\partial\hat{\psi}(\mathbf{n},\mathbf{m})}{\partial\mathbf{n}} + \mathbf{g}\right)\cdot\mathring{\mathbf{n}} + \left(\frac{\partial\hat{\psi}(\mathbf{n},\mathbf{m})}{\partial\mathbf{m}} + \mathbf{c}\right)\cdot\mathring{\mathbf{m}} + fV \le 0. \tag{4.44}$$

Bear in mind that $\mathbf{c}$ is orthogonal to $\mathbf{m}$, and that $\mathbf{n}$ and $\mathbf{m}$ are unit vectors, so that $\partial\hat{\psi}/\partial\mathbf{n}$ and $\partial\hat{\psi}/\partial\mathbf{m}$ are orthogonal to $\mathbf{n}$ and $\mathbf{m}$, respectively. Then a sufficient condition that (4.44) hold identically is that $\mathbf{g}$, $\mathbf{c}$, and f have the forms

$$\left.\begin{aligned} \mathbf{g} &= \alpha\mathbf{n} - \frac{\partial\hat{\psi}(\mathbf{n},\mathbf{m})}{\partial\mathbf{n}} - \beta_1(\mathbf{n},\mathbf{m})\,\mathring{\mathbf{n}},\\ \mathbf{c} &= -\frac{\partial\hat{\psi}(\mathbf{n},\mathbf{m})}{\partial\mathbf{m}} - \beta_2(\mathbf{n},\mathbf{m})\,\mathring{\mathbf{m}},\\ f &= -\beta_3(\mathbf{n},\mathbf{m})\,V, \end{aligned}\right\} \tag{4.45}$$

where α is a constitutively indeterminate interfacial field that arises because $\mathbf{g}$ need not be orthogonal to $\mathbf{n}$ and β_1, β_2, and β_3 are generalized viscosities consistent with

$\beta_i(\mathbf{n},\mathbf{m}) \geq 0$, $i = 1,2,3$. The field α is not independent of the bulk response. Indeed, by (4.20), $\alpha = \mathbf{g}\cdot\mathbf{n} = \boldsymbol{\alpha}\cdot\mathbf{m}$; α is thus determined by the interfacial normal component of the interfacial limit of the bulk multiplier $\boldsymbol{\alpha}$. Further, by (2.14) and $(4.19)_2$, $\alpha = \{(\partial\hat{\Psi}/\partial\mathbf{G})\mathbf{m}\}\cdot\mathbf{n}$.

Finally, we assume that the function $\hat{\psi}$ is isotropic and hence consistent with

$$\hat{\psi}(\mathbf{n},\mathbf{m}) = \hat{\psi}(\mathbf{Q}\mathbf{n},\mathbf{Q}\mathbf{m}) \tag{4.46}$$

for every rotation $\mathbf{Q}$; hence there is a function $\bar{\psi}$ such that

$$\psi = \hat{\psi}(\mathbf{n},\mathbf{m}) = \bar{\psi}(\xi), \qquad \xi = \mathbf{n}\cdot\mathbf{m}. \tag{4.47}$$

Furthermore, the viscosities β_1, β_2, and β_3 may depend on $(\mathbf{n},\mathbf{m})$ at most via ξ:

$$\beta_i(\mathbf{n},\mathbf{m}) = \beta_i(\xi), \qquad i = 1,2,3. \tag{4.48}$$

4.7 Basic partial differential equations for the interface

The final governing equations for the interface are

$$\beta_1\mathring{\mathbf{n}} + \sigma V\dot{\mathbf{n}} = -\frac{\partial\hat{\Psi}}{\partial\mathbf{G}}\mathbf{m}, -\frac{\mathrm{d}\bar{\psi}}{\mathrm{d}\xi}(\mathbf{m}-\xi\mathbf{n}) \tag{4.49}$$

which expresses director momentum balance, and

$$\beta_1\mathbf{G}\mathbf{m}\cdot\mathring{\mathbf{n}} + \mathsf{div}_s(\beta_2\mathring{\mathbf{m}}) + \beta_3 V = \psi K - \mathsf{div}_s\left(\frac{\partial\hat{\psi}}{\partial\mathbf{m}}\right) - \mathbf{G}\mathbf{m}\cdot\frac{\partial\hat{\psi}}{\partial\mathbf{n}} - (\Psi - \tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2), \tag{4.50}$$

which expresses normal configurational momentum balance (simplified by taking into account the director momentum balance (4.49)).

