

Theoretical Studies of Smectic Liquid Crystals in the Presence of Flow, Oscillatory Perturbations, and Edge Dislocations

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Chapter 5 of the thesis contains material published in an article of the same name, reference [64]; the results contained therein are the result of the author's original research in collaboration with the article's co-author, Prof. Iain W. Stewart.

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Smectic liquid crystals; continuum mechanics; rheology; nonlinear elasticity; viscoelasticity; non-Newtonian fluids; hydrodynamic stability; soft condensed matter.

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Abstract

A range of theoretical studies regarding the static and dynamic behaviour of smectic liquid crystals will be presented. The thesis is mainly concerned with the smectic A phase as modelled by the continuum theory of Stewart [69], though a working knowledge of the smectic C phase, modelled using the Leslie-Stewart-Nakagawa continuum theory [41], proves necessary.

In Chapter 3, reductions of Stewart's theory by appeal to certain physicallymotivated assumptions upon the smectic and the flow pattern to which it is subjected are outlined. The linear stability of each of the resultant systems is then analysed. Chapter 4 presents the derivation of a "lubrication-type" theory based on one of these resultant systems of equations, which is then analysed in general terms before being applied to the problem of flow past a finite obstacle.

Chapter 5 presents an investigation of a shear wave incident at a planar boundary between an isotropic elastic solid and a smectic A liquid crystal. The behaviour of the wave upon reflection and refraction at the interface is established, as is the response of the smectic; a comparison with the smectic C case as considered by Gill and Leslie [25] concludes the chapter.

Finally, Chapter 6 discusses the static configuration of a smectic A liquid crystal in the presence of an isolated edge dislocation. After constructing the energy density to fourth order, we first recover the results of previous investigations by assuming the director and layer normal always coincide, in addition to examining a perturbation to a known solution [9]. We then relax the constraint director-layer normal equivalence, obtaining exact solutions for the smectic's configuration for a quadratic energy density and deriving equilibrium equations for special cases for the fourth order formulation.

Chapter 1

Introduction

This chapter provides a brief introduction to a collection of phases of matter whose properties are mysterious, complex and still not fully understood, collectively known as liquid crystals. Section 1.1 gives information regarding the discovery of liquid crystals, as well as some historical background. For a fuller account, the interested reader is directed to the books by Dunmur and Sluckin [14], Mitov [50, Chapter 3] and the comprehensive review by Kelker [33]. Section 1.2 provides basic descriptions of two types of liquid crystal: nematics and smectics. Finally Section 1.3 concludes with a note on some essential background material.

1.1 "Un Nouvel État de la Matière" [28]

Most people have, at some stage, been taught that matter exists in three common states: solids, liquids and gases. Observation, however, has shown that this rather simple system of classification is not suitable for many materials. Other phases of matter falling outwith this restrictive framework that have been discovered over the years include plasmas, Bose-Einstein and Fermionic condensates, and superfluids, to name but a few. Liquid crystals are yet another example of a material for which the straightforward solid/liquid/gas distinction fails to provide an adequate classification system for matter as we know it. Liquid crystals are in fact examples of mesomorphic phases or mesophases: intermediate states of matter. As the name suggests, these bizarre and fascinating materials display flow properties like those of viscous fluids, while at the same time possessing structural features reminiscent of solid crystals, details of which will be discussed below.

The discovery of liquid crystals is attributed to the Austrian botanist and chemist Friedrich Reinitzer [54, 55]. Whilst heating a sample of cholesteryl benzoate (a solid at room temperature), he observed that it appeared to "melt" twice: first, at around $145.5^{\circ}C$, where the substance appeared to take the form of a "cloudy liquid", then again at around $178.5^{\circ}C$, at which it became a fully transparent liquid. It is now known that this "cloudy liquid" was a particular phase of liquid crystal: a cholesteric (also known as a chiral nematic). Further, the higher "melting point" is now termed to be the clearing point, that is, the point at which the material is no longer in a mesomorphic phase, and is a fully isotropic liquid¹; see Fig. 1.1 for a representation of the molecular arrangement in the smectic A and nematic phases.

Reinitzer, aware of the work of the German physicist Otto Lehmann on the observation of birefringence during crystallisation, sent a letter to Lehmann, along with two samples, asking him to confirm these observations [33]. After examination of the samples, Lehmann originally used the expression "flowing crystals" [38] to describe them, eventually coining the term "liquid crystal" some years later, in 1900.

In 1907, Vorländer, a German chemist, noted that anisotropic (either rodlike or disc-like) molecules were essential for a given material to exhibit the two melting points described above [61, 78]. Knowledge of the structure of these constituent molecules has proved invaluable for theoretical modelling of liquid crystalline phases of matter exactly as undertaken in this thesis.

In 1922, Friedel, the French mineralogist, proposed a classification scheme for liquid crystals consisting of three categories [19]: nematic, cholesteric and smectic. Before and during the years of the second world war, experimental investigations into the viscosities of liquid crystals were undertaken [47]. See, for example, reference [46], in which Miesowicz first reports the determination of the anisotropic viscosities for nematics. A historical review containing details of experiments carried out by Miesowicz may be found in [48]. This was also the time period during which the **order parameter** (discussed in more detail below in Section 1.2.1) was first defined and used.

After the Second World War, the study of liquid crystals went into something of a decline, then underwent a rekindling in the late 1950s and early 1960s in the UK, USA and the Soviet Union. Liquid crystals are now the focus of an active and highly interdisciplinary research community, with the widely-attended biennial International Liquid Crystal Conference, European Conference on Liquid Crystals, International Conference on Ferroelectric Liquid Crystals and International Liquid Crystal Elastomers Conference (in addition to multiple other events

¹A material is said to be isotropic when its physical properties are uniform in all directions.



Figure 1.1: Schematic representation of the molecular arrangements in different phases of matter.

such as the annual meeting of the British Liquid Crystal Society and the Optics of Liquid Crystals Conference), testifying to the worldwide endeavour to understand the properties and applications of these materials.

1.2 Basic Descriptions of Liquid Crystals

Most of the materials that are known to exhibit liquid crystal phases are organic substances. There are two ways of bringing about a liquid crystal phase in a given material:

- 1. by changing the temperature of the material. Such materials are referred to as **thermotropic** liquid crystals;
- 2. by changing the concentration of material in a given solvent: **lyotropic** liquid crystals.

This thesis will treat only thermotropic liquid crystals in an isothermal setting.

As has been alluded to in the previous section, liquid crystals tend to be thought of as consisting of elongated molecules with a preferred local average direction. Details of both nematic and smectic liquid crystals are presented below, cholesterics being outwith the scope of the present work. Moreover, while we do not concern ourselves with any in-depth study of the behaviour of nematics, a discussion of their properties and a detailed summary of the Ericksen-Leslie continuum theory for nematics [17, 40] will be presented. The reason for this is as follows: nematics have been studied to a far greater extent and their behaviour is successfully described by the aforementioned theory. As a consequence of this, comparisons and analogies between the two types of material may be drawn via the physical predictions of their respective continuum theories, allowing for an understanding of which physical processes in smectics are attributable to "nematic-like" effects, and which are a consequence of the layering that is unique to smectics. For details on the various liquid crystal phases (including, for example, cholesteric and columnar phases), see the book of de Gennes and Prost [23] or the Handbook of Liquid Crystals [27].

1.2.1 Nematics

The term "nematic" has its origins in the Greek word $\nu \eta \mu \alpha$, meaning thread, so named for the thread-like structures observed in materials exhibiting this phase. (These lines are a consequence of a type of defect referred to as **disclinations**.) The molecules making up a nematic tend to align parallel to one another along an average preferred direction, which is termed the anisotropic axis. The deviation in the degree of local alignment is represented by the **order parameter** S, given by

$$S = \langle P_2(\cos\theta) \rangle = \left\langle \frac{3}{2}\cos^2\theta - \frac{1}{2} \right\rangle, \qquad (1.2.1)$$

that is, the average of a single molecule over time or the average over an ensemble of molecules of the second Legendre polynomial, The Legendre polynomials $P_n(x)$ are solutions to Legendre's differential equation [1]:

$$\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}P_n(x)\right] + n(n+1)P_n(x) = 0.$$

Nematics exhibit no long-range positional order, being able to translate freely while remaining approximately parallel to one another, as is depicted schematically in Fig. 1.2. These materials have a rotational symmetry about their anisotropic axis, which means that nematics are uniaxial. Although the constituent molecules may themselves be polar, there is no reason to suppose that this polarity should be apparent on a larger scale. As such, the axis of uniaxial symmetry is not assumed to have polarity. This is the case in classical continuum mechanics, and is assumed to hold throughout this thesis. The molecules of *para*-Azoxyanisole (PAA), a typical nematic, are rigid rods with a length of roughly 20Å and a width of 5Å. (Note that 1Å is one Angstrom: 10^{-10} metres.)

The local direction of average molecular alignment of a given sample is described by the unit vector \mathbf{n} , commonly referred to as the **director**. In mathematical terms, the absence of polarity in nematics corresponds to an invariance under the transformation $\mathbf{n} \to -\mathbf{n}$. As such, any physical properties modelled mathematically (such as the elastic energy, introduced in Section 2.1.1) must be invariant under this transformation.

1.2.2 Smectics

The word "smectic" is taken from the Ancient Greek word $\sigma \mu \eta \gamma \mu \alpha$, which means soap. The name for these media was chosen based on the fact that they display mechanical properties reminiscent of soaps. The smectic phase, along with exhibiting the characteristic alignment property of nematics, also tends to arrange itself into a layered structure with a well-defined interlayer spacing, meaning that



Figure 1.2: Schematic representation of a nematic liquid crystal. The anisotropic axis, which denotes the local average molecular alignment and defines the director \boldsymbol{n} , is represented by the arrow.

smectic phases are more ordered than nematic phases. This thesis is mainly concerned with the smectic A phase, though we will also require an understanding of the smectic C phase, particularly in Chapter 5. Schematic representations of both of these phases are given in Fig. 1.3 below. Continuum theories will be presented for both in Sections 2.2 and 2.3 below. It should be noted that there are several more smectic phases that will not be discussed here; the reader is again referred to [23, 27] for further details regarding such phases.



Figure 1.3: Schematic representation of the molecular arrangement in smectics A and C.

In the smectic A phase, whose properties will be the main focus of this thesis, the molecules form layers such that the director \boldsymbol{n} is, on average, perpendicular to the layers; that is, \boldsymbol{n} is often taken to be equivalent to the unit layer normal, a vector referred to in the literature (and in the pages of this thesis) as \boldsymbol{a} . However, for reasons to be discussed in greater detail in Section 2.3, we will allow for the possibility of decoupling of n and a. The physical properties are invariant under the simultaneous transformations $n \to -n$ and $a \to -a$; the smectic A phase also displays uniaxial symmetry. In the thermotropic case, the interlayer distance ranges from roughly the length of the constituent molecules to around double their length. For lyotropics, the distance can be up to several thousand Angstroms.

In smectic C liquid crystals, the director \boldsymbol{n} is tilted by an angle θ relative to the layer normal \boldsymbol{a} ; θ is known as the **smectic tilt angle** or **smectic cone angle**, and is generally dependent on the temperature of a given sample of smectic C material. Smectic C is an example of a biaxial phase. The director will tend to align uniformly in the absence of any external influences.

Chiral smectic C phases can occur when the constituent molecules are **enantiomorphic**, that is, different from their mirror image. Again, such considerations would prove an unnecessary digression from our present considerations, and so we do not pursue this topic here, once again referring the interested reader to reference [23].

1.3 A Note on Background Material

Throughout the course of the thesis, we rely upon a working knowledge of continuum mechanics. There exists a plethora of textbooks on this subject from undergraduate to advanced graduate level, making the compilation of an exhaustive list of references on the field a task possibly tantamount in both time and effort to the completion of a Ph.D. thesis. The reader is referred to the books by Malvern [43], Spencer [66], and Tanner [74, Chapter 2]. In particular, we will make extensive use of index notation and the Einstein summation convention for vectors and tensors, of which a cursory account is presented in Appendix A. Some introductory accounts on this topic are the books of Aris [4] and Goodbody [26], though again this list is by no means comprehensive.

Further, the results in Chapter 6 follow from application of standard methods of the Calculus of Variations. Appendix C provides an overview of the key results for dealing with the case where there is only one function of one independent variable. For introductory accounts of the theory, the reader is directed to [20,59]. A generalisation to several multivariable functions may be found in [11].

Chapter 2

A Review of Some Continuum Theories for Liquid Crystals

In this section, an outline of continuum theories for nematics as well as smectics A and C are given. As discussed above, nematics are described using the Ericksen-Leslie continuum theory, while the smectic C and smectic A phases will be modelled using the theories of Leslie, Stewart & Nakagawa and Stewart, respectively.

2.1 Nematics

The first attempt at a theory describing the dynamics of nematics was undertaken by Anzelius in 1931 [3]. Some thirty years later, Ericksen made use of the balance laws of classical continuum mechanics in order to construct the first widely-accepted theory [16,17]. In 1968, Leslie derived constitutive equations [39], proposing expressions for dynamic contributions. The combined results of these two works form what is referred to as Ericksen-Leslie theory. This model is one of the most successful and widely-employed theories used in the modelling of nematics. Leslie published an alternative derivation of the theory under the assumptions of incompressibility and isothermality [40]. Given that this thesis will only deal with incompressible liquid crystals under isothermal conditions, it makes sense for us to outline the results of the latter derivation. We will follow the book of Stewart [68] and start in Section 2.1.1 by introducing various kinematic quantities and pieces of terminology that frequently arise in the modelling of fluids possessing a mechanically significant microstructure (for example, polar fluids [12] and polymeric fluids [74]).

2.1.1 Kinematics

The Eulerian description of the instantaneous motion of a fluid with a microstructure makes use of two independent vector fields: the velocity vector $\boldsymbol{v}(\boldsymbol{x},t)$ and an axial vector $\boldsymbol{w}(\boldsymbol{x},t)$ which, in a polar fluid, represents the angular velocity of the polar fluid particle at position \boldsymbol{x} at time t. In the context of liquid crystals, \boldsymbol{w} is the **local angular velocity** of the liquid crystal material element i.e. the local angular velocity of the director \boldsymbol{n} . In "ordinary" continuum theory, the only independent field is the velocity of the fluid, since the angular velocity in such theories is given by $\frac{1}{2}\nabla \times \boldsymbol{v}$. For liquid crystals, this particular angular velocity is referred to as the **regional angular velocity**, denoted $\hat{\boldsymbol{w}}$, and defined, as previously stated, by

$$\widehat{\boldsymbol{w}}(\boldsymbol{x},t) = \frac{1}{2} \nabla \times \boldsymbol{v}. \tag{2.1.1}$$

This provides a measure of the average rotation of the fluid over a neighbourhood of the material element. We define $\boldsymbol{\omega}$ to be the **relative angular velocity**, that is, the angular velocity of the material element relative to the regional angular velocity in which the material element is embedded, viz.,

$$\boldsymbol{\omega} = \boldsymbol{w} - \hat{\boldsymbol{w}} = \boldsymbol{w} - \frac{1}{2} \nabla \times \boldsymbol{v}, \qquad (2.1.2)$$

the difference between the local angular velocity \boldsymbol{w} of the director and the regional angular velocity $\hat{\boldsymbol{w}}$ of the fluid in the neighbourhood of the director.

The director itself is a unit vector, and is therefore required to satisfy

$$\boldsymbol{n} \cdot \boldsymbol{n} = n_i n_i = 1. \tag{2.1.3}$$

Since \boldsymbol{w} represents the angular velocity of \boldsymbol{n} , it follows from the above constraint that

$$\dot{\boldsymbol{n}} = \boldsymbol{w} \times \boldsymbol{n}, \tag{2.1.4}$$

with the superposed dot representing the **material time derivative**:

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + (\boldsymbol{v} \cdot \nabla) = \partial_t + v_i \partial_i.$$
(2.1.5)

Details on the physical interpretation of the material time derivative may be found in the books by Acheson [2] and Aris [4], while useful discussions regarding angular momentum and axial vectors are to be found in [34].

The usual rate of strain tensor or velocity gradient tensor A and vorticity tensor W have components A_{ij} and W_{ij} , respectively, defined in the usual way by

$$A_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i})$$
 and $W_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i}).$ (2.1.6)

Note that A is symmetric, while W is anti-symmetric. Leslie introduced the vector N [40], defined by

$$\boldsymbol{N} := \boldsymbol{\omega} \times \boldsymbol{n}. \tag{2.1.7}$$

It then follows from this and equations (2.1.2), (2.1.4), (2.1.6) and (A.7) that

$$N_i = \varepsilon_{ijk}\omega_j n_k = \dot{n}_i + \frac{1}{2}(v_{k,i} - v_{i,k}) = \dot{n}_i - W_{ij}n_j, \qquad (2.1.8)$$

so that equation (2.1.7) is equivalent to

$$\boldsymbol{N} = \dot{\boldsymbol{n}} - \boldsymbol{\mathsf{W}}\boldsymbol{n}. \tag{2.1.9}$$

The vector N is sometimes referred to as the **co-rotational time flux** of the director, for example in the terminology employed by Truesdell & Noll [76]. From the definition (2.1.7), it is clear that N is connected to the relative angular velocity ω : it is a measure of the rotation of n relative to the fluid. The requirement (2.1.3) leads to

$$n_i \dot{n}_i = 0,$$
 (2.1.10)

while equation (2.1.7) gives

$$n_i N_i = 0.$$
 (2.1.11)

Material Frame-Indifference

A well-known fundamental principle of classical physics is that of material frameindifference, which states that the constitutive equations for a given material must be invariant under changes of reference frame. Formally, under a motion defined by

$$\boldsymbol{x}^*(t-\tau) = \boldsymbol{\mathsf{Q}}(t)\boldsymbol{x}(t) + \boldsymbol{c}(t), \qquad (2.1.12)$$

where τ is any real number, c(t) an arbitrary function of time, and Q(t) an arbitrary rotation represented by a proper orthogonal tensor function of time, a vector \boldsymbol{a} and second-order tensor B are **frame-indifferent** or **objective** if they transform according to

$$\boldsymbol{a}^* = \boldsymbol{\mathsf{Q}}\boldsymbol{a}, \qquad \boldsymbol{\mathsf{B}}^* = \boldsymbol{\mathsf{Q}}\boldsymbol{\mathsf{B}}\boldsymbol{\mathsf{Q}}^T, \tag{2.1.13}$$

a starred symbol corresponding to its non-starred quantity after the motion (2.1.12) has occurred. The components Q_{ij} of \mathbf{Q} will be identified with entries in a matrix. Note that a matrix \mathbf{Q} is **proper orthogonal** if

$$\mathbf{Q}\mathbf{Q}^T = \mathbf{I} \iff Q_{ik}Q_{jk} = Q_{kj}Q_{ki} = \delta_{ij}, \qquad \det \mathbf{Q} = 1, \tag{2.1.14}$$

where I represents the identity matrix, whose components are $I_{ij} \equiv \delta_{ij}$.

Of the quantities introduced above, n_i , N_i and A_{ij} are frame-indifferent. Details of the calculations involved in proving this are omitted here for brevity, but the interested reader is directed to [68, Section 4.2.1].