Of these, (4.49) follows immediately on using $(4.45)_1$ and the identity

$$\frac{\partial\hat{\psi}}{\partial\mathbf{n}} = \frac{\mathrm{d}\bar{\psi}}{\mathrm{d}\xi}(\mathbf{m}-\xi\mathbf{n}), \tag{4.51}$$

which is a consequence of (4.47), in (4.21). Each term of (4.49) is orthogonal to $\mathbf{n}$.

Next, the normal configurational momentum balance (4.40) and the constitutive equations (4.45) yield

$$\mathsf{div}_s(\beta_2\mathring{\mathbf{m}}) + (\beta_3 - \sigma\mathbf{G}\mathbf{m}\cdot\dot{\mathbf{n}})V = \psi K - \mathsf{div}_s\left(\frac{\partial\hat{\psi}}{\partial\mathbf{m}}\right) - \left(\Psi - \tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2 - \mathbf{G}\mathbf{m}\cdot\frac{\partial\hat{\psi}}{\partial\mathbf{G}}\mathbf{m}\right), \tag{4.52}$$

which, when combined with the director momentum balance (4.49), yields (4.50).

A potentially useful alternative to (4.50) is

$$\begin{aligned}\beta_1\mathbf{G}\mathbf{m}\cdot\mathring{\mathbf{n}} + (\beta_2|\mathbf{K}|^2 + \beta_3)V - \beta_2\mathring{K} + \frac{\mathrm{d}\beta_2}{\mathrm{d}\xi}(\mathbf{G}^\top\mathbf{m} - \mathbf{K}\mathbf{n})\cdot\mathring{\mathbf{m}} \\ = \left(\psi - \xi\frac{\mathrm{d}\bar{\psi}}{\mathrm{d}\xi}\right)K + \frac{\mathrm{d}^2\bar{\psi}}{\mathrm{d}\xi^2}\mathbf{n}\cdot\mathbf{K}\mathbf{n} + \xi\frac{\mathrm{d}^2\bar{\psi}}{\mathrm{d}\xi^2}\mathbf{m}\cdot\mathbf{G}\mathbf{m} - \frac{\mathrm{d}\bar{\psi}}{\mathrm{d}\xi}\mathsf{tr}\,\mathbf{G} - \Psi + \tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2.\end{aligned} \tag{4.53}$$

To obtain this, we first note that, by

$$\mathsf{grad}_s\xi = (\mathsf{grad}_s\mathbf{m})^\top\mathbf{n} + (\mathsf{grad}_s\mathbf{n})^\top\mathbf{m} = -\mathbf{K}\mathbf{n} + \mathbf{P}\mathbf{G}^\top\mathbf{m} \tag{4.54}$$

and (Gurtin and Jabbour 2002, eqt. $(2.19)_2$)

$$\mathsf{div}_{\mathcal{S}}\big(\mathring{\mathbf{m}}\big) = -\mathring{K} + |\mathbf{K}|^2 V, \tag{4.55}$$

it follows that

$$\mathsf{div}_{\mathcal{S}}(\beta_2\mathring{\mathbf{m}}) = -\beta_2\mathring{K} + \beta_2|\mathbf{K}|^2 V + \frac{\mathrm{d}\beta_2}{\mathrm{d}\xi}(\mathbf{G}^\top\mathbf{m} - \mathbf{K}\mathbf{n})\cdot\mathring{\mathbf{m}}. \tag{4.56}$$

Further, by $(4.51)_2$ and (4.54)

$$\mathsf{div}_{\mathcal{S}}\left(\frac{\partial\hat{\psi}}{\partial\mathbf{m}}\right) = -\frac{\mathrm{d}^2\bar{\psi}}{\mathrm{d}\xi^2}\,(\mathbf{n}\cdot\mathbf{K}\mathbf{n} + \xi\mathbf{m}\cdot\mathbf{G}\mathbf{m}) + \frac{\mathrm{d}\bar{\psi}}{\mathrm{d}\xi}(\mathsf{tr}\,\mathbf{G} - \mathbf{m}\cdot\mathbf{G}\mathbf{m} + \xi K). \tag{4.57}$$

Thus, using (4.56) and (4.57) in (4.50), we obtain (4.50). A similar alternative exists for (4.52).