The Frank-Oseen Elastic Energy

It is, at this point, pertinent to introduce a free energy density associated with distortions of n, that is, corresponding to deformations of a given sample of nematic material. This is referred to as the **Frank-Oseen elastic energy**, and is assumed to be of the form

$$w_f = w_f(n_i, n_{i,j});$$
 (2.1.15)

 w_f is also taken to be quadratic in the gradients of \boldsymbol{n} . Assuming incompressibility, the free energy is generally defined to within the addition of an arbitrary constant; it proves advantageous to choose this constant such that $w_f = 0$ for any relaxed orientation (in the absence of forces, fields and boundary conditions) and suppose that any other configuration produces an energy greater than or equal to that of this relaxed orientation. This leads to the inequality

$$w_f(\boldsymbol{n}, \nabla \boldsymbol{n}) \ge 0. \tag{2.1.16}$$

Given the general absence of polarity in nematics, \boldsymbol{n} and $-\boldsymbol{n}$ are physically indistinguishable. In fact, this holds even if the constituent molecules are polar, as they can be thought of as having a local arrangement at any given point such that they are divided equally into two groups possessing opposite orientations. This means that w_f is required to be invariant under the change $\boldsymbol{n} \to -\boldsymbol{n}$:

$$w_f(\boldsymbol{n}, \nabla \boldsymbol{n}) = w_f(-\boldsymbol{n}, -\nabla \boldsymbol{n}). \tag{2.1.17}$$

The free energy is also subject to the condition of frame-indifference, so that

$$w_f(\boldsymbol{n}, \nabla \boldsymbol{n}) = w_f(\boldsymbol{\mathsf{Q}}\boldsymbol{n}, \boldsymbol{\mathsf{Q}}\nabla \boldsymbol{n}\boldsymbol{\mathsf{Q}}^T). \tag{2.1.18}$$

With these restrictions in mind, it is possible to construct the Frank-Oseen elastic energy for nematics in the form

$$w_f = \frac{1}{2}K_1(\nabla \cdot \boldsymbol{n})^2 + \frac{1}{2}K_2(\boldsymbol{n} \cdot \nabla \times \boldsymbol{n})^2 + \frac{1}{2}K_3(\boldsymbol{n} \times \nabla \times \boldsymbol{n})^2 + \frac{1}{2}(K_2 + K_4)\nabla \cdot [(\boldsymbol{n} \cdot \nabla)\boldsymbol{n} - (\nabla \cdot \boldsymbol{n})\boldsymbol{n}], \qquad (2.1.19)$$

or, equivalently, in component form:

$$w_f = \frac{1}{2}(K_1 - K_2 - K_4)(n_{i,i})^2 + \frac{1}{2}K_2n_{i,j}n_{i,j} + \frac{1}{2}K_4n_{i,j}n_{j,i} + \frac{1}{2}(K_3 - K_2)n_jn_{i,j}n_kn_{i,k}.$$
(2.1.20)

Again, details of the derivation of these terms may be found in [68, Section 2.2]. Respectively, K_1 , K_2 , K_3 , and $K_2 + K_4$ are known as the **splay**, **twist**, **bend**, and **saddle-splay** constants. See p.16 of [68] along with relevant comments to be found on pages, 21, 38 ("Null Lagrangians"), and 47 (problems involving strong anchoring) for details on the physical interpretation of these constants. The reader is also directed to Section 3.3 of the book by Virga [77]. Finally, it is worth pointing out that another derivation of (2.1.19) has been provided by Clark [10].

2.1.2 Balance Laws

As stated above, we only deal with isothermal conditions, so thermal effects are ignored. For a volume $\Omega \subset \mathbb{R}^3$ of nematic bounded by the surface S, the conservation laws for mass, linear momentum and angular momentum are, respectively,

$$\frac{D}{Dt} \int_{\Omega} \rho \, dV = 0, \tag{2.1.21}$$

$$\frac{D}{Dt} \int_{\Omega} \rho \boldsymbol{v} \, dV = \int_{\Omega} \rho \boldsymbol{f} \, dV + \int_{S} \boldsymbol{t} \, dA, \qquad (2.1.22)$$

$$\frac{D}{Dt} \int_{\Omega} \rho(\boldsymbol{x} \times \boldsymbol{v}) \, dV = \int_{\Omega} \rho(\boldsymbol{x} \times \boldsymbol{f} + \boldsymbol{K}) \, dV + \int_{S} (\boldsymbol{x} \times \boldsymbol{t} + \boldsymbol{l}) \, dA, \qquad (2.1.23)$$

where dV and dA denote, respectively, the volume and area elements, ρ is the mass density, \boldsymbol{x} the position vector, \boldsymbol{v} the velocity, \boldsymbol{f} the external body force per unit mass, \boldsymbol{t} the surface force per unit area (traction), \boldsymbol{K} the external body moment per unit mass, and \boldsymbol{l} the surface moment per unit area (or couple stress vector). We note that no director inertial term has been incorporated into the

above formulation, since it is generally regarded as negligible in nematic flow problems. (A discussion of such terms is to be found on pp. 147-149 of [68].) Also, there seems to be a convention in static theory whereby \boldsymbol{f} will appear in place of $\rho \boldsymbol{f}$, so that in static considerations, \boldsymbol{f} will represent the external body force per unit volume. An analogous comment applies to \boldsymbol{K} .

The mass conservation law may be manipulated via the well-known Reynolds' transport theorem (see, for instance, [68, Appendix B] or [74, Section 2.4.1]) to yield the continuity equation

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}) = 0. \tag{2.1.24}$$

A fluid is said to be **incompressible** if its mass density is constant: that is, $\dot{\rho} = 0$. It follows that the mass conservation law for an incompressible fluid may be replaced with

$$\nabla \cdot \boldsymbol{v} = v_{i,i} = 0, \qquad (2.1.25)$$

with the density constant throughout the volume Ω . Note that (2.1.25) is equivalent to

$$\mathrm{Tr}\mathsf{A} = A_{ii} = 0. \tag{2.1.26}$$

The usual tetrahedron argument [66] allows the surface force t_i and the surface moment l_i to be written in terms of the stress tensor t_{ij} and the couple stress tensor l_{ij} , respectively, as

$$t_i = t_{ij}\nu_j, \qquad l_i = l_{ij}\nu_j,$$
 (2.1.27)

where $\boldsymbol{\nu}$ denotes the outward unit normal to the surface S. The last term in equation (2.1.22) may be re-written via the divergence theorem as

$$\int_{S} t_i \, dA = \int_{\Omega} t_{ij,j} \, dV. \tag{2.1.28}$$

Inserting this back into (2.1.22), making further use of Reynolds' transport theorem and noting that the balance law holds for an arbitrary choice of volume finally allows us to write it in point form as

$$\rho \dot{v}_i = \rho f_i + t_{ij,j}. \tag{2.1.29}$$

Yet another application of the transport theorem gives

$$\frac{D}{Dt} \int_{\Omega} \rho \varepsilon_{ijk} x_j v_k \, dV = \int_{\Omega} \rho \varepsilon_{ijk} x_j \dot{v}_k \, dV, \qquad (2.1.30)$$

whilst the divergence theorem may be employed to show that

$$\int_{S} \varepsilon_{ijk} x_j t_k \, dA = \int_{\Omega} \varepsilon_{ijk} (t_{kj} + x_j t_{kl,l}) \, dV. \tag{2.1.31}$$

Using the second relation in (2.1.27) and the divergence theorem, the balance law for angular momentum (2.1.23) may be cast into the form

$$\int_{\Omega} \varepsilon_{ijk} x_j (\rho \dot{v}_k - \rho f_k - t_{kl,l}) \, dV = \int_{\Omega} (\rho K_i + \varepsilon_{ijk} t_{kj} + l_{ij,j}) \, dV.$$
(2.1.32)

But, by (2.1.29), the left-hand side of this must vanish. Recalling that this holds for arbitrary V allows the angular momentum balance equation to be expressed in point form:

$$\rho K_i + \varepsilon_{ijk} t_{kj} + l_{ij,j} = 0. \tag{2.1.33}$$

The specific forms of t_{ij} and l_{ij} may be deduced from the rate-of-work postulate proposed by Leslie [40],

$$\int_{\Omega} \mathcal{D} \, dV = \int_{V} \rho(f_i v_i + K_i w_i) \, dV + \int_{S} (t_i v_i + l_i w_i) \, dA$$
$$- \frac{D}{Dt} \int_{\Omega} \left(\frac{1}{2} \rho v_i v_i + w_f\right) \, dV, \qquad (2.1.34)$$

where \boldsymbol{w} is the local angular velocity and w_f the **Frank-Oseen elastic energy** as discussed in Section 2.1.1 above, and \mathcal{D} is the rate of viscous dissipation per unit volume, most commonly referred to as the **dissipation function**. For brevity, we simply state the forms of the stress and couple stress tensors, directing the interested reader to the book by Stewart [68, pp.141-142] for details on the necessary calculations.

$$t_{ij} = -p\delta_{ij} - n_{k,i}\frac{\partial w_f}{\partial n_{k,j}} + \tilde{t}_{ij}, \qquad (2.1.35)$$

$$l_{ij} = \varepsilon_{ikl} n_k \frac{\partial w_f}{\partial n_{l,j}} + \tilde{l}_{ij}, \qquad (2.1.36)$$

with p an arbitrary pressure arising from incompressibility and \tilde{t}_{ij} , l_{ij} denote dynamic contributions. Note that here and in subsequent discussion \tilde{t}_{ij} is referred

to as the **viscous stress**. Further calculation allows for the establishment of the following inequality:

$$\mathcal{D} = \tilde{t}_{ij} v_{i,j} + \tilde{l}_{ij} w_{i,j} - w_i \varepsilon_{ijk} \tilde{t}_{kj} \ge 0.$$
(2.1.37)

This proves very important when considering constitutive equations and in establishing restrictions on the forms of the dynamic terms.

2.1.3 Constitutive Equations

To proceed further, it proves necessary to make further assumptions about the dynamic contributions to the stress and couple stress tensors. We therefore need to introduce relations between the stresses \tilde{t}_{ij} , \tilde{l}_{ij} and the motion of the material. Such relations lead to the establishment of **constitutive equations**. It seems natural to use the director, velocity gradients and local angular velocity of the director as the continuum variables. As such, it is assumed that at any material point at any instant, the terms \tilde{t}_{ij} and \tilde{l}_{ij} are functions of these terms evaluated at that point at that instant. In fact, the viscous couple stress \tilde{l}_{ij} is assumed not to be dependent on the gradients of the local angular velocity $w_{i,j}$ of the director. It may then be deduced from inequality (2.1.37) that

$$\tilde{l}_{ij} = 0,$$
(2.1.38)

so that

$$\mathcal{D} = \tilde{t}_{ij} v_{i,j} - w_i \varepsilon_{ijk} \tilde{t}_{kj} \ge 0, \qquad (2.1.39)$$

which imposes restrictions on the form of \tilde{t}_{ij} .

By considering a rigid-body motion, straightforward calculations show that \tilde{t}_{ij} may be equivalently taken to be a function of n_i , N_i and A_{ij} . Further, material frame-indifference requires that \tilde{t}_{ij} be a hemitropic function of these variables². This gives

$$\tilde{t}_{ij}^*(n_i^*, N_i^*, A_{ij}^*) = Q_{ik} \tilde{t}_{kl}(n_i, N_i, A_{ij}) Q_{jl}, \qquad (2.1.40)$$

where Q is a second order proper orthogonal tensor. Further, the experiments of Miesowicz [46] suggest that \tilde{t}_{ij} is a linear function of its above named variables, i.e.

$$\tilde{t}_{ij} = X_{ij} + Y_{ijk}N_k + Z_{ijkl}A_{kl}, \qquad (2.1.41)$$

²A material is *hemitropic* if its symmetry group consists of all rotations but no reflections [66].

where the coefficients are subject to

$$X_{ij}^{*} = Q_{ik}Q_{jl}X_{kl}, Y_{ijk}^{*} = Q_{il}Q_{jm}Q_{kp}Y_{lmp}, Z_{ijkl}^{*} = Q_{im}Q_{jp}Q_{kq}Q_{lr}Z_{mpqr}, (2.1.42)$$

and are functions of n_i . Nematic symmetry requires that these coefficients are transversely isotropic [66, p.110] with respect to n_i . Smith and Rivlin [62] showed that such tensors are expressible as a linear combination of products of n_i and $\delta_{ij}-n_in_j$ (or, equivalently, δ_{ij} and n_i), so that, expanding these coefficients in their general forms and making use of equations (2.1.11), (2.1.26) and the symmetries $A_{ij} = A_{ji}$, $n_in_j = n_jn_i$, allows, after some tedious but routine manipulation, for the following expressions to be deduced for the viscous stress and dissipation function, respectively:

$$\tilde{t}_{ij} = \alpha_1 n_k A_{kl} n_l n_i n_j + \alpha_2 N_i n_j + \alpha_3 n_i N_j + \alpha_4 A_{ij} + \alpha_5 n_j A_{ik} n_k + \alpha_6 n_i A_{jk} n_k,$$
(2.1.43)

$$\mathcal{D} = \alpha_1 (n_i A_{ij} n_j)^2 + (\alpha_2 + \alpha_3 + \gamma_2) N_i A_{ij} n_j + \alpha_4 A_{ij} A_{ij} + (\alpha_5 + \alpha_6) n_i A_{ij} A_{jk} n_k + \gamma_1 N_i N_i \ge 0, \qquad (2.1.44)$$

where $\gamma_1 := \alpha_3 - \alpha_2$ and $\gamma_2 := \alpha_6 - \alpha_5$. The coefficients $\alpha_n, n \in \{1, \ldots, 6\}$ are known as the **Leslie viscosity coefficients**, or simply the **Leslie viscosities**. Restrictions on the Leslie viscosities may be derived via inequality (2.1.44). An elementary example is given on p.146 of reference [68].

2.1.4 The Ericksen-Leslie Dynamic Equations

Making use of the expressions for t_{ij} and l_{ij} in equations (2.1.35) and (2.1.36) (keeping in mind that $\tilde{l}_{ij} = 0$), along with the Ericksen identity

$$\varepsilon_{ijk} \left(n_j \frac{\partial w_f}{\partial n_k} + n_{j,l} \frac{\partial w_f}{\partial n_{k,l}} + n_{l,j} \frac{\partial w_f}{\partial n_{l,k}} \right) = 0, \qquad (2.1.45)$$

and the assumption that the external body moment per unit mass K is related to the generalised body force G via

$$\rho K_i = \varepsilon_{ijk} n_j G_k, \qquad (2.1.46)$$

calculations allow the final form of angular momentum balance to be given as

$$\left(\frac{\partial w_f}{\partial n_{i,j}}\right)_{,j} - \frac{\partial w_f}{\partial n_i} + \tilde{g}_i + G_i = \lambda n_i, \qquad (2.1.47)$$

where

$$\tilde{g}_i = -\gamma_1 N_i - \gamma_2 A_{ij} n_j, \qquad (2.1.48)$$

and λ is an arbitrary scalar function. Taking the scalar product of equation (2.1.47) with $n_{i,k}$ and some straightforward manipulation then gives the final form of the balance of linear momentum equation as

$$\rho \dot{v}_i = \rho f_i - \tilde{p}_{,i} + \tilde{g}_j n_{j,i} + G_j n_{j,i} + \tilde{t}_{ij} = 0, \qquad (2.1.49)$$

where

$$\tilde{p} = p + w_f. \tag{2.1.50}$$

Summary of the Ericksen-Leslie Dynamic Equations

For convenience, a summary of the complete Ericksen-Leslie equations will be given. Similar summaries will be given for the smectic A and C dynamic theories proposed below without any discussion of the derivation; these derivations follow a similar approach to that outlined above. For further details, it is suggested that the interested reader consult the appropriate references.

In isothermal conditions, an incompressible nematic liquid crystal is subject to the constraints

$$n_i n_i = 1, \tag{2.1.3}$$

$$v_{i,i} = 0.$$
 (2.1.25)

and the balance laws

$$\rho \dot{v}_i = \rho f_i - \tilde{p}_{,i} + \tilde{g}_j n_{j,i} + G_j n_{j,i} + \tilde{t}_{ij}, \qquad (2.1.49)$$

and

$$\left(\frac{\partial w_f}{\partial n_{i,j}}\right)_{,j} - \frac{\partial w_f}{\partial n_i} + \tilde{g}_i + G_i = \lambda n_i, \qquad (2.1.47)$$

for linear and angular momentum, respectively. In the above, f_i denotes the external body force per unit mass, G_i is the generalised body force, which is related to the external body moment per unit mass K_i via equation (2.1.46), ρ is the mass density, $\tilde{p} = p + w_f$ with p the pressure and w_f the elastic energy of

the nematic, given by

$$w_f = \frac{1}{2}(K_1 - K_2 - K_4)(n_{i,i})^2 + \frac{1}{2}K_2n_{i,j}n_{i,j} + \frac{1}{2}K_4n_{i,j}n_{j,i} + \frac{1}{2}(K_3 - K_2)n_jn_{i,j}n_kn_{i,k}, \qquad (2.1.20)$$

The K_i $(i \in \{1, ..., 4\})$ are the elastic constants discussed in Section 2.1.1 above. The scalar function λ is a Lagrange multiplier, which is generally evaluated on taking the scalar product of (2.1.47) with \boldsymbol{n} . The constitutive relations for the viscous stress \tilde{t}_{ij} and the vector \tilde{g}_i are

$$\tilde{t}_{ij} = \alpha_1 n_k A_{kl} n_l n_i n_j + \alpha_2 N_i n_j + \alpha_3 n_i N_j + \alpha_4 A_{ij} + \alpha_5 n_j A_{ik} n_k + \alpha_6 n_i A_{jk} n_k,$$
(2.1.43)

$$\tilde{g}_i = -\gamma_1 N_i - \gamma_2 A_{ij} n_j, \qquad (2.1.48)$$

with $\gamma_1 = \alpha_3 - \alpha_2$, $\gamma_2 = \alpha_6 - \alpha_5$, and

$$N_i = \dot{n}_i - W_{ij} n_j. \tag{2.1.8}$$

The result

$$\gamma_2 = \gamma_1, \tag{2.1.51}$$

known as the **Parodi relation** [69], is often taken to be the case, so that only 5 of the Leslie viscosities are linearly independent. The stress tensor and couple stress tensor are given by

$$t_{ij} = -p\delta_{ij} - n_{k,i}\frac{\partial w_f}{\partial n_{k,j}} + \tilde{t}_{ij}, \qquad (2.1.35)$$

$$l_{ij} = \varepsilon_{ikl} n_k \frac{\partial w_f}{\partial n_{l,j}},\tag{2.1.36}$$

on recalling that the dynamic contribution to the couple stress must be zero in order to satisfy the dissipation inequality. This concludes our summary of the Ericksen-Leslie equations.

2.2 Smectic C

In this section, we present a brief outline of the nonlinear continuum theory for smectic C (SmC) liquid crystals as presented in Chapter 6 of [68], which in turn is drawn from the continuum theory originally proposed by Leslie, Stewart, and



Figure 2.1: Configuration of (a) the constituent molecules and (b) the vectors \boldsymbol{a} , \boldsymbol{b} and \boldsymbol{c} , as well as the fictitious cone on which the director \boldsymbol{n} in constrained to lie. (Figure reproduced from reference [68] with permission from the author.)

Nakagawa in 1991 [41]. Essentially, the principles used in deriving this theory are analogous to those found in the continuum theory for nematics as discussed above in Section 1.2.1. Because of this, and for the sake of brevity, only a summary need be presented. However, as remarked by Stewart [68], the extensions presented are by no means trivial, and the reader is directed to the relevant literature for further details.

2.2.1 Static Theory and the Elastic Energy

As mentioned above, the director in the SmC phase makes a so-called smectic tilt angle θ with the layer normal, which is generally temperature-dependent. However, as this thesis concerns itself only with the incompressible isothermal case, θ may be taken as a constant angle for our purposes. Further, it will be supposed that the layers are spaced equidistantly by some interlayer distance d. Note that, while these assumptions have proved reasonable in a variety of circumstances, for certain situations they may be considered too restrictive (for example, in the case of a sample of SmC under a high level of stress). The basic mathematical description follows that of de Gennes and Prost [23], introducing two unit vectors: \boldsymbol{a} , which defines the layer normal; and \boldsymbol{c} , referred to as the \boldsymbol{c} -director, which is the unit orthogonal projection of the director \boldsymbol{n} onto the plane of the layers. Referring to Fig. 2.1, it is easily seen that

$$\boldsymbol{n} = \boldsymbol{a}\cos\theta + \boldsymbol{c}\sin\theta. \tag{2.2.1}$$

It also proves convenient to employ the vector \boldsymbol{b} , defined by

$$\boldsymbol{b} = \boldsymbol{a} \times \boldsymbol{c}. \tag{2.2.2}$$

Based on this, along with the restriction in equation (2.1.3), it is readily observed that

$$\boldsymbol{a} \cdot \boldsymbol{a} = 1, \qquad \boldsymbol{c} \cdot \boldsymbol{c} = 1, \qquad \boldsymbol{a} \cdot \boldsymbol{c} = 0.$$
 (2.2.3)

It is worth noting that these restrictions, via a straightforward exercise in partial differentiation, lead to the results

$$a_i a_{i,j} = 0,$$
 $c_i c_{i,j} = 0,$ $a_i c_{i,j} + c_i a_{i,j} = 0.$ (2.2.4)

In addition, we have the Oseen constraint [52]:

$$\nabla \times \boldsymbol{a} = 0, \tag{2.2.5}$$

which holds in the absence of any defects or singularities. This constraint was first derived by Oseen for the smectic A phase (that is, when $\theta \equiv 0$), and may be derived in the following way. Given incompressible, equidistant smectic layers, with the constant interlayer spacing d, the integral

$$\frac{1}{d} \int_{x_1}^{x_2} \boldsymbol{a} \cdot d\boldsymbol{x} \tag{2.2.6}$$

represents the number of layers crossed by an observer travelling along the path from point x_1 to point x_2 . Given the absence of defects, the layer normal \boldsymbol{a} must be differentiable at all points. Now, considering the scenario where $x_1 = x_2$, the path traversed will form a closed loop Γ , from which it follows that the number of layers crossed "going up" is the same as those crossed when "coming down". Therefore

$$\int_{\Gamma} \boldsymbol{a} \cdot d\boldsymbol{x} = 0 \implies \int_{S} (\nabla \times \boldsymbol{a}) \cdot \boldsymbol{\nu} \, dA = 0, \qquad (2.2.7)$$

by an application of Stokes' Theorem, with $\boldsymbol{\nu}$ denoting the outward unit normal to the area S enclosed by the contour Γ . Given that Γ , and therefore S, is arbitrary, this result yields exactly the Oseen constraint as given in (2.2.5): $\nabla \times \boldsymbol{a} = 0$. Expressing this in component form allows for the deduction

$$\varepsilon_{ijk}a_{k,j} = 0 \implies a_{i,j} = a_{j,i}.$$
 (2.2.8)

The Elastic Energy

As for nematics, it will be assumed that there is a free energy density associated with deformations of the material, which may be related to distortions in n and, thereby, distortions in a and c. The resulting energy is taken to be of the form

$$w = w(a_i, c_i, a_{i,j}, c_{i,j}), (2.2.9)$$

and is assumed to be quadratic in the gradients of a and c. As before, the condition of frame-indifference is imposed on the material, so that

$$w(\boldsymbol{a}, \boldsymbol{c}, \nabla \boldsymbol{a}, \nabla \boldsymbol{c}) = w(\boldsymbol{Q}\boldsymbol{a}, \boldsymbol{Q}\boldsymbol{c}, \boldsymbol{Q}\nabla \boldsymbol{a}\boldsymbol{Q}^{T}, \boldsymbol{Q}\nabla \boldsymbol{c}\boldsymbol{Q}^{T}), \qquad (2.2.10)$$

where Q denotes a proper orthogonal matrix. Note that this requirement also holds for chiral SmC, denoted by SmC^{*}. In fact, for achiral smectic C, requirement (2.2.10) must hold for any orthogonal matrix Q – that is, det $Q = \pm 1$. The energy is also invariant under the simultaneous changes

$$\boldsymbol{a} \to -\boldsymbol{a} \quad \text{and} \quad \boldsymbol{c} \to -\boldsymbol{c}, \quad (2.2.11)$$

this being a natural requirement of invariance under the transformation $n \rightarrow -n$. Imposing these requirements leads, through extensive calculation, to the expression

$$w = \frac{1}{2}K_1(\nabla \cdot \boldsymbol{a})^2 + \frac{1}{2}K_2(\nabla \cdot \boldsymbol{c})^2 + \frac{1}{2}K_3(\boldsymbol{a} \cdot \nabla \times \boldsymbol{c})^2 + \frac{1}{2}K_4(\boldsymbol{c} \cdot \nabla \times \boldsymbol{c})^2 + \frac{1}{2}K_5(\boldsymbol{b} \cdot \nabla \times \boldsymbol{c})^2 + K_6(\nabla \cdot \boldsymbol{a})(\boldsymbol{b} \cdot \nabla \times \boldsymbol{c}) + K_7(\boldsymbol{a} \cdot \nabla \times \boldsymbol{c})(\boldsymbol{c} \cdot \nabla \times \boldsymbol{c}) + K_8(\nabla \cdot \boldsymbol{c})(\boldsymbol{b} \cdot \nabla \times \boldsymbol{c}) + K_9(\nabla \cdot \boldsymbol{a})(\nabla \cdot \boldsymbol{c}),$$
(2.2.12)

or the equivalent component form

$$w = \frac{1}{2}K_1(a_{i,i})^2 + \frac{1}{2}(K_2 - K_4)(c_{i,i})^2 + \frac{1}{2}(K_3 - K_4)c_{i,j}c_jc_{i,k}c_k + \frac{1}{2}K_4c_{i,j}c_{i,j}$$

+ $\frac{1}{2}(K_5 - K_3)(c_ia_{i,j}c_j)^2 + K_6a_{i,i}(c_ja_{j,k}c_k) - K_7c_{i,j}c_jc_{i,k}a_k$
+ $(K_8 - K_7)c_{i,i}(c_ja_{j,k}c_k) + K_9a_{i,i}c_{j,j}.$ (2.2.13)

The reader is directed to Section 6.2.1 and the references therein for an exhaustive account of the interpretation of the constants K_i $(i \in \{1, ..., 9\})$ and how they relate to the elastic constants found in, for example, the work of the Orsay group [23] and those introduced by Saupe in an earlier description of smectics [60].

2.2.2 The Dynamic Theory

Recall the balance laws for mass, linear momentum and angular momentum, which still apply to a given sample volume Ω of SmC enclosed by a bounding surface S:

$$\frac{D}{Dt} \int_{\Omega} \rho \, dV = 0, \qquad (2.2.14)$$

$$\frac{D}{Dt} \int_{\Omega} \rho \boldsymbol{v} \, dV = \int_{\Omega} \rho \boldsymbol{f} \, dV + \int_{S} \boldsymbol{t} \, dA, \qquad (2.2.15)$$

$$\frac{D}{Dt} \int_{\Omega} \rho(\boldsymbol{x} \times \boldsymbol{v}) \, dV = \int_{\Omega} \rho(\boldsymbol{x} \times \boldsymbol{f} + \boldsymbol{k}) \, dV + \int_{S} (\boldsymbol{x} \times \boldsymbol{t} + \boldsymbol{l}) \, dA.$$
(2.2.16)

Consequently, we arrive, as before, at the incompressibility condition, expressed in the form

$$v_{i,i} = 0, (2.2.17)$$

along with the linear and angular momentum balance laws

$$\rho \dot{v}_i = \rho f_i + t_{ij,j}, \tag{2.2.18}$$

$$\rho K_i + \varepsilon_{ijk} t_{kj} + l_{ij,j} = 0, \qquad (2.2.19)$$

with the symbols retaining their meanings as set out in Section 2.1.2, with identical comments applying to f_i and K_i . Again the director inertial term has been assumed negligible and therefore is omitted in the present formulation. The derivation of the theory relies on an analogous rate-of-work postulate to that given in equation (2.1.34), with the nematic energy w_f replaced by w as given in equations (2.2.12), (2.2.13) and the assumption that the rate of viscous dissipation per unit volume, \mathcal{D} , is non-negative. Therefore, by considering the rate of work done on an arbitrary volume of smectic C material, it is readily shown that

$$t_{ij}v_{i,j} + l_{ij}w_{i,j} - w_i\varepsilon_{ijk}t_{kj} = \dot{w} + \mathcal{D}, \qquad (2.2.20)$$

where the vector \boldsymbol{w} represents the local angular velocity of a material element of SmC and must satisfy

$$\dot{\boldsymbol{a}} = \boldsymbol{w} \times \boldsymbol{a}, \qquad \dot{\boldsymbol{c}} = \boldsymbol{w} \times \boldsymbol{c}, \qquad (2.2.21)$$

the smectic analogues of equation (2.1.4). Motivated by the static theory (see equations (6.70) and (6.90) in [68]), we take

$$t_{ij} = -p\delta_{ij} + \beta_l \varepsilon_{ljk} a_{k,i} - a_{k,i} \frac{\partial w}{\partial a_{k,j}} - c_{k,i} \frac{\partial w}{\partial c_{k,i}} + \tilde{t}_{ij}, \qquad (2.2.22)$$

$$l_{ij} = \beta_k a_k \delta_{ij} - \beta_i a_j + \varepsilon_{ikl} \left(a_k \frac{\partial w}{\partial a_{l,j}} + c_k \frac{\partial w}{\partial c_{l,j}} \right) + \tilde{l}_{ij}, \qquad (2.2.23)$$

where \tilde{t}_{ij} and \tilde{l}_{ij} denote dynamic contributions to stress and couple stress, respectively. Following a similar procedure to that outlined for nematics, the viscous terms are taken to be functions of a_i , c_i , w_i and $v_{i,j}$, with frame-indifference requiring the dependences to instead be upon the variables a_i , c_i , A_i , C_i and D_{ij} , where

$$A_i = \dot{a}_i - W_{ij}a_j, \qquad C_i = \dot{c}_i - W_{ij}c_j,$$
 (2.2.24)

with

$$D_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i}), \qquad W_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i}).$$
 (2.2.25)

The vectors \boldsymbol{A} and \boldsymbol{C} denote the co-rotational time flux of the vectors \boldsymbol{a} and \boldsymbol{c} , respectively; these are analogous to the vector \boldsymbol{N} as defined in equation (2.1.8) above. The terms D_{ij} and W_{ij} are simply the components of the velocity gradient and vorticity tensors, and we note the change in symbol for the velocity gradient tensor from A_{ij} to D_{ij} : this is to avoid any notational confusion with the corotational time flux of the vector \boldsymbol{a} , i.e. \boldsymbol{A} as given in equation (2.2.24) above. Working backwards with an analogous argument to that used in the derivation of equation (2.1.8), it is readily shown that

$$A = \boldsymbol{\omega} \times \boldsymbol{a}, \qquad C = \boldsymbol{\omega} \times \boldsymbol{c}, \qquad (2.2.26)$$

with $\boldsymbol{\omega}$ denoting the relative angular velocity as in (2.1.2).

Given the assumed form of the viscous stress and viscous couple stress in (2.2.22) and (2.2.23), the rate-of-work postulate of equation (2.2.20) may be expressed in the form

$$\mathcal{D} = \tilde{t}_{ij} v_{i,j} + \tilde{l}_{ij} w_{i,j} - w_i \varepsilon_{ijk} \tilde{t}_{kj} \ge 0.$$
(2.2.27)

As outlined in reference [41], this inequality combined with the assumption that \tilde{l}_{ij} is a function of the above named variables (and therefore not $w_{i,j}$) leads to the requirement

$$\tilde{l}_{ij} = 0,$$
(2.2.28)

reducing the inequality (2.2.27) to

$$\mathcal{D} = \tilde{t}_{ij} v_{i,j} - w_i \varepsilon_{ijk} \tilde{t}_{kj} \ge 0.$$
(2.2.29)

Assuming that \tilde{t}_{ij} is a linear function of A_i , C_i and D_{ij} and that the requirement that w, the elastic energy, be frame-indifferent, the dependence of \tilde{t}_{ij} on the variables listed above can easily be shown to require that \tilde{t}_{ij} must then be an isotropic function of its variables [66, p.22]. It can then be shown [70] that the viscous stress consists of forty-one terms. Four of these are found to equate to zero via use of the dissipation inequality (2.2.29) and another five may be shown to be linearly dependent on others, reducing the total to thirty-two. Finally, the use of Onsager relations allows us to reduce this number further to twenty. The final form of the viscous stress is given via

$$\tilde{t}_{ij} = \tilde{t}^s_{ij} + \tilde{t}^{as}_{ij},$$
(2.2.30)

where \tilde{t}^s_{ij} denotes the symmetric part

$$\begin{split} \hat{t}_{ij}^{s} &= \mu_{0} D_{ij} + \mu_{1} a_{l} D_{l}^{a} a_{i} a_{j} + \mu_{2} (D_{i}^{a} a_{j} + D_{j}^{a} a_{i}) + \mu_{3} c_{k} D_{k}^{c} c_{i} c_{j} + \mu_{4} (D_{i}^{c} c_{j} + D_{j}^{c} c_{i}) \\ &+ \mu_{5} c_{k} D_{k}^{a} (a_{i} c_{j} + c_{i} a_{j}) + \lambda_{1} (A_{i} a_{j} + A_{j} a_{i}) + \lambda_{2} (C_{i} c_{j} + C_{j} c_{i}) \\ &+ \lambda_{3} c_{k} A_{k} (a_{i} c_{j} + c_{i} a_{j}) + \kappa_{1} (D_{i}^{a} c_{j} + D_{j}^{a} c_{i} + D_{i}^{c} a_{j} + D_{j}^{c} a_{i}) \\ &+ \kappa_{2} \left\{ a_{k} D_{k}^{a} (a_{i} c_{j} + c_{i} a_{j}) + 2a_{l} D_{l}^{c} a_{i} a_{j} \right\} \\ &+ \kappa_{3} \left\{ c_{k} D_{k}^{c} (a_{i} c_{j} + c_{i} a_{j}) + 2a_{k} D_{k}^{c} c_{i} c_{j} \right\} + \tau_{1} (C_{i} a_{j} + C_{j} a_{i}) \\ &+ \tau_{2} (A_{i} c_{j} + A_{j} c_{i}) + 2 \tau_{3} c_{k} A_{k} a_{i} a_{j} + 2 \tau_{4} c_{k} A_{k} c_{i} c_{j}, \end{split}$$

and \tilde{t}^{as}_{ij} is the anti-symmetric part

$$\tilde{t}_{ij}^{as} = \lambda_1 (D_j^a a_i - D_i^a a_j) + \lambda_2 (D_j^c c_i - D_i^c c_j) + \lambda_3 c_k D_k^a (a_i c_j - c_i a_j) + \lambda_4 (A_j a_i - A_i a_j) + \lambda_5 (C_j c_i - C_i c_j) + \lambda_6 c_k a_k (a_i c_j - c_i a_j) + \tau_1 (D_j^a c_i - D_i^a c_j) + \tau_2 (D_j^c a_i - D_i^c a_j) + \tau_3 a_l D_k^a (a_i c_k - c_i a_j) + \tau_4 c_k D_k^c (a_i c_j - c_i a_j) + \tau_5 (A_j c_i - A_i c_j + C_j a_i - C_i a_j),$$
(2.2.31b)

where we have introduced the notation

$$D_i^a = D_{ij}a_j, \qquad D_i^c = D_{ij}a_j.$$
 (2.2.32)

The twelve viscosity coefficients μ_0 to μ_5 and λ_1 to λ_6 are associated with dynamic stress contributions even in the vector \boldsymbol{c} ; the remaining eight viscosities, τ_1 to τ_5

and κ_1 to κ_3 , are associated with those terms which are odd in c.

Some of the above expressions may be written in a more convenient fashion via certain manipulations. Without going into detail, we note that the intrinsic torque arising from equation (2.2.31b) may be expressed in the form

$$\varepsilon_{ijk}\tilde{t}^{as}_{kj} = \varepsilon_{ijk}(a_j\tilde{g}^a_k + c_j\tilde{g}^c_k), \qquad (2.2.33)$$

on introducing the terms

$$\tilde{g}_i^a = -2\left(\lambda_1 D_i^a + \lambda_3 c_i c_j D_j^a + \lambda_4 A_i + \lambda_6 c_i c_j A_j + \tau_2 D_i^c + \tau_3 c_i a_j D_j^a\right), \qquad (2.2.34)$$

$$\tilde{g}_{i}^{c} = -2\left(\lambda_{2}D_{i}^{c} + \lambda_{5}C_{i} + \tau_{1}D_{i}^{a} + \tau_{5}A_{i}\right).$$
(2.2.35)

This allows for a reformulation of the dissipation inequality:

$$\mathcal{D} = \tilde{t}_{ij}^s D_{ij} - \tilde{g}_i^a A_i - \tilde{g}_i^c C_i \ge 0, \qquad (2.2.36)$$

which may be obtained in an analogous fashion to that used in deriving the result (2.1.39). This inequality can be used to derive restrictions on the smectic viscosity coefficients.

Similarly to the form given for nematics, the external body moment may be assumed to obey the relation

$$\rho K_i = \varepsilon_{ijk} (a_j G_k^a + c_k G_k^c), \qquad (2.2.37)$$

 G^a and G^c denoting the external body forces introduced in a similar way to those mentioned in the static theory [68]. Making use of the technique as employed in nematic theory, it is possible to employ certain constitutive relations, along with the above result for the external body moment and equation (2.2.28), apply these to the balance law for angular momentum (2.2.19), and thereby obtain the smectic analogue of equation (2.1.47) in the form of two coupled sets of component equations:

$$\left(\frac{\partial w}{\partial a_{i,j}}\right)_{,j} - \frac{\partial w}{\partial a_i} + G_i^a + \tilde{g}_i^a + \gamma a_i + \mu c_i + \varepsilon_{ijk}\beta_{k,j} = 0, \qquad (2.2.38a)$$

$$\left(\frac{\partial w}{\partial c_{i,j}}\right)_{,j} - \frac{\partial w}{\partial c_i} + G_i^c + \tilde{g}_i^c + \tau c_i + \mu a_i = 0, \qquad (2.2.38b)$$

where the scalar functions γ , μ , and τ , and the vector function β are Lagrange multipliers arising from constraints (2.2.3) and the Oseen constraint (2.2.5). In turn, these equations allow for convenient reformulation of the balance of linear momentum equation (2.2.18); viz.,

$$\rho \dot{v}_i = \rho f_i - \tilde{p}_{,i} + G^a_j a_{j,i} + G^c_j c_{j,i} + \tilde{g}^a_j a_{j,i} + \tilde{g}^c_j c_{j,i} + \tilde{t}_{ij,j}, \qquad (2.2.39)$$

where $\tilde{p} = p + w$, p denoting an arbitrary pressure arising from incompressibility.