5 Approximate equations for a perturbed planar interface

The balances (4.49) and, especially, (4.53) are complicated. A somewhat simpler system ensues when the interface is nearly planar and the interfacial energy is of the form (Rapini & Papoular 1969)

$$\hat{\psi}(\mathbf{n},\mathbf{m}) = \psi_0 - c(\mathbf{n}\cdot\mathbf{m})^2, \tag{5.1}$$

with $c > 0$ and ψ_0 a given constant, so that $\bar{\psi}(\xi) = \psi_0 - c\xi^2$. Precisely, given an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}\}$, let $\mathcal{S}_0$ denote the family of moving planes with parametric representation $\mathbf{r} = \mathbf{r}(x,y,t) = x\mathbf{e}_1 + y\mathbf{e}_2 + F_0(t)\mathbf{e}$, and let $\mathcal{S}$ be a perturbation of $\mathcal{S}_0$ given parametrically by

$$\mathbf{r} = \mathbf{r}(x,y,t) = x\mathbf{e}_1 + y\mathbf{e}_2 + (F_0(t) + \epsilon F_1(x,y,t))\mathbf{e}. \tag{5.2}$$

On denoting by $\mathsf{grad}_{\mathcal{S}_0}$ the gradient in the plane perpendicular to $\mathbf{e}$, it follows that

$$\left.\begin{aligned}
&\mathbf{m} = \mathbf{m}_0 + \epsilon\mathbf{m}_1 + o(\epsilon) = \mathbf{e} - \epsilon\mathsf{grad}_{\mathcal{S}_0}F_1 + o(\epsilon),\\
&V = V_0 + \epsilon V_1 + o(\epsilon) = \dot{F}_0 + \epsilon\dot{F}_1 + o(\epsilon),\\
&\mathbf{K} = \epsilon\mathbf{K}_1 + o(\epsilon) = -\epsilon\mathsf{grad}_{\mathcal{S}_0}\mathbf{m}_1 + o(\epsilon) = \epsilon\mathsf{grad}_{\mathcal{S}_0}\mathsf{grad}_{\mathcal{S}_0}F_1 + o(\epsilon),\\
&K = \epsilon K_1 + o(\epsilon) = \epsilon\Delta_{\mathcal{S}_0}F_1 + o(\epsilon),\\
&\mathring{K} = \epsilon\dot{K}_1 + o(\epsilon) = \epsilon\Delta_{\mathcal{S}_0}\dot{F}_1 + o(\epsilon),
\end{aligned}\right\} \tag{5.3}$$

with $\Delta_{\mathcal{S}_0}$ the Laplacian in the plane perpendicular to $\mathbf{e}$. Also, for $z \geq F_0(t) + \epsilon F_1(t)$, we assume that

$$\mathbf{n} = \mathbf{e} + \epsilon\mathbf{n}_1(x,y,z,t), \tag{5.4}$$

so that

$$\left.\begin{aligned}
&\mathbf{n}|_{\mathcal{S}} = \mathbf{e} + \epsilon\mathbf{n}_1(x,y,F_0(t)) + o(\epsilon),\\
&\mathbf{G} = \epsilon\mathbf{G}_1 + o(\epsilon) = \epsilon\mathsf{grad}\,\mathbf{n}_1 + o(\epsilon),\\
&\mathring{\mathbf{n}} = \epsilon(\dot{\mathbf{n}}_1 + V_0\mathbf{G}_1\mathbf{e}) + o(\epsilon),\\
&\xi = 1 + o(\epsilon).
\end{aligned}\right\} \tag{5.5}$$

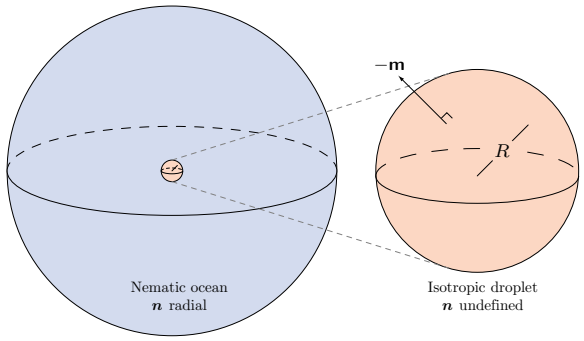

Figure 2: Schematic of an isotropic drop of radius R in an nematic ocean with radial director field. The interfacial unit normal $\mathbf{m}$ is directed outward from the nematic phase toward the origin.