2.3 Smectic A

The continuum theory of Stewart [69] will provide the model used for the description of smectic A liquid crystals, which will be the main focus of this thesis. This continuum theory allows for the separation of the director \boldsymbol{n} and the layer normal \boldsymbol{a} where many others do not. This decoupling was motivated by the work of Auernhammer *et al.* [5–7] and Soddemann *et al.* [65], which established that this phenonmenon does indeed occur for smectic A subjected to simple shear. The theory also incorporates the possibility of permeation between the smectic layers. Finally, the Oseen constraint on the layer normal \boldsymbol{a} as discussed above in Section 2.2.1 at equation (2.2.5) is not imposed. The theory is derived using principles identical to those used in the derivation of Ericksen-Leslie theory for nematics (another reason for the inclusion of a somewhat more detailed account of that derivation in Section 1.2.1 above), and is based on ideas used in a variety of treatises on smectic A dynamics, such as those of Martin et al. [45], de Gennes [21,23] and E [15].

Finally, we note that the layers are conveniently described by a scalar function Φ such that

$$\boldsymbol{a} = \frac{\nabla \Phi}{|\nabla \Phi|}.\tag{2.3.1}$$

For example, in an undistorted sample of SmA whose director and layer normal lie parallel to the z-axis, the layer function is given by $\Phi = z$, so that $\nabla \Phi = (0, 0, 1)$, $|\nabla \Phi| = 1$ and thus $\boldsymbol{a} = (0, 0, 1)$. This is a particularly trivial example: for samples exhibiting departure from equilibrium, $\nabla \Phi$ and its magnitude are generally nonconstant, giving rise to the possibility $\nabla \times \boldsymbol{a} \neq 0$ and requiring us to discard the Oseen constraint under general perturbations to the smectic layer structure. As discussed by Stewart [69], the phenomenon of permeation turns out to be intricately linked to Φ .

While the presentation of the theory to be outlined will follow the paper of

Stewart from which said theory is taken [69], a great deal of detail will be omitted in the interest of brevity.

2.3.1 Balance Laws

The balance laws as given in equations (2.2.14) - (2.2.16) once again allow us to write

$$\rho \dot{v}_i = \rho f_i + t_{ij,j}, \qquad (2.3.2)$$

and

$$\rho K_i + \varepsilon_{ijk} t_{kj} + l_{ij,j} = 0, \qquad (2.3.3)$$

where all the algebraic terms remain as before. A slightly altered rate-of-work postulate is required for smectic A:

$$\int_{\Omega} \mathcal{D} \, dV = \int_{\Omega} \rho(f_i v_i + K_i w_i) \, dV + \int_S (t_i v_i + l_i w_i + \dot{\Phi} \tau_i \nu_i) \, dA$$
$$- \frac{D}{Dt} \int_{\Omega} \left(\frac{1}{2} \rho v_i v_i + w_{\rm DS}\right) dV, \qquad (2.3.4)$$

where we find all the same physical quantities as in our previous rate-of-work postulates, as well as the terms w_{DS} corresponding to the smectic A energy energy density, which is that proposed by De Vita and Stewart [13] to be discussed below in Section 2.3.2 and $\dot{\Phi}\tau_i\nu_i$, the rate of work done by the layers at the boundary surface S as introduced by E [15]. Since Φ provides a description of the orientation of the smectic layers, $\dot{\Phi}$ is interpreted as their rate of displacement, with τ representing the permeation force at the bounding surface S applied to the layers in the volume Ω . Following a process analogous to that for SmC in Section 2.2.2 above, the equation (2.3.4) reduces for arbitrary volumes to the dissipation function,

$$\mathcal{D} = t_{ij}v_{i,j} + l_{ij}w_{i,j} - w_i\varepsilon_{ijk}t_{kj} + (\Phi\tau_i)_{,i} - \dot{w}_{\rm DS}, \qquad (2.3.5)$$

which is, as before, taken to be non-negative.

The energy will be assumed to take the form

$$w_{\rm DS} = w_{\rm DS}(n_i, n_{i,j}, a_i, a_{i,j}, \Phi_{,i}).$$
(2.3.6)

Given that \boldsymbol{a} may by derived directly from Φ , it is equally valid to suppose that the dependence of w_{DS} is only on \boldsymbol{n} , $\nabla \boldsymbol{n}$ and $\nabla \Phi$; however, it proves useful to consider contributions that can be expressed in terms of \boldsymbol{a} or Φ , or both. Following the argument put forward by Stewart, one finds the forms of the stress and couple stress tensors to be

$$t_{ij} = -p\delta_{ij} + |\nabla\Phi|a_i J_i - n_{k,i} \frac{\partial w_{\rm DS}}{\partial n_{k,j}} - a_{k,i} \frac{\partial w_{\rm DS}}{\partial a_{k,j}} + \tilde{t}_{ij}, \qquad (2.3.7)$$

$$l_{ij} = \varepsilon_{ikl} \left(n_k \frac{\partial w_{\rm DS}}{\partial n_{l,j}} + a_k \frac{\partial w_{\rm DS}}{\partial a_{l,j}} \right) + \tilde{l}_{ij}, \qquad (2.3.8)$$

respectively, where p is the usual arbitrary pressure arising from incompressibility, and \tilde{t}_{ij} and \tilde{l}_{ij} denote the viscous stress and viscous couple stress, respectively.

The permeation force $\boldsymbol{\tau}$ has components given by $\tau_i = -J_i$, where, for convenience, the vector \boldsymbol{J} is defined via

$$J_{i} = -\frac{\partial w_{\mathrm{A}}}{\partial \Phi_{,i}} + \frac{1}{|\nabla \Phi|} \left\{ \left(\frac{\partial w_{\mathrm{A}}}{\partial a_{j,k}} \right)_{,k} - \frac{\partial w_{\mathrm{A}}}{\partial a_{j}} \right\} (\delta_{ji} - a_{j}a_{i}).$$
(2.3.9)

The forms given above allow the dissipation inequality to be expressed in the form

$$\mathcal{D} = \tilde{t}_{ij} v_{i,j} + \tilde{l}_{ij} w_{i,j} - w_i \varepsilon_{ijk} \tilde{t}_{kj} - \dot{\Phi} J_{i,i} \ge 0.$$
(2.3.10)

This inequality, in an analogous fashion to those considered for the nematic and smectic A continuum descriptions, will be vital in the establishment of the appropriate constitutive equations in Section 2.3.3 below, imposing restrictions on the possible forms of dynamic contribution.

2.3.2 The Energy Density

In this section, we depart from the formulation set forth by Stewart, and instead present the energy density w_{DS} as provided by De Vita & Stewart [13], which takes the form

$$w_{\rm DS} = \frac{1}{2} K_1^a (\nabla \cdot \boldsymbol{a})^2 + \frac{1}{2} K_1^n (\nabla \cdot \boldsymbol{n} - s_0)^2 + \frac{1}{2} K_2 \nabla \cdot \{ (\boldsymbol{n} \cdot \nabla) \boldsymbol{n} - (\nabla \cdot \boldsymbol{n}) \boldsymbol{n} \} + \frac{1}{2} B_0 |\nabla \Phi|^{-2} (1 - |\nabla \Phi|)^2 + \frac{1}{2} B_1 \{ 1 - (\boldsymbol{n} \cdot \boldsymbol{a})^2 \} + B_2 (\nabla \cdot \boldsymbol{n}) (1 - |\nabla \Phi|^{-1}), \qquad (2.3.11)$$

where K_1^a , K_1^n , and K_2 are elastic constants and B_0 , B_1 , and B_2 are constant energy densities. The first term on the right-hand side is the energy associated with bending of the smectic layers; the second term is the splay energy, with s_0 denoting the spontaneous splay; the third term is the saddle-splay energy; the
fourth is the energy associated with layer compression/expansion; the fifth is the energy attributed to coupling between n and a; the sixth and final term is the energy due to coupling between splay and compression of the layers. This energy density provides a general description of the deformation of a lipid bilayer. Note that we will be concerned only with SmA liquid crystals with no polarisability, i.e. those which have no spontaneous splay. We will therefore assume $s_0 = 0$ in all that follows. In this case $K_2 = 0$ and $B_2 = 0$ [13, equation (10)], and thus the energy we require is given by

$$w_{\rm A} = \frac{1}{2} K_1^a (\nabla \cdot \boldsymbol{a})^2 + \frac{1}{2} K_1^n (\nabla \cdot \boldsymbol{n})^2 + \frac{1}{2} B_0 |\nabla \Phi|^{-2} (1 - |\nabla \Phi|)^2 + \frac{1}{2} B_1 \left\{ 1 - (\boldsymbol{n} \cdot \boldsymbol{a})^2 \right\}.$$
(2.3.12)

Note that, for completeness, the calculations presented in this section will retain all six of the material constants of $w_{\rm DS}$ above, as well as the spontaneous splay, while in subsequent sections it will be assumed that we are working with $w_{\rm A}$ unless it is explicitly stated otherwise.

A comprehensive account of the physical properties of the energy density in equation (2.3.11), as well as a range of applications to problems concerning the behaviour of lipid bilayers, may be found in the paper of De Vita and Stewart [13].

Some Useful Identities

For convenience, we present some identities for the energy and derivatives thereof to be utilised in subsequent sections. First, note that w_{DS} has the equivalent representation

$$w_{\rm DS} = \frac{1}{2} K_1^a (\delta_{ij} a_{i,j})^2 + \frac{1}{2} K_1^n (\delta_{ij} n_{i,j} - s_0)^2 + \frac{1}{2} K_2 \{ n_{j,i} n_{i,j} - (\delta_{ij} n_{i,j})^2 + n_i (n_{j,ij} + n_{j,ji}) \} + \frac{1}{2} B_1 \{ 1 - (\delta_{ij} n_i a_j)^2 \} + B_2 (\delta_{ij} n_{i,j}) \{ 1 - (\delta_{kl} \Phi_{,kl})^{-1/2} \}, \qquad (2.3.13)$$

from which it follows that

$$\left(\frac{\partial w_{\rm DS}}{\partial n_{i,j}}\right)_{,j} - \frac{\partial w_{\rm DS}}{\partial n_i} = K_1^n (\nabla \cdot n - s_0)_{,i} + \frac{1}{2} K_2 \left(n_{j,ij} - n_{j,ji}\right) + B_1 (\boldsymbol{n} \cdot \boldsymbol{a}) a_i + \frac{B_2}{|\nabla \Phi|^2} a_j \Phi_{,ji}.$$
(2.3.14)

This expression will often be employed in a simplified form where spontaneous splay is neglected and partial derivatives commute:

$$\left(\frac{\partial w_{\rm DS}}{\partial n_{i,j}}\right)_{,j} - \frac{\partial w_{\rm DS}}{\partial n_i} = K_1^n (\nabla \cdot n)_{,i} + B_1 (\boldsymbol{n} \cdot \boldsymbol{a}) a_i + \frac{B_2}{|\nabla \Phi|^2} a_j \Phi_{,ji}.$$
 (2.3.15)

Furthermore,

$$\left(\frac{\partial w_{\rm DS}}{\partial a_{i,j}}\right)_{,j} - \frac{\partial w_{\rm DS}}{\partial a_i} = K_1^a (\nabla \cdot \boldsymbol{a})_{,i} + B_1 (\boldsymbol{n} \cdot \boldsymbol{a}) n_i, \qquad (2.3.16)$$

and

$$\frac{\partial w_{\text{DS}}}{\partial \Phi_{,i}} = \frac{B_0}{|\nabla \Phi|^3} \left(|\nabla \Phi| - 1 \right) a_i + \frac{B_2}{|\nabla \Phi|^2} (\nabla \cdot \boldsymbol{n}) a_i.$$
(2.3.17)

Substitution of the latter two of these relations into equation (2.3.9) yields

$$J_{i} = \frac{1}{|\nabla\Phi|} \{ K_{1}^{a} (\nabla \cdot \boldsymbol{a})_{,j} - B_{1} (\boldsymbol{n} \cdot \boldsymbol{a}) n_{j} \} (\delta_{ij} + a_{j} a_{i}) + \frac{B_{0}}{|\nabla\Phi|^{3}} (1 - |\nabla\Phi|) a_{i}$$
$$- \frac{B_{2}}{|\nabla\Phi|^{2}} (\nabla \cdot \boldsymbol{n}) a_{i}$$
(2.3.18)

and thus

$$J_{i,i} = \frac{K_1^a}{|\nabla\Phi|^2} \Big\{ a_i \Phi_{,ij} \Big[a_k (\nabla \cdot \boldsymbol{a})_{,k} a_j - (\nabla \cdot \boldsymbol{a})_{,j} \Big] + |\nabla\Phi| \Big[a_{j,jii} - (a_j (\nabla \cdot \boldsymbol{a})_{,j} a_i)_{,i} \Big] \Big\}$$

+ $\frac{B_0}{|\nabla\Phi|^4} \Big\{ (2|\nabla\Phi| - 3) a_i \Phi_{,ij} a_j + |\nabla\Phi| (1 - |\nabla\Phi|) (\nabla \cdot \boldsymbol{a}) \Big\}$
+ $\frac{B_1}{|\nabla\Phi|^2} \Big\{ (\boldsymbol{n} \cdot \boldsymbol{a}) a_i \Phi_{,ij} \Big[(\boldsymbol{n} \cdot \boldsymbol{a}) a_j - n_j \Big] + |\nabla\Phi| \Big[(n_i - 2(\boldsymbol{n} \cdot \boldsymbol{a}) a_i) (\boldsymbol{n} \cdot \boldsymbol{a})_{,i}$
+ $(\boldsymbol{n} \cdot \boldsymbol{a}) (\nabla \cdot \boldsymbol{n} - (\boldsymbol{n} \cdot \boldsymbol{a}) (\nabla \cdot \boldsymbol{a})) \Big] \Big\}$
+ $\frac{B_2}{|\nabla\Phi|^3} \Big\{ (\nabla \cdot \boldsymbol{n}) a_i \Phi_{,ij} a_j - |\nabla\Phi| \Big[a_i (\nabla \cdot \boldsymbol{a})_{,i} + (\nabla \cdot \boldsymbol{n}) (\nabla \cdot \boldsymbol{a}) \Big] \Big\}.$ (2.3.19)

2.3.3 Constitutive Equations

The simplest constitutive assumption on $\dot{\Phi}$ is that it is linear in $J_{i,i}$, subject to the satisfaction of the dissipation inequality. This gives the permeation equation

$$\dot{\Phi} = -\lambda_p J_{i,i}, \qquad \lambda_p \ge 0, \tag{2.3.20}$$

where λ_p is the **permeation coefficient**, based upon concepts first discussed by Helfrich [29] in the study of cholesteric and smectic liquid crystals. This version of the permeation equation is clearly consistent with the special case as considered by E [15] as well as that calculated by Sukumaran & Ranganth [73] for smectic C.

Following arguments outlined above for nematics and smectic C, it is possible to establish that $\tilde{l}_{ij} = 0$, allowing us to express the dissipation inequality in the form

$$\mathcal{D} = \tilde{t}_{ij} v_{i,j} - w_i \varepsilon_{ijk} \tilde{t}_{kj} + \lambda_p (J_{i,i})^2 \ge 0, \qquad (2.3.21)$$

and, in a notation consistent with that introduced in previous sections, we conclude that \tilde{t}_{ij} is a function of a_i , n_i , N_i and A_{ij} , with frame-indifference requiring it to be a hemitropic function in the given variables. In fact, the symmetry of the SmA phase requires the dependence to be isotropic, as for nematics. The viscous stress \tilde{t}_{ij} will be taken to be invariant under simultaneous changes in sign $n \to -n$ and $a \to -a$.

Comment 2.1. Treating the director \boldsymbol{n} as if it were nematic in type should be feasible when it decouples from \boldsymbol{a} . When the layers are not allowed to distort independently of \boldsymbol{n} , results similar to those in equation (2.1.7) are available in terms of \boldsymbol{a} . Of course, one such example is to be found in the fixed layer Leslie-Stewart-Nakagawa theory for SmC, as given above in Section 2.2, in which the smectic analogue of \boldsymbol{N} was introduced. However, in the current framework, this analogy breaks down on no longer constraining \boldsymbol{n} and \boldsymbol{a} to be mutually parallel. It is therefore taken as a constitutive assumption that \tilde{t}_{ij} cannot be dependent upon \boldsymbol{A} as given in equation (2.2.24).

On supposing that t_{ij} has a linear dependence upon its variables, it follows that we may write

$$\tilde{t}_{ij} = X_{ij} + Y_{ijk}N_k + Z_{ijkl}A_{kl}, \qquad (2.3.22)$$

where the coefficients X_{ij} , Y_{ijk} , Z_{ijkl} are functions of a_i and n_i , and are required to be transversely isotropic by virtue of the symmetry of the SmA phase. This, in addition to the invariance under simultaneous changes in sign of \boldsymbol{n} and \boldsymbol{a} , the properties

$$A_{ii} = 0, \qquad A_{ij} = A_{ji}, \qquad n_i N_i = 0,$$
 (2.3.23)

the restrictions imposed by the dissipation inequality (2.3.21), and the use of Onsager relations, one arrives, after lengthy calculations [69] at the final form of

the viscous stress tensor

$$\tilde{t}_{ij} = \alpha_1 (n_k A_{kl} n_l) n_i n_j + \alpha_2 N_i n_j + \alpha_3 n_i N_j + \alpha_4 A_{ij} + \alpha_5 (n_j A_{ik} n_k + n_i A_{jk} n_k) + (\alpha_2 + \alpha_3) n_i A_{jk} n_k + \tau_1 (a_k A_{kl} a_l) a_i a_j + \tau_2 (a_i A_{jk} a_k + a_j A_{ik} a_k) + \kappa_1 (a_i N_j + N_i a_j + n_i A_{jk} a_k - n_j A_{ik} a_k) + \kappa_2 (n_k A_{kl} n_l) (n_i a_j + a_i n_j) + \kappa_3 \{ (n_k A_{kl} n_l) a_i a_j + (a_k A_{kl} a_l) n_i n_j \} + \kappa_4 \{ 2 (n_k A_{kl} a_l) n_i n_j + (n_k A_{kl} n_l) (a_i n_j + n_i a_j) \} + \kappa_5 \{ 2 (n_k A_{kl} a_l) a_i a_j + (a_k A_{kl} a_l) (n_i a_j + a_i n_j) \} + \kappa_6 (n_j A_{ik} a_k + n_i A_{jk} a_k + a_i A_{jk} n_k + a_j A_{ik} n_k).$$
(2.3.24)

Noting the anti-symmetric part of the viscous stress, it follows that

$$\varepsilon_{ijk}\tilde{t}_{kj} = \varepsilon_{ijk}n_j\tilde{g}_k, \qquad (2.3.25)$$

where

$$\tilde{g}_i = -(\alpha_3 - \alpha_2)N_i - (\alpha_2 + \alpha_3)A_{ij}n_j - 2\kappa_1 A_{ij}a_j.$$
(2.3.26)

It follows that the dissipation inequality (2.3.21) may be expressed in the form

$$\mathcal{D} = \tilde{t}_{ij}A_{ij} - N_i\tilde{g}_i + \lambda_p (J_{i,i})^2 \ge 0.$$
(2.3.27)

The form of \mathcal{D} as given in (2.3.27) suggests that we may also write

$$\tilde{t}_{ij} = \frac{1}{2} \frac{\partial \mathcal{D}}{\partial v_{i,j}},\tag{2.3.28}$$

provided the Onsager relations, as stated in [69, equations (3.21)-(3.24)], hold.