Finally, we assume that

$$\Psi = \Psi_0 + \epsilon\Psi_1 + o(\epsilon) \tag{5.6}$$

with Ψ_0 and Ψ_1 given constants.

Then, assuming that β_2 is constant and neglecting inertia, (4.53) yields at zeroth and first order in ϵ,

$$\left.\begin{aligned} \beta_3 V_0 &= -\Psi_0, \\ \beta_3 V_1 - \beta_2 \mathring{K}_1 &= (\psi_0 + c)K_1 + 2c\,\mathrm{div}_{\mathcal{S}_0}\mathbf{n}_1 - \Psi_1. \end{aligned}\right\} \tag{5.7}$$

When the interfacial free energy is constant (i.e., $c = 0$) this relation takes the form

$$-\beta_2 \mathring{K}_1 + \beta_3 V_1 = \psi_0 K_1 - \Psi_1, \tag{5.8}$$

which, for $\beta_2 = 0$, is the classical *curvature-flow equation* (Gurtin 2000).

6 Radial symmetry. Isotropic drop in a nematic ocean

6.1 Kinematics

Consider an isotropic spherical drop of time-dependent radius $R(t)$ surrounded by a nematic ocean with purely radial director field (Figure 2)

$$\mathbf{n}(\mathbf{x}) = \frac{\mathbf{x}}{|\mathbf{x}|}. \tag{6.1}$$

Then, for $|\mathbf{x}| > R(t)$,

$$\mathbf{G}(\mathbf{x}) = \frac{1}{|\mathbf{x}|}(\mathbf{1} - \mathbf{n}(\mathbf{x})\otimes\mathbf{n}(\mathbf{x})), \qquad \dot{\mathbf{n}}(\mathbf{x}) = \mathbf{0}, \qquad \text{and} \qquad \ddot{\mathbf{n}}(x) = \mathbf{0} \tag{6.2}$$

Moreover, for the phase interface $|\mathbf{x}| = R(t)$,

$$\left.\begin{aligned} \mathbf{m}(\mathbf{x},t) = -\frac{\mathbf{x}}{R(t)}, \quad \mathbf{K}(\mathbf{x},t) = \frac{1}{R(t)}\mathbf{P}(\mathbf{x},t), \quad K(\mathbf{x},t) = \frac{2}{R(t)}, \\ V(\mathbf{x},t) = -\dot{R}(t), \qquad \mathring{\mathbf{m}}(\mathbf{x},t) = \mathbf{0}, \qquad \mathring{K}(\mathbf{x},t) = -\frac{2\dot{R}(t)}{R^2(t)}, \end{aligned}\right\} \tag{6.3}$$

with $\mathbf{P} = \mathbf{1} - \mathbf{m}\otimes\mathbf{m}$. Also, on $|\mathbf{x}| = R(t)$,

$$\mathbf{n}(\mathbf{x}) = -\mathbf{m}(\mathbf{x},t), \quad \mathbf{G}(\mathbf{x}) = \frac{1}{R(t)}\mathbf{P}(\mathbf{x},t), \quad \dot{\mathbf{n}}(\mathbf{x}) = \mathring{\mathbf{n}}(\mathbf{x}) = \mathbf{0}, \quad \xi = -1, \tag{6.4}$$

the last of which is a consequence of $(6.4)_1$.