There are thirteen viscosity coefficients, and it proves instructive to consider certain special cases of the expression in equation (2.3.24) as a means of interpreting these viscosities physically. First, note that, if terms involving the layer normal \boldsymbol{a} are neglected and the Parodi relation for nematics (2.1.51) holds, the viscous stress takes the form

$$\tilde{t}_{ij} = \alpha_1 (n_k A_{kl} n_l) n_i n_j + \alpha_2 N_i n_j + \alpha_3 n_i N_j + \alpha_4 A_{ij} + \alpha_5 (n_j A_{ik} n_k + n_i A_{jk} n_k) + (\alpha_2 + \alpha_3) n_i A_{jk} n_k,$$

the coefficients α_1 to α_5 denoting the Leslie viscosities. One may therefore interpret these viscosities as being "nematic-like", with α_4 being related to usual Newtonian isotropic fluid viscosity η by $\alpha_4 = 2\eta$. Secondly, if instead the terms involving \boldsymbol{n} are neglected, the viscous stress takes the form

$$\tilde{t}_{ij} = \alpha_4 A_{ij} + \tau_1 (a_k A_{kl} a_l) a_i a_j + \tau_2 (a_i A_{jk} a_k + a_j A_{ik} a_k)$$

This is exactly the form known for from other descriptions of the SmA phase [15, 45], and coincides with the incompressible case as outlined by de Gennes & Prost [23, p.415] for a linearised description of planar samples. This will be explored further in Section 3.2 below. It follows that the viscosities τ_1 and τ_2 are "smectic-like". Finally, the coefficients κ_1 to κ_6 appear in contributions involving both \boldsymbol{a} and \boldsymbol{n} , so may be interpreted as "coupling terms", illustrating how the nematic-type and SmA-type modes of behaviour are linked.

2.3.4 The Dynamic Equations

From the balance laws (2.3.2), (2.3.3) and the incompressibility condition $v_{i,i} = 0$, it is possible to derive the main dynamic equations using the constitutive equations outlined above and the identity

$$\varepsilon_{ijk} \left(a_k \frac{\partial w_{\rm DS}}{\partial a_j} + a_{k,l} \frac{\partial w_{\rm DS}}{\partial a_{j,l}} + a_{l,k} \frac{\partial w_{\rm DS}}{\partial a_{l,j}} + a_k \frac{\partial w_{\rm DS}}{\partial n_j} + n_{k,l} \frac{\partial w_{\rm DS}}{\partial n_{j,l}} + n_{l,k} \frac{\partial w_{\rm DS}}{\partial a_{l,j}} + \Phi_{,k} \frac{\partial w_{\rm DS}}{\partial \Phi_{,j}} \right) = 0, \qquad (2.3.29)$$

derived from a modified version of the Ericksen identity for nematics [16,68] or SmC [41]. Details of the derivation, omitted here for brevity, may be found in reference [69]. The dynamic equations for SmA may be summarised as follows.

The layer normal \boldsymbol{a} is defined via a scalar function $\Phi(x, y, z, t)$, and satisfies

$$\boldsymbol{a} = \frac{\nabla \Phi}{|\nabla \Phi|}, \quad \text{i.e.}, \quad \boldsymbol{a}_i = \frac{\Phi_{,i}}{|\nabla \Phi|}.$$
 (2.3.30)

Further, the layer normal, along with the director \boldsymbol{n} , is a unit vector, so that the constraints

$$a_i a_i = 1$$
 and $n_i n_i = 1$ (2.3.31)

hold. Incompressibility requires that the velocity \boldsymbol{v} satisfies

$$v_{i,i} = 0. (2.3.32)$$

The balance of linear momentum equation takes the form

$$\rho \dot{v}_i = \rho f_i - \tilde{p}_{,i} + \tilde{g}_j n_{j,i} + G_j n_{j,i} + |\nabla \Phi| a_i J_{j,j} + \tilde{t}_{ij,j}, \qquad (2.3.33)$$

with ρ denoting the density, f_i the external body force per unit mass, $\tilde{p} = p + w_{\text{DS}}$, where p is the pressure and w_{DS} is the energy density, as discussed in Section 2.3.1 given by

$$w_{\rm DS} = \frac{1}{2} K_1^a (\nabla \cdot \boldsymbol{a})^2 + \frac{1}{2} K_1^n (\nabla \cdot \boldsymbol{n} - s_0)^2 + \frac{1}{2} K_2 \nabla \cdot \{ (\boldsymbol{n} \cdot \nabla) \boldsymbol{n} - (\nabla \cdot \boldsymbol{n}) \boldsymbol{n} \} + \frac{1}{2} B_0 |\nabla \Phi|^{-2} (1 - |\nabla \Phi|)^2 + \frac{1}{2} B_1 \{ 1 - (\boldsymbol{n} \cdot \boldsymbol{a})^2 \} + B_2 (\nabla \cdot \boldsymbol{n}) (1 - |\nabla \Phi|^{-1}), \qquad (2.3.11)$$

 \tilde{g}_i is as given in (2.3.26), G_i denote the components of the generalised external body force, which is related to the external body moment $\mathbf{K} = (K_i)$ per unit mass via

$$\rho K_i = \varepsilon_{ijk} n_j G_k, \qquad (2.3.34)$$

 \boldsymbol{J} is the negative of the permeative force $\boldsymbol{\tau}$, and has components as

$$J_{i} = -\frac{\partial w_{\rm DS}}{\partial \Phi_{,i}} + \frac{1}{|\nabla \Phi|} \left\{ \left(\frac{\partial w_{\rm DS}}{\partial a_{j,k}} \right)_{,k} - \frac{\partial w_{\rm DS}}{\partial a_{j}} \right\} (\delta_{ji} - a_{j}a_{i}),$$
(2.3.9)

and \tilde{t}_{ij} is the viscous stress, as given above in equation (2.3.24). Balance of angular momentum may be expressed in the form

$$\left(\frac{\partial w_{\rm DS}}{\partial n_{i,j}}\right)_{,j} - \frac{\partial w_{\rm DS}}{\partial n_i} + \tilde{g}_i + G_i = \lambda n_i, \qquad (2.3.35)$$

where λ is a Lagrange multiplier arising from the unit vector constraint on \boldsymbol{n} as given in equation (2.3.31), which can generally be either evaluated or manipulated on taking the scalar product of (2.3.35) with \boldsymbol{n} . Finally, the permeation equation is

$$\dot{\Phi} = -\lambda_p J_{i,i}, \qquad \lambda_p \ge 0, \tag{2.3.20}$$

where λ_p is the permeation coefficient.

Chapter 3

General Considerations for the Study of Flow Patterns in Smectic A Dynamic Theory

3.1 Introduction

In this chapter, we investigate a selection of properties and applications of Stewart's dynamic theory for SmA as outlined in Section 2.3 in the previous chapter. First, in Section 3.2, we show that the theory of Stewart reduces to a system of equations considered by de Gennes, provided the flow pattern considered satisfies certain conditions to be specified below. It will be seen, however, that this system must in general include an additional equation relating the director alignment to the component of velocity normal to the smectic layers. Next, a linear stability analysis of this system in the context of flow past a finite obstacle is presented in Section 3.3. In particular, it will be seen that the inclusion of this additional equation does not affect the stability properties of solutions in this framework. Section 3.4 is concerned with the derivation of a two-dimensional system of linear equations from Stewart's theory, incorporating all viscosity and energy terms. These allow for the study of a whole host of flow patterns, some elementary examples of which are outlined in Section 3.5. In section 3.6, we present a linear stability analysis of the system derived in Section 3.4, demonstrating via both analytical examinations and plots based on typical numerical values of SmA physical parameters, that instabilities in flow patterns of SmA are anticipated by Stewart's theory. The realisation of linear instability is found to be contingent upon the violation of a set inequalities, determined by the appropriate Routh-Hurwitz stability criteria (Appendix B), which involve the SmA material

parameters and the incident perturbative wave numbers.

3.2 An Important Simplification

In this section, it will be shown that the dynamic equations outlined above in Section 2.3.4 reduce to those considered by de Gennes in his seminal paper, "Viscous Flow in Smectic A Liquid Crystals" [22], provided that the flow pattern, and the consequent response thereto of the smectic, satisfies a particular set of assumptions. (The viscous flow equations of de Gennes are themselves derived as a simplification of the theory set forth by Martin *et al.* [45] under a set of physically pertinent assumptions similar to those to be considered below.) While de Gennes' equations do not take into account director motion, we show that this reduced form of Stewart's equations leads to an additional equation relating the component of velocity the perpendicular to the plane of the layers to the spatial gradient of the director across the sample. It will be shown that, in requiring such gradients to vanish, the resultant system is not valid for velocity profiles with zero (or at least vanishingly small) velocity perpendicular to the layers.

Consider a sample of SmA such that the layer normal a lies along the positive z-axis in an appropriately chosen Cartesian coordinate system. This corresponds to flat layers:

$$\Phi \equiv z \implies \boldsymbol{a} \equiv (0, 0, 1). \tag{3.2.1}$$

Let us assume that, on subjecting the system to flow, the director \boldsymbol{n} may deviate only a small amount from its unstrained alignment along the z-axis. More precisely, if θ denotes the angle between \boldsymbol{n} and the z-axis (and hence between \boldsymbol{n} and \boldsymbol{a} by equation (3.2.1)), terms of order θ^2 and above may be considered negligibly small in the calculations to follow.

Recall the balance of linear momentum equation from Section 2.3:

$$\rho \dot{v}_i = \rho f_i - \tilde{p}_{,i} + \tilde{g}_j n_{j,i} + G_j n_{j,i} + |\nabla \Phi| a_i J_{j,j} + \tilde{t}_{ij,j}.$$
(2.3.33)

Let us first consider flows in which body forces are absent, so that $f_i = G_i = 0$. Further, it is readily checked that $w_A = \mathcal{O}(\theta^2)$ and thus $\tilde{p} = p + \mathcal{O}(\theta^2)$. Equation (2.3.33) may then be written in the approximate form

$$\rho \dot{v}_i = -p_{,i} + \tilde{g}_j n_{j,i} + a_i J_{j,j} + \tilde{t}_{ij,j}.$$
(3.2.2)

The permeation equation, $\dot{\Phi} + \lambda_p J_{j,j} = 0$, reads $J_{j,j} = -v_z/\lambda_p$, which, on substi-

tuting into (3.2.2), leads to

$$\rho(\partial_t v_i + v_j \partial_j v_i) = -p_{,i} + \tilde{g}_j n_{j,i} - \frac{v_z a_i}{\lambda_p} + \tilde{t}_{ij,j}.$$
(3.2.3)

It is natural to expect that high velocities and velocity gradients would significantly affect the alignment of the sample, rendering our assumption that $\mathbf{n} \cdot \mathbf{a} \approx 1$ invalid. We therefore impose the requirements that flow is sufficiently slow and velocity gradients sufficiently small that the advection term $v_j \partial_j v_i$ may be neglected and $a_i v_z \approx n_i v_z$, and thus equation (3.2.3) may be approximated by

$$\rho \partial_t v_i = -p_{,i} + \tilde{g}_j n_{j,i} - \frac{v_z n_i}{\lambda_p} + \tilde{t}_{ij,j}.$$
(3.2.4)

Finally, if we take the often-employed symmetric approximation [80, 81]

$$\tilde{t}_{ij,j} \approx \sigma_{ij} = \alpha_4 A_{ij} + \tau_1 (a_k A_{kl} a_l) a_i a_j + \tau_2 (a_i A_{jk} a_k + a_j A_{ik} a_k), \qquad (3.2.5)$$

so that the physical properties that play a significant role lead to the elementary inclusion of only the isotropic and "smectic-like" viscosities, equation (3.2.4) reduces further to

$$\rho \partial_t v_i = \sigma_{ij,j} - p_{,i} - \frac{n_i v_z}{\lambda_p}, \qquad (3.2.6)$$

where the terms $\tilde{g}_j n_{j,i}$ vanish due to our neglect of the anti-symmetric part of the viscous stress in equation (3.2.5). (One could instead impose the additional constraint that spatial director gradients are negligibly small if it proved desirable to retain asymmetries in the viscous stress, though see Comment 3.1 below.) Equation (3.2.6) is exactly as in [22, equation (4)], provided one sets $2\nu_1 = \alpha_4$, $2\nu_1 = \alpha_4 + \tau_1 + 2\tau_2$, and $2\nu_3 = \alpha_4 + \tau_2$.

The angular momentum balance equations simply read

$$B_1 a_i = \lambda n_i \implies \lambda = B_1 + \mathcal{O}(\theta^2). \tag{3.2.7}$$

We have therefore shown that the dynamic equations of Stewart collapse to a reduced system of four equations in four continuum variables for a sample of SmA subject to the following set of physically motivated assumptions:

- 1. flat layers (though very slight deviations from this will still render equations (3.2.6) approximately valid).
- 2. No dislocations or other defects in the sample.
- 3. Sufficiently slow velocities to ensure little decoupling between n and a.

4. A symmetric viscous stress tensor.

This system reads

$$\rho \partial_t v_i = \sigma_{ij,j} - p_{,i} - \frac{n_i v_z}{\lambda_p}.$$
(3.2.6)

$$v_{i,i} = 0,$$
 (3.2.8)

Comment 3.1. Recall equation (2.3.19); when spontaneous splay is absent, it reads

$$J_{i,i} = \frac{K_1^a}{|\nabla\Phi|^2} \Big\{ a_i \Phi_{,ij} \Big[a_k (\nabla \cdot \boldsymbol{a})_{,k} a_j - (\nabla \cdot \boldsymbol{a})_{,j} \Big] + |\nabla\Phi| \Big[a_{j,jii} - (a_j (\nabla \cdot \boldsymbol{a})_{,j} a_i)_{,i} \Big] \Big\} \\ + \frac{B_0}{|\nabla\Phi|^4} \Big\{ (2|\nabla\Phi| - 3) a_i \Phi_{,ij} a_j + |\nabla\Phi| (1 - |\nabla\Phi|) (\nabla \cdot \boldsymbol{a}) \Big\} \\ + \frac{B_1}{|\nabla\Phi|^2} \Big\{ (\boldsymbol{n} \cdot \boldsymbol{a}) a_i \Phi_{,ij} \Big[(\boldsymbol{n} \cdot \boldsymbol{a}) a_j - n_j \Big] + |\nabla\Phi| \Big[(n_i - 2(\boldsymbol{n} \cdot \boldsymbol{a}) a_i) (\boldsymbol{n} \cdot \boldsymbol{a})_{,i} \\ + (\boldsymbol{n} \cdot \boldsymbol{a}) (\nabla \cdot \boldsymbol{n} - (\boldsymbol{n} \cdot \boldsymbol{a}) (\nabla \cdot \boldsymbol{a})) \Big] \Big\}.$$
(3.2.9)

It is readily observed that, under the assumptions of completely flat layers and very little decoupling of \boldsymbol{n} and \boldsymbol{a} , one arrives at $J_{i,i} \approx B_1 \theta_{,x}$, which, on substitution into the permeation equation, gives

$$v_z \approx -\lambda_p B_1 \theta_{,x},\tag{3.2.10}$$

providing a fifth governing equation relating the z-component of the velocity to the spatial variation of the director alignment. Imposing the strict equality $\mathbf{n} \equiv \mathbf{a}$ would require that either $\mathbf{n} = (0, 0, 1)$, from which $v_z \equiv 0$, or that \mathbf{a} is allowed to vary via

$$\Phi = z - u(x, y, z, t).$$

The former case restricts us to the study flows whose velocity components lie strictly in the xy-plane. In this case, equations (2.1.25) and (3.2.6) may be written

$$v_{x,x} + v_{y,y} = 0, (3.2.11)$$

$$\rho \partial_t v_x + p_{,x} = \frac{1}{2} \alpha_4 \left(v_{x,xx} + v_{x,yy} + v_{x,zz} \right) + \frac{1}{2} \tau_2 v_{x,zz}, \qquad (3.2.12)$$

$$\rho \partial_t v_y + p_{,y} = \frac{1}{2} \alpha_4 \left(v_{y,xx} + v_{y,yy} + v_{y,zz} \right) + \frac{1}{2} \tau_2 v_{y,zz}, \qquad (3.2.13)$$

$$p_{z} = \frac{1}{2}(\alpha_4 + \tau_2)(v_{x,zx} + v_{y,zy}) = 0.$$
(3.2.14)

In the latter case, we would then require a further governing equation relating u

to the other variables in the system, though the requirement $\boldsymbol{n} = \boldsymbol{a}$ to order θ would imply $u + \theta_{,x} \approx 0$.

It follows from this comment that, for de Gennes' equations to be a complete description of SmA subject to flow under assumptions 1-4 outlined above, they must be supplemented by equation (3.2.10), leading to a system of five equations in five variables.

The more general case of flows in which both n and a are allowed to vary with $n \neq a$ is considered below in Section 3.4.

3.3 Linear Stability Analysis of Flow Past a Finite Obstacle

We now examine the stability of a two-dimensional system of equations, derived from (2.1.25) and (3.2.6) above, governing rectilinear flow of a sample of SmA in the presence of an obstacle. Specifically, consider a finite barrier of unit length placed in the sample. The barrier is taken to lie along the z-axis with its centre at the origin, as outlined in reference [82]. In addition to the assumptions 1–4 outlined above, we impose steady flow and a sufficiently high aspect ratio to allow for the validity of a lubrication approximation (see [22] and Chapter 4). With the possible exception of the region in the immediate vicinity of the obstacle, flow within the xy-plane will be a straight line (in fact, we anticipate $v_z = 0$ in regions far from the obstacle, so for the most part flow is a straight line parallel to the xy-plane), and thus we may choose our axes such that there is no velocity component in the y-direction, and none of the terms has any y-dependence. In this case, the governing equations (3.2.6) and (3.2.8) reduce to

$$v_{x,x} + v_{z,z} = 0, (3.3.1)$$

$$p_{,x} = \nu_3 v_{x,zz}, \tag{3.3.2}$$

$$p_{,z} = -v_z/\lambda_p,\tag{3.3.3}$$

with $2\nu_3 = \alpha_4 + \tau_2$. Boundary conditions are given by

$$v_x(0,z) = \begin{cases} 0 & \text{when } |z| < 1/2, \\ v_0 & \text{when } |z| > 1/2, \end{cases} \qquad v_z(0,z) = 0. \tag{3.3.4}$$



Figure 3.1: Schematic representation of the obstacle problem, with the finite barrier of unit length located at the origin. See also references [75,82].

An exact solution for this problem has been found [82]:

$$v_x = v_0 + \frac{v_0}{2} \left\{ \operatorname{erf}\left(\frac{2z+1}{4\sqrt{\delta|x|}}\right) - \operatorname{erf}\left(\frac{2z-1}{4\sqrt{\delta|x|}}\right) \right\},\tag{3.3.5}$$

$$v_z = \pm \frac{v_0 \sqrt{\delta}}{\sqrt{\pi |x|}} \sinh\left(\frac{z}{4\delta |x|}\right) \exp\left(-\frac{4z^2 + 1}{16\delta |x|}\right),\tag{3.3.6}$$

where v_0 is the value of v_x far downstream of the obstacle, erf is the usual error function, defined via

$$\operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt,$$

and $\delta = \sqrt{\lambda_p \nu_3}$. The plus (minus) sign is taken for x < 0 (x > 0). The pressure p may be found by integrating (3.3.3) with respect to z and applying an appropriate boundary condition.

We now investigate the response of this system by imposing time-dependent perturbations to the known solutions of the form

$$\hat{v}_x = v_x + \varepsilon \exp\{\omega t + i(k_x x + k_z z)\},\tag{3.3.7}$$

$$\hat{v}_z = v_z + \zeta \exp\{\omega t + i(k_x x + k_z z)\},$$
(3.3.8)

$$\hat{p} = p + \varphi \exp\{\omega t + i(k_x x + k_z z)\},\tag{3.3.9}$$

where $k_x, k_z \in \mathbb{R}$. Substitution of these into the unsteady system

$$v_{x,x} + v_{z,z} = 0, (3.3.10)$$

$$\rho v_{x,t} + p_{,x} - \nu_3 v_{x,zz} = 0, \qquad (3.3.11)$$

$$\rho v_{z,t} + p_{,z} + \frac{v_z}{\lambda_p} = 0, \qquad (3.3.12)$$

leads to the linear system

$$\begin{bmatrix} ik_x & ik_z & 0\\ \omega\rho + \nu_3 k_z^2 & 0 & ik_x\\ 0 & \omega\rho - 1/\lambda_p & ik_z \end{bmatrix} \begin{bmatrix} \varepsilon\\ \zeta\\ \varphi \end{bmatrix} = \begin{bmatrix} 0\\ 0\\ 0 \end{bmatrix}.$$
 (3.3.13)

For non-trivial solutions, the determinant of the 3×3 matrix on the left-hand side of (3.3.13) must be zero [34], which leads to the condition

$$\omega = -\frac{1}{\rho(k_x^2 + k_z^2)} \left(\frac{k_x^2}{\lambda_p} + \nu_3 k_z^4\right).$$
(3.3.14)

Given that ρ , λ_p , $\nu_3 > 0$, it is clear that $\omega < 0$ for all k_x , k_z , and hence the solutions (3.3.5) and (3.3.6) to equations (3.3.1)–(3.3.3) are linearly stable to small oscillatory perturbations.

Comment 3.2. Including the equation $\theta_{,x} = -v_z/\lambda_p B_1$ and carrying out the same stability analysis for the resultant 4×4 system does not change this outcome: ω is exactly as given in (3.3.14).

The problem of flow past an obstacle will be discussed further in Section 4.3 below.

3.4 Linearising the Full System of Equations

Motivated by the stability properties displayed by solutions to the system of equations above, we wish to ascertain in a more general setting the linear stability of solutions for flow patterns and resultant configurations in Stewart's theory. It has already been shown by Stewart [69, Section 5] that, if one assumes the viscous stress to be of the form given above in equation (3.2.5) and a somewhat simplified energy density, a sample of planar-aligned SmA remains stable to small oscillatory perturbations of the form of those given in equations (3.3.7)-(3.3.9). It is as yet unknown whether the full system of equations which form Stewart's theory permits instability, and, if so, under what conditions on both the physical

parameters characterising the smectic, and the frequency and wave number of the perturbation such instability should arise. It is towards the aim of investigating such properties that the work of this section is directed.

As above, we consider a sample of SmA, initially in an unstrained configuration such that $\Phi \equiv z$ and $\mathbf{n} = \mathbf{a} \equiv (0, 0, 1)$, and subject to the following

- 1. The sample is free of defects and remains so in the presence of flow. Again, this requires sufficiently slow velocities, and small spatial gradients thereof.
- 2. The flow may be treated as two-dimensional, enabling a choice of axes such that

$$\boldsymbol{v} = (v_x(x, z, t), 0, v_z(x, z, t)), \qquad |v_x|, |v_z| \ll 1, \qquad (3.4.1)$$

for simplicity.

3. The director and layer normal are allowed to vary and, moreover, to do so independently of one another. We take

$$\Phi = z - u(x, z, t), \qquad |u| \ll 1, \qquad (3.4.2)$$

$$\boldsymbol{n} = (\theta(x, z, t), 0, 1), \qquad |\theta| \ll 1.$$
 (3.4.3)

Equation (3.4.2) suggests that

$$\nabla \Phi = (-u_{,x}, 0, 1 - u_{,z}), \qquad |\nabla \Phi| \approx 1 - u_{,z}, \tag{3.4.4}$$

from which

$$a \approx (-u_{,x}, 0, 1).$$
 (3.4.5)

Once again, we assume that body forces are absent. Stewart's equations may then be written in the form

$$n_i n_i = 1 + \mathcal{O}(\theta^2), \qquad (3.4.6)$$

$$v_{x,x} + v_{z,z} = 0,$$
 (3.4.7)

$$v_{x,x} + v_{z,z} = 0,$$
 (3.4.7)
 $\dot{\Phi} + \lambda_p J_{j,j} = 0,$ (3.4.8)

$$\rho \dot{v}_i = -p_{,i} + \Phi_i J_{j,j} + \tilde{g}_j n_{j,i} + \tilde{t}_{ij,j}, \qquad (3.4.9)$$

$$\left(\frac{\partial w_{\rm A}}{\partial n_{i,j}}\right)_{,j} - \frac{\partial w_{\rm A}}{\partial n_i} + \tilde{g}_i = \lambda n_i. \tag{3.4.10}$$

The vector $\tilde{\boldsymbol{g}} = (\tilde{g}_x, 0, \tilde{g}_z)$ is given by

$$\tilde{g}_x = -(\gamma_1 \theta_{,t} + \nu_1 v_{x,z} + \nu_2 v_{z,x}), \qquad (3.4.11)$$

$$\tilde{g}_z = (\gamma_1 + 2\nu_2)v_{x,x},$$
(3.4.12)

where

$$\nu_1 = \alpha_2 + \kappa_1, \qquad \nu_2 = \alpha_3 + \kappa_1, \qquad \gamma_1 = \alpha_3 - \alpha_2 = \nu_2 - \nu_1.$$
 (3.4.13)

Then, since we anticipate only small director gradients, it follows that the terms $\tilde{g}_j n_{j,i}$ are of a magnitude which allows us to treat them as negligibly small in equation (3.4.9). Making use of identity (2.3.18) in Section 2.3.2, one finds

$$\boldsymbol{J} = \left(B_1(\theta + u_{,x}) - K_1^a u_{,xxx}, 0, B_0 u_{,z}\right), \qquad (3.4.14)$$

$$\implies J_{i,i} = B_0 u_{,zz} + B_1(\theta_{,x} + u_{,xx}) - K_1^a u_{,xxxx}, \qquad (3.4.15)$$

while some tedious calculations yield

$$\tilde{t}_{xj,j} = \eta_1 v_{x,xx} + \eta_2 v_{x,zz} + \nu_1 \theta_{,tz}, \qquad (3.4.16)$$

$$\tilde{t}_{yj,j} = 0,$$
(3.4.17)

$$\tilde{t}_{zj,j} = \eta_3 v_{z,xx} + \eta_4 v_{z,zz} + \nu_2 \theta_{,tx}, \qquad (3.4.18)$$

where

$$2\eta_1 = \alpha_4 - \alpha_2 - \alpha_5 - \tau_2 - 2\kappa_6, \tag{3.4.19}$$

$$2\eta_2 = \alpha_4 - \alpha_2 + \alpha_5 + \tau_2 - 2\kappa_1 + 2\kappa_6, \qquad (3.4.20)$$

$$2\eta_3 = \alpha_2 + 2\alpha_3 + \alpha_4 + \alpha_5 + \tau_2 + 2(\kappa_1 + \kappa_6), \qquad (3.4.21)$$

$$2\eta_4 = 2\alpha_1 + \alpha_2 + 2\alpha_3 + \alpha_4 + 3\alpha_5 + 2\tau_1 + 3\tau_2 + 4(\kappa_2 + \kappa_3) + 8(\kappa_4 + \kappa_5) + 6\kappa_6.$$
(3.4.22)

Finally, if we take advective terms to be negligible as above, the balance of linear momentum equations read

$$\rho v_{x,t} + p_{,x} = \eta_1 v_{x,xx} + \eta_2 v_{x,zz} + \nu_1 \theta_{,tz}, \qquad (3.4.23)$$

$$p_{,y} = 0, (3.4.24)$$

$$\rho v_{z,t} + p_{,z} = \eta_3 v_{z,xx} + \eta_4 v_{z,zz} + \nu_2 \theta_{,tx} - K_1^a u_{,xxxx} + B_0 u_{,zz} + B_1 (\theta_{,x} + u_{,xx}).$$
(3.4.25)

On employing relation (2.3.15), it follows that the balance of angular momentum equations may be written

$$K_1^n \theta_{,xx} - B_1 u_{,x} - \gamma_1 \theta_{,t} - \nu_1 v_{x,z} - \nu_2 v_{z,x} = \lambda \theta, \qquad (3.4.26)$$

$$K_1^n \theta_{,xz} + B_1 + (\gamma_1 + 2\nu_2) v_{x,x} = \lambda.$$
(3.4.27)

Equation (3.4.27) provides us with an exact expression for λ , and, on substitution into (3.4.26), yields the relation

$$K_1^n \theta_{,xx} - B_1(\theta + u_{,x}) - \gamma_1 \theta_{,t} - \nu_1 v_{x,z} - \nu_2 v_{z,x} = \mathcal{O}(\theta^2).$$
(3.4.28)

Finally, the permeation equation may be written

$$v_z - u_{,t} = \lambda_p \left\{ K_1^a u_{,xxxx} - B_0 u_{,zz} - B_1(\theta_{,x} + u_{,xx}) \right\}.$$
 (3.4.29)

Equations (3.2.8), (3.4.23), (3.4.25), (3.4.28) and (3.4.29) provide a system of five equations in the five unknown variables p, v_x , v_z , θ and u. A detailed analysis of this system will be carried out in Section 3.6.

3.5 Flows Between Parallel Plates: Some Illustrative Examples

This section serves to illustrate some applications of the linearised two-dimensional system derived above, which consists of equations (3.6.1), (3.4.23), (3.4.25), (3.4.28) and (3.4.29). Via three simple examples, we show that the velocity profiles of flow parallel to the layers displays Newtonian behaviour in this limit, while flow normal to the layers leads to a plug-like velocity profile as derived by de Gennes [22]. We also establish solutions for the director profile and layer configurations via the equations for angular momentum balance and permeation.

3.5.1 Simple Shear Flow

Consider a sample of SmA confined between two infinite parallel plates placed at z = 0 and z = d. The sample is initially at rest, then, at a given moment, is subject to a simple shear induced by moving the top plate at a constant velocity v_0 along the x-axis. We ignore transients that may be induced by the initial acceleration of the top plate, and seek steady-state (i.e., time-independent) solutions for the velocity profile, pressure, director, and layer normal. It is natural to



Figure 3.2: Configuration for simple shear flow. The top plate is moved with a constant velocity v_0 , while the constant pressure gradient $G = p_{,x}$ is applied in the plane parallel to the smectic layers.

assume that the velocity takes the form

$$\boldsymbol{v} = (v(z), 0, 0),$$
 (3.5.1)

automatically satisfying requirement (3.2.8). The balance of linear momentum equations reduce to

$$p_{,x} = \eta_2 v''(z), \qquad p_{,y} = p_{,z} = 0,$$
 (3.5.2)

Then, with Φ and \boldsymbol{n} as given in (3.4.2) and (3.4.3), the equations governing angular momentum balance and permeation are, respectively,

$$K_1^n \theta_{,xx} = B_1(\theta + u_{,x}) + \nu_1 v'(z), \qquad (3.5.3)$$

$$K_1^a u_{,xxxx} = B_0 u_{,zz} + B_1(\theta_{,x} + u_{,xx}).$$
(3.5.4)

Equations (3.5.2) show that p is a function of x only, and, on integrating the first of these equations with respect to x, we see that

$$p = \eta_2 x v''(z) + f_1(z) \implies v'''(z) = -\frac{f_1'(z)}{\eta_2 x},$$

but, since v is a function of z only, it follows that $f'_1(z) = 0$ and thus $p_{,x} = G$ (say), a constant. Thus

$$v(z) = \frac{Gz^2}{2\eta_2} + b_1 z + b_2, \qquad (3.5.5)$$

where the constants b_1 and b_2 may be determined by imposing no-slip conditions at the bounding plates, viz., v(0) = 0, $v(d) = v_0$; from this, we have

$$v(z) = \frac{Gz(z-d)}{2\eta_2} + \frac{v_0 z}{d}.$$
(3.5.6)

Note that this is exactly the velocity profile one finds when analysing the same problem for an isotropic Newtonian fluid with viscosity η_2 . In order to determine the director profile and the layer displacement we must substitute this expression into equation (3.5.3) then solve this and equation (3.5.4) together. For instance, if it is assumed that the director alignment and layer displacement do not vary along the x-direction and the layer normal is fixed, we obtain

$$\theta = -\frac{\nu_1 v'(z)}{B_1} = \frac{G\nu_1(d-2z)}{2B_1\eta_2} - \frac{\nu_1 v_0}{B_1 d}, \qquad u \equiv u(z) = b_3 z + b_4, \tag{3.5.7}$$

for some constants b_3 and b_4 . The local layer normal remains undisturbed. Other configurations of the SmA may of course be possible under this simple shear flow, but for brevity we omit such explorations from this illustrative digression.

3.5.2 Plane Poiseuille flow

Here, we choose to fix two bounding plates at $z = \pm d$ and impose a constant pressure gradient $G = p_{,x}$ along the x-direction; assuming the velocity is as in (3.5.1), we arrive at the following relations for balance of linear momentum

$$v''(z) = G/\eta_2, \qquad p_{,y} = p_{,z} = 0.$$
 (3.5.8)

The boundary velocities are now v(-d) = v(d) = 0, so that

$$v(z) = \frac{G(z^2 - d^2)}{2\eta_2}.$$
(3.5.9)

The equations for angular momentum balance and permeation are then

$$K_1^n \theta_{,xx} = B_1(\theta + u_{,x}) + \frac{G\nu_1 z}{\eta_2}, \qquad (3.5.10)$$

$$K_1^a u_{,xxxx} = B_0 u_{,zz} + B_1 (\theta_{,x} + u_{,xx}).$$
(3.5.11)

Combining these yields

$$K_1^a u_{,xxxx} = B_0 u_{,zz} + K_1^n \theta_{,xxx}.$$
 (3.5.12)



Figure 3.3: Schematic demonstrating plane Poiseuille flow. The top and bottom plates are stationary and a constant pressure gradient $G = p_{,x}$ is applied in the *x*-direction.

There are a few possible cases here, of which we consider only the following three.

Case 1: Director Alignment Independent of x

We may solve equation (3.5.12) by assuming variables-separable solution for u of the form $u(x, z) = \varphi(x)\psi(z)$, which leads to the following eigenvalue problem:

$$\lambda_a^2 \frac{\varphi^{(4)}(x)}{\varphi(x)} = \frac{\psi''(z)}{\psi(z)} = \kappa, \qquad (3.5.13)$$

where $\lambda_a^2 = K_1^a/B_0$ and κ is some constant to be determined. We anticipate symmetry about the z-axis in the layer displacement u and director θ , so that u(x, z) = u(x, -z), and require that both remain finite as $x \to \pm \infty$, from which it readily follows that equations (3.5.13) yield non-trivial solutions only when $\kappa > 0$. The general solutions are

$$\varphi(x) = c_1 \sinh\left\{\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x\right\} + c_2 \cosh\left\{\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x\right\} + c_3 \sin\left\{\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x\right\} + c_4 \cos\left\{\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x\right\},\qquad(3.5.14)$$

$$\psi(z) = c_5 \sinh\left(\sqrt{\kappa}z\right) + c_6 \cosh\left(\sqrt{\kappa}z\right). \qquad (3.5.15)$$

Imposing the conditions that u is finite for all x and that u(x, z) = u(x, -z) yields

$$u(x,z) = \left\{ c_7 \sin\left[\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x \right] + c_8 \cos\left[\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x \right] \right\} \cosh\left(\sqrt{\kappa}z\right), \quad (3.5.16)$$

where $c_7 = c_3 c_6$, $c_8 = c_4 c_6$. The director alignment θ is then determined by differentiation with respect to x of our expression for u in (3.5.16) and substitution into equation (3.5.10), viz.,

$$\theta(x,z) = -\partial_x u - \frac{G\nu_1 z}{\eta_2 B_1}$$

$$= \left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} \left\{ c_8 \sin\left[\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x\right] - c_7 \cos\left[\left(\frac{\kappa}{\lambda_a^2}\right)^{1/4} x\right]\right\} \cosh\left(\sqrt{\kappa}z\right)$$

$$- \frac{G\nu_1 z}{\eta_2 B_1}.$$
(3.5.17)

Since the director alignment has been assumed independent of x, it follows that either

(i)
$$\kappa = 0$$
, or

(ii)
$$c_7 = c_8 = 0$$
.

Both cases correspond to constant u and therefore no change in the layer displacement, with the director simply a linear function of z.

Case 2: Layer Displacement Independent of x

This is equivalent to the assumption that the layer normal remains constant. The equations for angular momentum balance and permeation read

$$K_1^n \theta_{,xx} = B_1 \theta + \frac{G\nu_1 z}{\eta_2}, \qquad (3.5.18)$$

$$0 = B_0 u_{,zz} + B_1 \theta_{,x}. \tag{3.5.19}$$

From the latter of these, it is evident that $\theta_{x} = \theta_{x}(z) \implies \theta = x\theta_{x} + g_{1}(z)$. Substitution into (3.5.18) then yields

$$\theta = x\theta_{,x} + g_1(z) = \frac{G\nu_1 z}{\eta_2 B_1},$$
(3.5.20)

revealing that θ is a function of z only. Finally, one finds from equation (3.5.19) that u is a linear function of z.

Taken together, cases 1 and 2 reveal that the director is independent of x if and only if the layer displacement is also independent of x, and making either of these assumptions leads to the solution $\theta = G\nu_1 z/\eta_2 B_1$ as well as no change in the local layer normal.

Case 3: No Decoupling of n and a

In this case, $\theta + u_{,x} = 0$, and thus we may use separation of variables to obtain the solution (3.5.16) for u. However, angular momentum balance then requires

$$K_1^n \theta_{,xx} = -K_1^n u_{,xxx} = \frac{G\nu_1 z}{\eta_2}, \qquad (3.5.21)$$

leading to an immediate inconsistency. If instead one solves the angular momentum balance equation first, it follows that u must be an arbitrary linear function of z in order to preserve finiteness of u as $x \to \infty$. It then follows that $\theta \equiv 0$ and both the director and layer normal remain unchanged from their initial states.

3.5.3 Plug Flow

As a final example, consider a sample of SmA confined between two parallel plates, this time lying along the yz-plane at $x = \pm d$. Applying a constant pressure gradient $G = p_{z}$ and anticipating a velocity profile of the form

$$\boldsymbol{v} = (0, 0, v(x)), \tag{3.5.22}$$

we find that condition (3.2.8) holds and equations (3.4.23)-(3.4.25) may be written

$$p_{,x} = p_{,y} = 0, \qquad v''(x) - \frac{v(x)}{\delta_3^2} = \frac{G}{\eta_3},$$
 (3.5.23)

where $\delta_3 = \sqrt{\lambda_p \eta_3}$, while equations (3.4.28) and (3.4.29) reduce to

$$K_1^n \theta''(x) = B_1\{\theta(x) + u'(x)\} + \nu_2 v'(x)$$
(3.5.24)

d
$$\frac{v(x)}{\lambda_p} = K_1^a u^{(4)}(x) + B_1 \{\theta(x) + u'(x)\}',$$
 (3.5.25)

respectively. Note that we have assumed that θ and u are functions of x only.