6.2 Bulk results

We take the relative free-energy density of the nematic phase to have the standard form

$$\hat{\Psi}(\mathbf{n}, \operatorname{grad}\mathbf{n}) = \Psi_0 + \tfrac{1}{2}k_1(\operatorname{div}\mathbf{n})^2 + \tfrac{1}{2}k_2(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + \tfrac{1}{2}k_3|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 + \tfrac{1}{2}(k_2+k_4)(|\operatorname{grad}\mathbf{n}|^2 - (\operatorname{div}\mathbf{n})^2), \tag{6.5}$$

due to Oseen (1933), Zöcher (1933), and Frank (1958). Here, following Ericksen (1966), we assume that the splay, twist, bend, and saddle-splay moduli k_1, k_2, k_3, and k_4 obey $k_1 \geq 0$, $k_2 \geq |k_4|$, $k_3 \geq 0$, and $2k_1 \geq k_2 + k_4$. The term Ψ_0 contains information about the free-energy density of the nematic phase relative to that of the isotropic phase. For fixed compositions and in the absence of external electromagnetic fields, we might expect Ψ_0 to be negative at sufficiently low temperatures, positive at sufficiently high temperatures, and zero at some intermediate temperature. Similar remarks can be made about what to expect when the temperature is fixed, external fields are absent, but compositional fluctuations are allowed, etc. We refer to Ψ_0 as the *ambient free-energy difference*.

In view of (6.1) and (6.2), the free-energy density (6.5) specializes to

$$\hat{\Psi}(\mathbf{n}(\mathbf{x}), \mathbf{G}(\mathbf{x})) = \Psi_0 + \frac{\kappa}{|\mathbf{x}|^2}, \tag{6.6}$$

where we have introduced

$$\kappa = 2k_1 - (k_2 + k_4) \geq 0. \tag{6.7}$$

Further, direct calculations show that

$$\frac{\partial\hat{\Psi}(\mathbf{n}(\mathbf{x}), \mathbf{G}(\mathbf{x}))}{\partial\mathbf{G}} = \frac{\kappa}{|\mathbf{x}|}(\mathbf{1} - \mathbf{n}(\mathbf{x})\otimes\mathbf{n}(\mathbf{x})), \qquad \frac{\partial\hat{\Psi}(\mathbf{n}(\mathbf{x}), \mathbf{G}(\mathbf{x}))}{\partial\mathbf{n}} = \mathbf{0}. \tag{6.8}$$

Satisfaction of the bulk director momentum balance (2.15) on $|\mathbf{x}| > R(t)$ then follows from (6.2) and (6.8).

6.3 Interfacial results

By (6.4) and (6.8), a direct calculation shows that the interfacial director momentum balance (4.49) is satisfied on $|\mathbf{x}| = R(t)$.

Further, by (6.3), (6.4), (6.6), and (6.8), the normal configurational force balance (4.53) simplifies to an ordinary differential equation

$$\beta\dot{R} = \Psi_0 - \frac{2\sigma}{R} + \frac{\kappa}{R^2} \tag{6.9}$$

for the position R of the phase interface. Here, we have introduced

$$\beta = \beta_3 \qquad \text{and} \qquad \sigma = \bar{\psi}(-1). \tag{6.10}$$

Table 1: Equilibria for the ordinary differential equation (6.9).

$\Psi_0 < 0$	$R_* = \left(\sqrt{1 + \frac{\kappa\lvert\Psi_0\rvert}{\sigma^2}} - 1\right)\frac{\sigma}{\lvert\Psi_0\rvert}$
$\Psi_0 = 0$	$R_* = \frac{\kappa}{2\sigma}$
$0 < \Psi_0 < \frac{\sigma^2}{\kappa}$	$R_*^{\pm} = \left(1 \pm \sqrt{1 - \frac{\kappa\Psi_0}{\sigma^2}}\right)\frac{\sigma}{\Psi_0}$
$\Psi_0 = \frac{\sigma^2}{\kappa}$	$R_* = \frac{\sigma}{\Psi_0} = \frac{\kappa}{\sigma}$ (unstable)
$\Psi_0 > \frac{\sigma^2}{\kappa}$	$R_* \to \infty$

We assume the interfacial free-energy density is defined so that

$$\sigma > 0. \tag{6.11}$$

The equilibria of the ordinary differential equation (6.9) are synopsized in Table 1 and the qualitative behavior of the solutions is depicted in Figure 3. Suppose that the isotropic drop initially occupies a sphere of radius R_0:

$$R(0) = R_0 \tag{6.12}$$

To discuss the initial-value problem formed by (6.9) and (6.12), we consider separetly three regimes:

$$\Psi_0 < 0, \qquad \Psi_0 = 0, \qquad \text{and} \qquad \Psi_0 > 0.$$

For $\Psi_0 < 0$, (6.9) has a single equilibrium point

$$R_* = \left(\sqrt{1 + \frac{\kappa\lvert\Psi_0\rvert}{\sigma^2}} - 1\right)\frac{\sigma}{\lvert\Psi_0\rvert}. \tag{6.13}$$

Thus, when the ambient energy of the nematic phase is less than that of the isotropic phase, the competition between nematic curvature elasticity and interfacial tension allows for the existence of a unique two-phase equilibrium state with an isotropic spherical drop in a nematic ocean. In a dynamical process, the radius R of the drop grows or shrinks from its initial value R_0 until it reaches R_* as given by (6.14) depending on whether $0 < R_0 < R_*$ or $R_* < R_0 < \infty$, respectively.

For $\Psi_0 = 0$, (6.9) still has a single stable equilibrium point

$$R_* = \frac{\kappa}{2\sigma}, \tag{6.14}$$

and the qualitative behavior is the same as above.

For $\Psi_0 > 0$, we consider three subregimes:

$$\Psi_0 < \frac{\sigma^2}{\kappa}, \qquad \Psi_0 = \frac{\sigma^2}{\kappa}, \qquad \text{and} \qquad \Psi_0 > \frac{\sigma^2}{\kappa}.$$

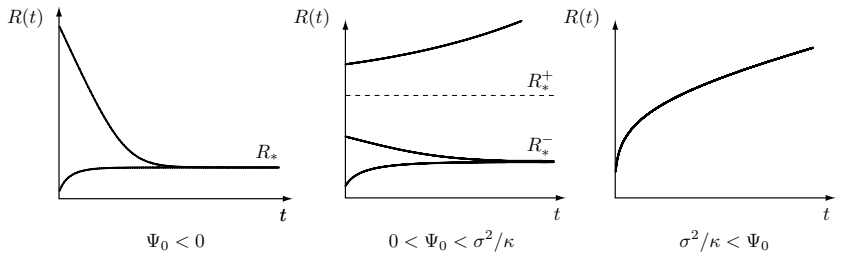

Figure 3: Plots of the time-dependence of the radius of an isotropic drop in a radial nematic ocean, at different values of the ambient energy.

First, for $\Psi_0 < \sigma^2/2\kappa$, (6.9) has two equilibrium points

$$R_*^{\pm} = \left(1 \pm \sqrt{1 - \frac{\kappa\Psi_0}{\sigma^2}}\right)\frac{\sigma}{\Psi_0}, \tag{6.15}$$

and R_*^- is stable while R_*^+ is unstable. In this regime the ambient energy of the nematic phase exceeds that of the isotropic phase, but the competition between nematic curvature elasticity and interfacial tension allows for the presence of stable isotropic spherical drops in a nematic ocean. For $0 < R_0 < R_*^+$, the radius R of the drop grows or shrinks from its initial value R_0 until it reaches R_*^- as given by (6.15), depending on whether $0 < R_0 < R_*^-$ or $R_*^- < R_0$, respectively. For $R_*^+ < R_0 < \infty$, the region occupied by the isotropic phase grows at the expense of the nematic phase. Hence R_*^+ is a critical radius for the phase transition: the drop must be sufficiently large to initiate a complete transformation to the isotropic phase. The fact that a nematic to isotropic transition that initiated with the nucleation of isotropic droplets requires that the drops coalesce to proceed further is consistent with observations.

Next, for $\Psi_0 = \sigma^2/\kappa$, (6.9) has a single saddle equilibrium point

$$R_* = \frac{\sigma}{\Psi_0} = \frac{\kappa}{\sigma}. \tag{6.16}$$

Thus, in a dynamical process, the radius of the drop will always grow.

Finally, for $\Psi_0 > \sigma^2/\kappa$, the isotropic phase grows without bound. Thus, when the ambient energy of the nematic phase exceeds that of the isotropic phase to the extent that it is greater than σ^2/κ, the nematic phase is unstable.