The general solution of equation $(3.5.23)_3$ is

$$v(x) = \beta_1 \sinh(x/\delta_3) + \beta_2 \cosh(x/\delta_3) - \lambda_p G, \qquad (3.5.26)$$



Figure 3.4: Schematic diagram showing the geometry for plug flow. A constant pressure gradient $G = p_{,z}$ is applied in the z-direction, normal to the planar layers.

where the constants β_1 and β_2 are determined via the no-slip boundary conditions: $v(\pm d) = 0$, yielding

$$v(x) = \lambda_p G \left\{ \frac{\cosh(x/\delta_3)}{\cosh(d/\delta_3)} - 1 \right\}.$$
(3.5.27)

Note that this is exactly the velocity profile derived by de Gennes [22, equation (8)] for this problem. Differentiation of equation (3.5.24) with respect to x yields

$$B_1(\theta' + u'') = K_1^n \theta''' - \nu_2 v'',$$

which may be substituted into (3.5.25) to give

$$K_1^a u^{(4)} = K_1^n \theta^{\prime\prime\prime} - \nu_2 v^{\prime\prime} + v/\lambda_p, \qquad (3.5.28)$$

i.e.,

$$K_1^a(\theta + u')''' = (K_1^n + K_1^a)\theta''' + G\left\{\left(1 - \frac{\lambda_p\nu_2}{\delta_3^2}\right)\frac{\cosh(x/\delta_3)}{\cosh(d/\delta_3)} - 1\right\}.$$
 (3.5.29)

Integration of equation (3.5.25) three times with respect to x yields

$$K_1^a(\theta + u') = (K_1^a + K_1^n)\theta + G\left\{\frac{\delta_3(\delta_3^2 - \lambda_p \nu_2)\sinh(x/\delta)}{\cosh(d/\delta_3)} - \frac{x^3}{6}\right\} + \beta_3 x^2 + \beta_4 x + \beta_5,$$
(3.5.30)

for some constants β_3 , β_4 , β_5 . There are two cases to consider: one in which the director and layer normal are coincident, and the more general case in which they

are not.

Case 1: n = a

In this case the left-hand side, and thereby the right-hand side, of equation (3.5.30) is zero. One simply rearranges this relation to obtain

$$\theta = \frac{G}{K_1^a + K_1^n} \left\{ \frac{\delta_3(\lambda_p \nu_2 - \delta_3^2) \sinh(x/\delta_3)}{\cosh(d/\delta_3)} + \frac{x^3}{6} \right\} + \beta_6 x^2 + \beta_7 x + \beta_8. \quad (3.5.31)$$

It is reasonable to expect asymmetry in the director profile, so that θ is an odd function of x, leading us to conclude that $\beta_6 = \beta_8 = 0$. An anchoring condition at either boundary will serve to uniquely determine the constant β_7 . The function u is then given by rearranging and integrating $\theta + u' = 0$ to give

$$u = \frac{G}{K_1^a + K_1^n} \left\{ \frac{\delta_3^2(\delta_3^2 - \lambda_p \nu_2) \cosh(x/\delta_3)}{\cosh(d/\delta_3)} - \frac{x^4}{24} \right\} + \frac{\beta_7 x^2}{2} + \beta_9, \qquad (3.5.32)$$

where β_9 is an arbitrary constant.

Case 2: $n \neq a$

Substitution of equation (3.5.30) into (3.5.24) yields the differential equation

$$K_{1}^{n}\theta'' = \frac{B_{1}(K_{1}^{a} + K_{1}^{n})\theta}{K_{1}^{a}} + \left\{\frac{\delta_{3}(\delta_{3}^{2} - \lambda_{p}\nu_{2})}{K_{1}^{n}} + \frac{\lambda_{p}\nu_{2}}{\delta_{3}}\right\}\frac{GB_{1}\sinh(x/\delta_{3})}{\cosh(x/\delta_{3})} - \frac{GB_{1}x^{3}}{6K_{1}^{a}} + p_{1}x,$$
(3.5.33)

where, as in case 1 above, we have assumed that the director profile is such that $\theta(x) = -\theta(-x)$. Solving this equation for θ , we find that

$$\theta = \left\{ \frac{\delta_3^2(\delta_3^2 - \lambda_p \nu_2)}{K_1^a} + \lambda_p \nu_2 \right\} \frac{GK_1^a B_1 \delta_3 \sinh(x/\delta_3)}{\{K_1^a + K_1^n - B_1 \delta_3^2 (K_1^a + K_1^n)\} \cosh(d/\delta_3)} + p_2 \sinh\left\{ \sqrt{B_1 \left(\frac{1}{K_1^a} + \frac{1}{K_1^n}\right)} x \right\} + \frac{Gx^3}{6(K_1^a + K_1^n)} + p_3 x, \qquad (3.5.34)$$

where p_2 and p_3 are constants to be determined via anchoring conditions. Finally, a solution for u may be obtained by substitution of (3.5.34) into (3.5.30) and integrating with respect to x. Performing the integration, we obtain

$$u = \frac{\Gamma G \delta_3^2}{\cosh(d/\delta_3)} \cosh(x/\delta_3) + p_4 \cosh\left\{\sqrt{B_1\left(\frac{1}{K_1^a} + \frac{1}{K_1^n}\right)}x\right\} + \left\{\frac{K_1^n}{(K_1^a + K_1^n)} - 1\right\} \frac{Gx^4}{24K_1^a} + \frac{p_5x^2}{2} + p_6,$$
(3.5.35)

where

$$\Gamma = \frac{K_1^n B_1}{K_1^a K_1^n - B_1 \delta_3^2 (K_1^a + K_1^n)} \left[\frac{\delta_3^2 (\delta_3^2 - \lambda_p \nu_2)}{K_1^a} - \lambda_p \nu_2 \right] + \frac{\delta_3^2 - \lambda_p \nu_2}{K_1^a} \quad (3.5.36)$$

and

$$p_4 = \frac{K_1^n p_2}{K_1^a} \left\{ B_1 \left(\frac{1}{K_1^a} + \frac{1}{K_1^n} \right) \right\}^{-1/2},$$

while p_5 and p_6 are constants to be determined by suitable conditions on the layer displacement.

Note that a more detailed account of pressure-driven flow applied perpendicularly to the layered structure may be found in the work of Stewart et al. [72], in which the asymptotic properties of the fully nonlinear system are analysed and multiple boundary layers identified.

3.6 Linear Stability Analysis for the Full System

The theory of Stewart under the simplifying assumptions 1-4 in Section 3.4 above takes the approximate reduced form

$$v_{x,x} + v_{z,z} = 0, (3.6.1)$$

$$\rho v_{x,t} + \tilde{p}_{,x} = \eta_1 v_{x,xx} + \eta_2 v_{x,zz} + \nu_1 \theta_{,tz}, \qquad (3.6.2)$$

$$\rho v_{z,t} + \tilde{p}_{,z} = \eta_3 v_{z,xx} + \eta_4 v_{z,zz} + \nu_2 \theta_{,tx} - K_1^a u_{,xxxx} + B_0 u_{,zz} + B_1 (\theta_{,x} + u_{,xx}),$$
(3.6.3)

$$K_1^n \theta_{,xx} = B_1(\theta + u_{,x}) - (\gamma_1 \theta_{,t} + \nu_1 v_{x,z} + \nu_2 v_{z,x}), \qquad (3.6.4)$$

$$v_z - u_t = \lambda_p \{ K_1^a u_{,xxxx} - B_0 u_{,zz} - B_1(\theta_{,x} + u_{,xx}) \}, \qquad (3.6.5)$$

Following our approach in Section 3.3, we assume that we have a sample of SmA, either initially at rest and in a relaxed configuration or subject to a flow pattern such that equations (3.6.1)-(3.6.5) are valid. We therefore anticipate a velocity

profile of the form

$$\boldsymbol{v} = (v_x(x, z, t), 0, v_z(x, z, t)), \qquad (3.6.6)$$

while the director and layer normal are given by

$$\boldsymbol{n} = (\theta(x, z, t), 0, 1), \qquad \boldsymbol{a} = (-\partial_x u(x, z, t), 0, 1), \qquad |\theta|, |u| \ll 1, \quad (3.6.7)$$

with $\theta + \partial_x u \approx 0$. We wish to consider a set of oscillatory perturbations to the quantities v_x , v_z , p, θ , and u. Motivated by Section 5 in [69], in which solutions to a simplified version of this system was shown to be linearly stable to all such perturbations, we assume the perturbed quantities take the form

$$v_x^* = v_x + \hat{v}_x \exp\{\omega t + i(q_x x + q_z z)\},$$
(3.6.8)

$$v_z^* = v_z + \hat{v}_z \exp\{\omega t + i(q_x x + q_z z)\}, \qquad (3.6.9)$$

$$p^* = p + \hat{p} \exp\{\omega t + i(q_x x + q_z z)\}, \qquad (3.6.10)$$

$$\theta^* = \theta + \hat{\theta} \exp\{\omega t + i(q_x x + q_z z)\}, \qquad (3.6.11)$$

$$u^* = u + \hat{u} \exp\{\omega t + i(q_x x + q_z z)\}, \qquad (3.6.12)$$

where the amplitudes of the perturbations denoted by hats have modulus $\ll 1$ and $q_x, q_z \in \mathbb{R}$ are wave numbers making up the wave vector $\boldsymbol{q} = (q_x, 0, q_z)$. Substitution of these quantities into the dynamic equations (3.6.1)–(3.6.5) leads to a 5 × 5 linear system of the form $\Lambda_{ij}\xi_j = 0$, where

$$[\Lambda_{ij}] = \begin{bmatrix} 0 & 0 & 0 & q_x & q_z \\ iq_x & -iq_z\nu_1\omega & 0 & X & 0 \\ iq_z & -iq_x(B_1 + \nu_2\omega) & Q & 0 & Y \\ 0 & B_1 + K_1^n q_x^2 + \gamma_1\omega & iB_1q_x & i\nu_1q_z & i\nu_2q_z \\ 0 & i\lambda_p B_1q_x & -(\omega + \lambda_p Q) & 0 & 1 \end{bmatrix}, \quad (3.6.13)$$

with

$$X = \rho\omega + \eta_1 q_x^2 + \eta_2 q_z^2, \tag{3.6.14}$$

$$Y = \rho\omega + \eta_3 q_x^2 + \eta_4 q_z^2, \qquad (3.6.15)$$

$$Q = K_1^a q_x^4 + B_0 q_z^2 + B_1 q_x^2, (3.6.16)$$

and

$$\boldsymbol{\xi} = \left(\hat{p}, \, \hat{\theta}, \, \hat{u}, \, \hat{v}_x, \, \hat{v}_z\right)^T. \tag{3.6.17}$$

This linear system yields non-trivial solutions for the quantities making up the entries of the vector $\boldsymbol{\xi}$ provided the determinant of the matrix $[\Lambda_{ij}]$ is zero. That is,

$$0 = q_x^2 \Big\{ Y \left[\left(B_1 + K_1^n q_x^2 + \gamma_1 \omega \right) (\omega + \lambda_p Q) - \lambda_p B_1^2 q_x^2 \right] \\ + q_x^2 \nu_2 \left[\lambda_p Q B_1 - (B_1 + \nu_2 \omega) (\omega + \lambda_p Q) \right] \\ - B_1 q_x^2 (B_1 + \nu_2 \omega) + Q \left(B_1 + K_1^n q_x^2 + \gamma_1 \omega \right) \Big\} \\ + q_x^2 q_z^2 \Big\{ \nu_1 \left[(B_1 + \nu_2 \omega) (\omega + \lambda_p Q) - \lambda_p Q B_1 \right] + \nu_1 \left[\nu_2 (\omega^2 + \lambda_p Q \omega) + B_1 \omega \right] \Big\} \\ + q_z^2 \Big\{ X \left[\left(B_1 + K_1^n q_x^2 + \gamma_1 \omega \right) (\omega + \lambda_p Q - \lambda_p B_1^2 q_x^2) \right] \\ - q_z^2 \nu_1^2 \left(\omega^2 + \lambda_p Q \omega \right) \Big\}.$$
(3.6.18)

After some tedious but routine algebraic manipulation, equation (3.6.18) may be written in the form

$$\omega^3 + p_1 \omega^2 + p_2 \omega + p_3 = 0, \qquad (3.6.19)$$

where

$$\begin{split} \rho\gamma_{1}q^{2}p_{1} &= \gamma_{1}\left\{(\eta_{1}+\eta_{4})q_{x}^{2}q_{z}^{2}+\eta_{2}q_{z}^{4}+\eta_{3}q_{x}^{4}\right\} \\ &+ \rho q^{2}\left(B_{1}+K_{1}^{n}q_{x}^{2}+\gamma_{1}\lambda_{p}Q\right)-\left(\nu_{1}q_{z}^{2}-\nu_{2}q_{x}^{2}\right)^{2}, \quad (3.6.20) \\ \rho\gamma_{1}q^{2}p_{2} &= \left\{(\eta_{1}+\eta_{4})q_{x}^{2}q_{z}^{2}+\eta_{2}q_{z}^{4}+\eta_{3}q_{x}^{4}\right\}\left(B_{1}+K_{1}^{n}q_{x}^{2}+\gamma_{1}\lambda_{p}Q\right) \\ &+ \rho\lambda_{p}q^{2}\left\{B_{1}\left(K_{1}^{a}q_{x}^{4}+B_{0}q_{z}^{2}\right)+QK_{1}^{n}q_{x}^{2}\right\}-\lambda_{p}Q\left(\nu_{1}q_{z}^{2}-\nu_{2}q_{x}^{2}\right)^{2} \\ &+ q_{x}^{2}\left[\gamma_{1}Q+2B_{1}\left(\nu_{1}q_{z}^{2}-\nu_{2}q_{x}^{2}\right)^{2}\right] \quad (3.6.21) \\ \rho\gamma_{1}q^{2}p_{3} &= \lambda_{p}\left\{(\eta_{1}+\eta_{4})q_{x}^{2}q_{z}^{2}+\eta_{2}q_{z}^{4}+\eta_{3}q_{x}^{4}\right\}\left\{B_{1}\left(K_{1}^{a}q_{x}^{4}+B_{0}q_{z}^{2}\right)+QK_{1}^{n}q_{x}^{2}\right\}, \end{split}$$

on introducing the notation $q^2 = q_x^2 + q_z^2$. The criteria for stability are simply the Routh-Hurwitz conditions for a cubic polynomial (see Appendix B): for the zeros of equation (3.6.19) to lie in the left half-plane, we require:

$$p_1 > 0, \qquad p_3 > 0, \qquad p_1 p_2 > p_3.$$
 (3.6.23)

(3.6.22)

Since $\rho \gamma_1 q^2 > 0$, these criteria are equivalent to

$$0 < \gamma_{1} \{ (\eta_{1} + \eta_{4}) q_{x}^{2} q_{z}^{2} + \eta_{2} q_{z}^{4} + \eta_{3} q_{x}^{4} \} + \rho q^{2} (B_{1} + K_{1}^{n} q_{x}^{2} + \gamma_{1} \lambda_{p} Q) - (\nu_{1} q_{z}^{2} - \nu_{2} q_{x}^{2})^{2}, \qquad (3.6.24) 0 < \{ \lambda_{p} [(\eta_{1} + \eta_{4}) q_{x}^{2} q_{z}^{2} + \eta_{2} q_{z}^{4} + \eta_{3} q_{x}^{4}] + q_{x}^{2} \} \{ B_{1} (K_{1}^{a} q_{x}^{4} + B_{0} q_{z}^{2}) + Q K_{1}^{n} q_{x}^{2} \}, (3.6.25) 0 < \{ \gamma_{1} [(\eta_{1} + \eta_{4}) q_{x}^{2} q_{z}^{2} + \eta_{2} q_{z}^{4} + \eta_{3} q_{x}^{4}] + \rho q^{2} (B_{1} + K_{1}^{n} q_{x}^{2} + \gamma_{1} \lambda_{p} Q) - (\nu_{1} q_{z}^{2} - \nu_{2} q_{x}^{2})^{2} \} \{ [(\eta_{1} + \eta_{4}) q_{x}^{2} q_{z}^{2} + \eta_{2} q_{z}^{4} + \eta_{3} q_{x}^{4}] (B_{1} + K_{1}^{n} q_{x}^{2} + \gamma_{1} \lambda_{p} Q) + \rho \lambda_{p} q^{2} [B_{1} (K_{1}^{a} q_{x}^{4} + B_{0} q_{z}^{2}) + Q K_{1}^{n} q_{x}^{2}] - \lambda_{p} Q (\nu_{1} q_{z}^{2} - \nu_{2} q_{x}^{2})^{2} + q_{x}^{2} [\gamma_{1} Q + 2B_{1} (\nu_{1} q_{z}^{2} - \nu_{2} q_{x}^{2})^{2}] \} - \rho \gamma_{1} q^{2} \{ \lambda_{p} [(\eta_{1} + \eta_{4}) q_{x}^{2} q_{z}^{2} + \eta_{2} q_{z}^{4} + \eta_{3} q_{x}^{4}] + q_{x}^{2} \} \{ B_{1} (K_{1}^{a} q_{x}^{4} + B_{0} q_{z}^{2}) + Q K_{1}^{n} q_{x}^{2} \}, \qquad (3.6.26)$$

respectively.

3.6.1 Analytical Examination of the Stability Criteria

If one or more of the conditions (3.6.24)-(3.6.26) is not satisfied for a given set of values of the physical parameters and incident wave numbers, the SmA structure and flow pattern will exhibit an instability. Let us first consider condition (3.6.24): setting $q_x = q \cos \psi$ and $q_z = q \sin \psi$ allows us to write this inequality in the form

$$\chi_2 q^4 + \chi_1 q^2 + \chi_0 > 0, \qquad (3.6.27)$$

where

$$\chi_{0} = \rho B_{1}, \qquad (3.6.28)$$

$$\chi_{1} = \gamma_{1} \left\{ (\eta_{1} + \eta_{4}) \sin^{2} \psi \cos^{2} \psi + \eta_{2} \sin^{4} \psi + \eta_{3} \cos^{4} \psi \right\}$$

$$+ \rho \left\{ K_{1}^{n} \cos^{2} \psi + \gamma_{1} \lambda_{p} \left(B_{0} \sin^{2} \psi + B_{1} \cos^{2} \psi \right) \right\}$$

$$- \left(\nu_{1} \sin^{2} \psi - \nu_{2} \cos^{2} \psi \right)^{2}, \qquad (3.6.29)$$

$$\chi_2 = \lambda_p \gamma_1 K_1^a \cos^4 \psi. \tag{3.6.30}$$

We know from references [13, equation (9)], [69, equation (3.1)], and [79, equation (B.9)] that

$$K_1^a \ge 0, \qquad B_1 \ge 0, \qquad \lambda_p \ge 0, \qquad \gamma_1 \ge 0,$$
 (3.6.31)

from which it follows that

$$\chi_0 \ge 0, \qquad \chi_2 \ge 0.$$
 (3.6.32)

From the inequalities in (3.6.32) and an application of Descartes' rule of signs (see Appendix B, Theorem B.1), we deduce that criterion (3.6.24) is always satisfied provided $\chi_1 \geq 0$. If, however, $\chi_1 < 0$, the polynomial yields either two or zero positive real values of q^2 , and thus either one or zero positive real value(s) for q. The roots of the polynomial on the left-hand side of inequality (3.6.27) are given by

$$q_0^2 = \frac{-\chi_1 \pm \sqrt{\chi_1^2 - 4\chi_0\chi_2}}{2\chi_2} \implies q_0 = \pm \sqrt{\frac{-\chi_1 \pm \sqrt{\chi_1^2 - 4\chi_0\chi_2}}{2\chi_2}}.$$
 (3.6.33)

Clearly q_0^2 is real and positive if and only if the following conditions hold

$$\chi_1^2 - 4\chi_0\chi_2 \ge 0 \text{ and } \chi_1 < 0. \tag{3.6.34}$$

Otherwise, the polynomial has no positive real roots, and inequality (3.6.27) is always satisfied. We are therefore guaranteed that the flow pattern will be unstable to small oscillatory perturbations provided conditions (3.6.34) are satisfied.