Remarks

(i) Reasonable orders of magnitude for the parameters κ and σ are (Stephen & Straley 1974) $\kappa \sim 10^{-7}$ erg/cm Thus, when the ambient energy difference vanishes, (6.14) gives $R_* \sim 10^{-1}$ μm. Assuming that $|\Psi_0| \ll \sigma^2/\kappa$ and expanding (6.13) accordingly, we find that this value for $R_* \sim \sigma/\kappa \sim 10^{-1}$ μm as well. Further, for $\Psi_0 \ll \sigma^2/\kappa$, (6.15) gives $R_*^- \sim \kappa/\sigma \sim 10^{-1}$ μm and $R_*^+ \sim 2\sigma/\Psi_0 \gg R_*^-$. In each of these cases, the theory therefore yields drop radii on the order of 10^{-1} μm. Thus, since the characteristic dimension of a mesogen is 1 nm, R_* as predicted by our theory is on the order of 10^2 molecular lengths.

(ii) For $\Psi_0 > \sigma^2/\kappa$, i.e., when the isotropic to nematic transition is favored, different time scales characterize nucleation and growth. In fact, when R is sufficiently small, (6.9) should be well-approximated by

$$\beta\dot{R} \sim \frac{\kappa}{R^2},$$

which implies that the, in the initial stage of growth immediately after nucleation, the drop radius evolves according to

$$R(t) \sim \sqrt[3]{R_0 + 3\kappa t}.$$

Subsequently, there is a cross-over time where both terms $-2\sigma/R$ and κ/R^2 become important. Thereafter, the term $\Psi_0 - 2\sigma/R$ will dominate and the growth is diffusive ($\sim \sqrt{t}$). Finally, once the radius is large enough, the constant term will dominate, and the growth is linear in time. Hence, the initial growth after nucleation is much faster than the steady growth of sufficiently large inclusions (cf. Figure 3).

(iii) If we considered instead a radially-aligned nematic drop is an isotropic ocean, the foregoing results would be unchanged. (To achieve it all we would need to do is alter a few words and signs ($\mathbf{m}$ would be outward).) The analog of the foregoing result concerning a initial stage of rapid growth would then be consistent with the experiments of Ostner, Chan & Kahlweit (1973).

(iv) Small isotropic spherical drops in a nematic radially oriented phase for $\Psi_0 \leq 0$, may be used to model the cores of hedgehog defects. Indeed, we may explicitly calculate the net (bulk plus surface) free-energy in a sphere of radius $\bar{R} > R_*$ containing as isotropic drop to yield

$$4\pi\big(\tfrac{1}{3}\Psi_0\bar{R}^3 + \kappa\bar{R}\big) + 4\pi\big(\sigma R_*^2 - \tfrac{1}{3}\Psi_0 R_* - \kappa R_*\big). \tag{6.17}$$

Of the two terms in (6.17) the first is the bulk energy of a hedgehog defect while the second is the correction due to the isotropic core; a straightforward calculation shows that, for $\Psi_0 \leq 0$ and R_* given by (6.13) or (6.14), this correction is negative, so that the presence of the core decreases the free energy stored in the hedgehog.

Appendix

Variation Lemma:

(a) Let $\Phi = \Phi(\mathbf{x}, t)$ and $\Theta = \Theta(\mathbf{x}, t)$ be scalar bulk fields, and $\mathbf{h} = \mathbf{h}(\mathbf{x}, t)$ a bulk vector field. If

$$\int_{\mathcal{R}} \Phi \, dv + \int_{\partial\mathcal{R}} \mathbf{h}\cdot\mathbf{m}_{\partial\mathcal{R}} \, da \leq \int_{\partial\mathcal{R}} \Theta V_{\partial\mathcal{R}} \, da, \tag{6.18}$$

for all migrating control volumes $\mathcal{R}$, then

$$\Theta = 0. \tag{6.19}$$

(b) Let $u = u(\mathbf{x}, t)$ and $w = w(\mathbf{x}, t)$ be superficial fields: if

$$\int_{\mathcal{A}} u \, da \leq \int_{\partial\mathcal{A}} w V_{\partial\mathcal{A}} \, ds, \tag{6.20}$$

for all migrating pillboxes $\mathcal{A} \subset \mathcal{S}$, then

$$w = 0. \tag{6.21}$$

Proof:

(a) Fix $t = t_0$, and choose arbitrarily a fixed region $\mathcal{R}_0$. Letting $\mathbf{r}_0(\boldsymbol{\xi})$, $\boldsymbol{\xi} = (\xi_1, \xi_2)$, be a parametrization of $\partial\mathcal{R}_0$, define a migrating control volume $\mathcal{R}(t)$ so that

$$\mathbf{r}(\boldsymbol{\xi}, t) = \mathbf{r}_0(\boldsymbol{\xi}) + c(t - t_0)\phi(\boldsymbol{\xi})\mathbf{m}_{\partial\mathcal{R}}(\boldsymbol{\xi}),$$

is a parametrization of $\partial\mathcal{R}(t)$, where c is an arbitrary constant, ϕ is an arbitrary smooth function and $\mathbf{m}_{\partial\mathcal{R}}$ is the outward unit normal to $\partial\mathcal{R}_0$. Clearly, $\mathcal{R}(t_0) = \mathcal{R}_0$ and $V_{\partial\mathcal{R}}(\boldsymbol{\xi}, t_0) = c\phi(\boldsymbol{\xi})$. Hence, letting

$$A := \int_{\mathcal{R}_0} \Phi \, dv + \int_{\partial\mathcal{R}_0} \mathbf{h}\cdot\mathbf{m}_{\partial\mathcal{R}} \, da, \qquad B := \int_{\partial\mathcal{R}_0} \Theta\phi \, da,$$

(6.18) becomes $A \le cB$ for any constant c. Now, if $B \neq 0$, choosing $c < A/B$ when $B > 0$ and $c > A/B$ when $B < 0$, we obtain $A < A$, which is impossible. Hence, $\int_{\partial\mathcal{R}_0} \Theta\phi \, da = 0$ for arbitrary ϕ and $\mathcal{R}_0$, and this implies (6.19).

(b) Now let $\mathbf{r}(\boldsymbol{\xi}, t)$ be a parametrization of $\mathcal{S}(t)$, fix t_0 and $\mathcal{A}_0 \subset \mathcal{S}(t_0)$. If $\mathbf{r}(\boldsymbol{\xi}_0(s), t_0)$ is a parametrization of the curve $\partial\mathcal{A}_0$, define

$$\boldsymbol{\xi}(s, t) = \boldsymbol{\xi}_0(s) + c(t - t_0)\phi(s)\mathbf{m}(s),$$

where $\mathbf{m}(s)$ is the 2-dimensional vector such that

$$\left[\frac{\partial \mathbf{r}}{\partial \boldsymbol{\xi}}(\boldsymbol{\xi}_0(s), t_0)\right] \mathbf{m}(s) = \mathbf{m}_{\partial\mathcal{A}}(\boldsymbol{\xi}_0(s), t_0),$$

c is an arbitrary constant, and $\phi(s)$ and arbitrary real function. Then $\mathbf{r}(\boldsymbol{\xi}(s, t), t)$ is the parametrization of the boundary $\partial\mathcal{A}(t) \subset \mathcal{S}(t)$ of a migrating pillbox such that $\mathcal{A}(t_0) = \mathcal{A}_0$. Moreover, at $t = t_0$,

$$\mathbf{v}_{\partial\mathcal{A}} = \mathbf{v} + c\phi\mathbf{m}_{\partial\mathcal{A}}, \qquad V_{\partial\mathcal{A}} = \mathbf{v}\cdot\mathbf{m}_{\partial\mathcal{A}} + c\phi,$$

with $\mathbf{v} = \partial\mathbf{r}/\partial t$. Hence, letting

$$\alpha := \int_{\mathcal{A}_0} u \, da - \int_{\partial\mathcal{A}_0} w\mathbf{v}\cdot\mathbf{m}_{\partial\mathcal{A}} \, ds, \qquad \beta := \int_{\partial\mathcal{A}_0} w\phi \, ds,$$

(6.20) becomes $\alpha \le c\beta$ for any c. Proceeding as in (a) we obtain (6.21).

Appendix

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