By further appeal to [13, equation (9)], it follows that the second stability criterion in equation (3.6.25) may be recast in the form

$$\lambda_p \left\{ (\eta_1 + \eta_4) q_x^2 q_z^2 + \eta_2 q_z^4 + \eta_3 q_x^4 \right\} + q_x^2 > 0, \qquad (3.6.35)$$

or, making further use of the substitutions $q_x = q \cos \psi$, $q_z = q \sin \psi$,

$$\lambda_p q^2 \left\{ (\eta_1 + \eta_4) \sin^2 \psi \cos^2 \psi + \eta_2 \sin^4 \psi + \eta_3 \cos^4 \psi \right\} + \cos^2 \psi > 0.$$
 (3.6.36)

The polynomial on the left-hand side of the above inequality has one positive real root $(q_0^+, \text{ say})$ if and only if

$$(\eta_1 + \eta_4)\sin^2\psi\cos^2\psi + \eta_2\sin^4\psi + \eta_3\cos^4\psi < 0, \qquad (3.6.37)$$

a criterion which guarantees instability. Otherwise, the second Routh-Hurwitz stability criterion (3.6.25) holds.

Applying this substitution to the final stability criterion leads to a polynomial

of order ten in q, which is of the form

$$\sigma_5 q^{10} + \sigma_4 q^8 + \sigma_3 q^6 + \sigma_2 q^4 + \sigma_1 q^2, \qquad (3.6.38)$$

where the coefficients are given by

$$\sigma_{5} = \frac{(\lambda_{p} K_{1}^{a} \cos^{4} \psi)^{2}}{2\rho \gamma_{1}} \Big\{ \gamma_{1} \Big[(\eta_{1} + \eta_{4}) \sin^{2} \psi \cos^{2} \psi + \eta_{2} \sin^{4} \psi + \eta_{3} \cos^{4} \psi \Big] \\ + \rho K_{1}^{n} \cos^{2} \psi - (\nu_{1} \sin^{2} \psi - \nu_{2} \cos^{2} \psi)^{2} \Big\}, \qquad (3.6.39)$$

$$\sigma_{4} = \frac{\lambda_{p}K_{1}^{a}\cos^{4}\psi}{(\rho\gamma_{1})^{2}} \Big\{ \Big[\gamma_{1} \left((\eta_{1} + \eta_{4})\sin^{2}\psi\cos^{2}\psi + \eta_{2}\sin^{4}\psi + \eta_{3}\cos^{4}\psi \right) \\ + \rho \left(\gamma_{1}\lambda_{p}(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi) + K_{1}^{n}\cos^{2}\psi \right) - \left(\nu_{1}\sin^{2}\psi - \nu_{2}\cos^{2}\psi \right)^{2} \Big] \\ \times \Big[\gamma_{1} \left((\eta_{1} + \eta_{4})\sin^{2}\psi\cos^{2}\psi + \eta_{2}\sin^{4}\psi + \eta_{3}\cos^{4}\psi \right) + \rho K_{1}^{n}\cos^{2}\psi \\ - \left(\nu_{1}\sin^{2}\psi - \nu_{2}\cos^{2}\psi \right)^{2} \Big] + \rho\gamma_{1} \Big[\gamma_{1}\lambda_{p} \left((\eta_{1} + \eta_{4})\sin^{2}\psi\cos^{2}\psi + \eta_{2}\sin^{4}\psi \right) \\ + \eta_{3}\cos^{4}\psi \Big) \Big(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi \Big) + \rho\lambda_{p}\cos^{2}\psi \Big(K_{1}^{a}B_{1}\cos^{2}\psi \\ + K_{1}^{n}(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi) \Big) - \lambda_{p} \Big(\nu_{1}\sin^{2}\psi - \nu_{2}\cos^{2}\psi \Big)^{2} \Big(B_{0}\sin^{2}\psi \\ + B_{1}\cos^{2}\psi \Big) + \gamma_{1}K_{1}^{a}\cos^{6}\psi \Big] \Big\},$$
(3.6.40)

$$\begin{aligned} \sigma_{3} &= \frac{\lambda_{p}K_{1}^{a}\cos^{4}\psi}{\rho\gamma_{1}^{2}} \left\{ 2\gamma_{1}B_{1} \left[(\eta_{1} + \eta_{4})\sin^{2}\psi\cos^{2}\psi + \eta_{2}\sin^{4}\psi + \eta_{3}\cos^{4}\psi \right] \\ &+ \rho B_{1} \left(\gamma_{1}\lambda_{p}B_{0}\sin^{2}\psi + K_{1}^{n}\cos^{2}\psi \right) - B_{1} \left(\nu_{1}\sin^{2}\psi - \nu_{2}\cos^{2}\psi \right)^{2} \\ &+ \gamma_{1}^{2}\cos^{2}\psi \left(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi \right) \right\} + \frac{1}{(\rho\gamma_{1})^{2}} \left\{ \gamma_{1} \left[(\eta_{1} + \eta_{4})\sin^{2}\psi\cos^{2}\psi + \eta_{2}\sin^{4}\psi + \eta_{3}\cos^{4}\psi \right] + \rho \left[\gamma_{1}\lambda_{p} \left(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi \right) + K_{1}^{n}\cos^{2}\psi \right] \\ &- \left(\nu_{1}\sin^{2}\psi - \nu_{2}\cos^{2}\psi \right)^{2} \right\} \left\{ \left[(\eta_{1} + \eta_{4})\sin^{2}\psi\cos^{2}\psi + \eta_{2}\sin^{4}\psi + \eta_{3}\cos^{4}\psi \right] \left[\gamma_{1}\lambda_{p} \left(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi \right) + K_{1}^{n}\cos^{2}\psi \right] \\ &+ \rho\lambda_{p}\cos^{2}\psi \left[K_{1}^{a}B_{1}\cos^{2}\psi + K_{1}^{n} \left(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi \right) \right] - \lambda_{p} \left(\nu_{1}\sin^{2}\psi - \nu_{2}\cos^{2}\psi \right)^{2} \right] \right\} \\ &+ 2B_{1} \left(\nu_{1}\sin^{2}\psi - \nu_{2}\cos^{2}\psi \right)^{2} \right] \right\} + \frac{\cos^{2}\psi}{\rho\gamma_{1}} \left\{ K_{1}^{a}K_{1}^{n}\cos^{6}\psi \\ &+ \lambda_{p} \left[(\eta_{1} + \eta_{4})\sin^{2}\psi\cos^{2}\psi + \eta_{2}\sin^{4}\psi + \eta_{3}\cos^{4}\psi \right] \left[K_{1}^{a}B_{1}\cos^{2}\psi \\ &+ K_{1}^{n} \left(B_{0}\sin^{2}\psi + B_{1}\cos^{2}\psi \right) \right] \right\}, \end{aligned}$$

$$\begin{aligned} \sigma_{2} &= \frac{B_{1}}{\rho \gamma_{1}^{2}} \Big\{ \left[(\eta_{1} + \eta_{4}) \sin^{2} \psi \cos^{2} \psi + \eta_{2} \sin^{4} \psi + \eta_{3} \cos^{4} \psi \right] \left[\gamma_{1} \lambda_{p} \left(B_{0} \sin^{2} \psi \right. \\ &+ B_{1} \cos^{2} \psi \right) + K_{1}^{n} \cos^{2} \psi \right] + \rho \lambda_{p} \cos^{2} \psi \left[K_{1}^{a} B_{1} \cos^{2} \psi + K_{1}^{n} \left(B_{0} \sin^{2} \psi \right. \\ &+ B_{1} \cos^{2} \psi \right) \right] - \lambda_{p} \left(\nu_{1} \sin^{2} \psi - \nu_{2} \cos^{2} \psi \right)^{2} \left(B_{0} \sin^{2} \psi + B_{1} \cos^{2} \psi \right) \\ &+ \cos^{2} \psi \left[\gamma_{1} K_{1}^{a} \cos^{4} \psi + 2B_{1} \left(\nu_{1} \sin^{2} \psi - \nu_{2} \cos^{2} \psi \right)^{2} \right] \Big\} \\ &+ \frac{1}{(\rho \gamma_{1})^{2}} \Big\{ \gamma_{1} \left[(\eta_{1} + \eta_{4}) \sin^{2} \psi \cos^{2} \psi + \eta_{2} \sin^{4} \psi + \eta_{3} \cos^{4} \psi \right] \\ &+ \rho \left[\gamma_{1} \lambda_{p} \left(B_{0} \sin^{2} \psi + B_{1} \cos^{2} \psi \right) + K_{1}^{n} \cos^{2} \psi \right] - \left(\nu_{1} \sin^{2} \psi - \nu_{2} \cos^{2} \psi \right)^{2} \Big\} \\ &\times \Big\{ B_{1} \left[(\eta_{1} + \eta_{4}) \sin^{2} \psi \cos^{2} \psi + \eta_{2} \sin^{4} \psi + \eta_{3} \cos^{4} \psi \right] + \rho \lambda_{p} B_{0} B_{1} \sin^{2} \psi \\ &+ \gamma_{1} \cos^{2} \psi \left(B_{0} \sin^{2} \psi + B_{1} \cos^{2} \psi \right) \Big\} - \frac{1}{\rho \gamma_{1}} \Big\{ \cos^{4} \psi \left[K_{1}^{a} B_{1} \cos^{2} \psi \right] \\ &+ K_{1}^{n} \left(B_{0} \sin^{2} \psi + B_{1} \cos^{2} \psi \right) \Big\} + \lambda_{p} B_{0} B_{1} \sin^{2} \psi \left[(\eta_{1} + \eta_{4}) \sin^{2} \psi \cos^{2} \psi \right] \\ &+ \eta_{2} \sin^{4} \psi + \eta_{3} \cos^{4} \psi \Big] \Big\}, \quad (3.6.42) \end{aligned}$$

$$\sigma_{1} = \frac{B_{1}^{2}}{\rho \gamma_{1}^{2}} \left\{ \sin^{2} \psi \left[\rho \lambda_{p} B_{0} + (\eta_{1} + \eta_{4}) \cos^{2} \psi + \eta_{2} \sin^{2} \psi \right] + (\eta_{3} + \gamma_{1}) \cos^{4} \psi \right\}.$$
 (3.6.43)

It follows that for sufficiently high values of q, the negativity of σ_5 is enough to guarantee violation of the third criterion, inequality (3.6.26), and destabilise the system. However, as will be seen in the following subsection, such values of

Parameter	Representative value	Parameter	Representative value
K_1^n, K_1^a	$5 \times 10^{-12} \mathrm{N}$	α_1	$-0.0060 \mathrm{Pas}$
B_0	$8.95 imes 10^7 { m N} { m m}^{-2}$	α_2	$-0.0812\mathrm{Pas}$
B_1	$4 \times 10^7 \mathrm{Nm^{-2}}$	α_3	$-0.0036\mathrm{Pas}$
λ_p	$10^{-16} \mathrm{m^2} (\mathrm{Pas})^{-1}$	α_4, τ_1, τ_2	$0.0652\mathrm{Pas}$
ρ	$10^3 \rm kg m^{-3}$	α_5	$0.0640\mathrm{Pas}$

Table 3.1: Representative values of the SmA physical parameters as discussed in the text.

q are several orders of magnitude higher than those at which the first criterion is violated for typical values of the parameters characterising the sample. It is interesting to note that the sign of each of the coefficients $\sigma_2, \ldots, \sigma_5$ is determined by the magnitudes of the viscosities ν_1 and ν_2 : it follows that the viscosities α_2 , α_3 and κ_1 play important roles in determining whether instabilities are possible in a given sample of SmA, which is exactly as found by examining the first criterion. This will be demonstrated in Subsection 3.6.2 below, in which the quantities p_1 , p_3 and $p_1p_2 - p_3$ are plotted against κ_1 , allowing for the observation of a critical value of this coefficient above which one would expect to observe the onset of instability.

3.6.2 Plotting the Stability Criteria

In what follows, we explicitly demonstrate the prediction of instability in SmA via a series of plots of the quantities on the left-hand sides of the Routh-Hurwitz criteria (3.6.24)–(3.6.26) for physically plausible values of the SmA material parameters. Consideration of various parameter regimes demonstrates that instabilities can occur for sufficiently high wave numbers, with the instability threshold being determined by the particular values of the physical constants as well as the direction of the wave vector. We note the parameter values as given in Table 3.1 courtesy of Stewart & Stewart [71] and the following inequalities due to Walker [79, Appendix B]:

$$2\kappa_1^2 \le (\alpha_4 + \tau_2)(\alpha_2 - \alpha_3), \tag{3.6.44}$$

$$0 \le \frac{1}{2}(\alpha_2 + \alpha_3) + \alpha_4 + \alpha_5 + \tau_2 + \kappa_2, \tag{3.6.45}$$

$$(\alpha_4 + \kappa_3)^2 \le 2\left(\alpha_4 + \frac{1}{2}\tau_1 + \tau_2\right)\left\{\alpha_1 + \alpha_2 + \alpha_3 + 2(\alpha_4 + 2\alpha_5)\right\}, \qquad (3.6.46)$$

$$2(\kappa_4 + \kappa_6)^2 \le \left\{ \frac{1}{2}(\alpha_2 + \alpha_3) + \alpha_4 + \alpha_5 + \tau_2 + \kappa_2 \right\} \left\{ \alpha_1 + \alpha_2 + \alpha_3 + 2(\alpha_4 + \alpha_5) \right\},$$
(3.6.47)

$$(\kappa_5 + \kappa_6)^2 \le \left(\alpha_4 + \frac{1}{2}\tau_1 + \tau_2\right) \left\{ \frac{1}{2}(\alpha_2 + \alpha_3) + \alpha_4 + \alpha_5 + \tau_2 + \kappa_2 \right\}, \quad (3.6.48)$$

$$\kappa_6^2 \le (\alpha_4 + \tau_2) \left\{ \frac{1}{2} (\alpha_2 + \alpha_3) + \alpha_4 + \alpha_5 \right\}, \qquad (3.6.49)$$

from which one readily deduces that, for this particular sample,

$$|\kappa_1| \le 0.0712 \,\mathrm{Pa\,s}, \qquad \kappa_2 \ge -0.1520 \,\mathrm{Pa\,s}, \qquad |\kappa_6| \le 0.1063 \,\mathrm{Pa\,s}, \qquad (3.6.50)$$

as well as

$$-0.1685 \operatorname{Pas} \le \kappa_3 \le 0.2989 \operatorname{Pas}, \qquad 0.0340 \operatorname{Pas} \le \kappa_4 \le 0.1660 \operatorname{Pas}, 0.0007 \operatorname{Pas} \le \kappa_5 \le 0.1920 \operatorname{Pas}. \qquad (3.6.51)$$

Plots may be found at the end of the chapter. In Figs. 3.5–3.12, each of the quantities which determine the stability of the system, p_1 , p_3 , and $p_1p_2 - p_3$, is plotted against increasing magnitude q of the wave vector for selected directions of said vector (determined by the value of the angle ψ) and physically permissible values of the viscosities κ_i ($i \in \{1, \ldots, 6\}$). Note that, in the interest of brevity, a vast number of plots produced for various different values of these viscosity coefficients have been omitted. These plots neither add to nor detract from the conclusions to be drawn below, and the data for these figures may be obtained from the author upon request. As was established by the analytical work set forth in the previous subsection, sufficiently high values of q will lead to destabilisation of the system. What is apparent from these figures is that the first quantity to become negative as q increases is p_1 , at least for physically realisable values of the material constants. Moreover, the threshold value of q at which this instability manifests itself varies substantially according to the wave vector's direction and the values of the SmA parameters.

The latter fact is demonstrated both by this set of plots and those contained in Figs. 3.13–3.17, in which the effect of varying the viscosity κ_1 across its permissible range upon the threshold value of q is shown. It is evident from our analytical considerations that this particular viscosity plays a significant role in determining whether the Routh-Hurwitz criteria remain satisfied via its presence in the apparent viscosities ν_1 and ν_2 , hence our choosing to focus on its role here. In the case of the first stability criterion, one sees a nonlinear dependence of p_1 upon κ_1 , so that, as q is increased, the curve cuts the line $p_1 = 0$ at two points; samples of SmA with values of κ_1 between these points will not exhibit any instability for this wave vector, but those with values either side of these two points will. Once q is increased past a certain threshold, however, p_1 is always negative and one would expect to see instabilities for all samples. Generally speaking, for a particular range of q, the viscosity κ_1 acts as something of a "destabilising agent" for the material, as anticipated by the forms of the stability conditions outlined above.

3.7 Conclusions and Discussion

This chapter has outlined the details of some important predictions regarding the behaviour of SmA arising from Stewart's dynamic theory. Firstly, it was shown that the hydrodynamic description due to de Gennes [22] arises straightforwardly as a simplification of this framework provided one imposes the set of physical assumptions exactly as outlined by de Gennes in the above referenced seminal work. However, the resultant system is supplemented by additional governing equation (relation (3.2.10) above). A linear stability analysis of this reduced model in two dimensions allows us to conclude that solutions are always predicted to be stable to small oscillatory perturbations; interpreting this in the context of two-dimensional flow past a finite obstacle, however, one readily sees that this system cannot provide a complete description of flow in SmA, as both further theoretical investigation (see Chapter 4) and experimental evidence [75] clearly point to the existence of linear instability of the flow pattern.

Going a step further, we have linearised the full system of equations comprising Stewart's theory and utilised the resultant system to describe some simple two-dimensional flow patterns. Moreover, a linear stability analysis using this system of equations yields regimes in which one could realistically expect to see instabilities arise, as demonstrated by examination of the three stability criteria (3.6.24)–(3.6.26). Given that these criteria will vary between different samples of SmA, it follows that while one sample may exhibit instabilities for one particular range of values of perturbative wave vector (or, indeed, none at all), another sample may exhibit these for a different range of such values. An example of this is demonstrated in the figures below, in which each of the quantities determining stability is plotted against physically allowable values of the viscosity coefficient κ_1 , where all other physical parameters were held at some constant value. Increasing the value of κ_1 was seen to cause an instability in the system. Such information could, in principle, be useful in the synthesis of materials exhibiting SmA phases for particular applications to which the stability (or instability) of the material is conducive.

While the particular case of flow past a finite obstacle in two-dimensions is revisited in Chapter 4, let us now outline some possible general lines for future research following on from the work set forth in this chapter. The linearised twodimensional simplification of Stewart's theory as derived in Section 3.4 could readily be be made three-dimensional by relaxing the assumption of two-dimensional flow independent of the y coordinate, by which we may readily hope to describe more complicated flow patterns via an approach not dissimilar to that employed in Section 3.5, though of course it may prove more convenient in certain cases to work in an alternative choice of coordinate system. Alternatively, it may be of interest to work in two dimensions but relax the assumptions leading to the linearity of the system. This may lead to significantly more complicated governing equations, potentially resulting in the need to appeal to computational methods to obtain the resultant flow pattern and SmA configuration; however, such a framework might enable us to consider flow in the presence of defects, for example an edge dislocation as considered in Chapter 6, for which a key assumption regarding the validity of the linear model, that of flat layers, must break down, at least in a small region of the sample. For a problem such as this, an asymptotic approach should enable one to utilise equations (3.2.8), (3.4.23), (3.4.25), (3.4.28)and (3.4.8) in regions sufficiently far from the defect core, but a modified nonlinear system in a small neighbourhood around this core.

Finally, we note that further investigation is necessary in order to obtain a fuller understanding of the stability properties of SmA. It may be of interest to investigate the effects of the application of an oscillatory electric and/or magnetic field upon the aforementioned stability criteria, and thereby whether the stability/instability threshold might be "tuned" by variation of the applied field strength, direction or frequency. Preliminary calculations in this direction have already been undertaken by the author, and it is hoped that such considerations will form the basis of future work. It may also prove fruitful to consider the effects of varying other viscosity coefficients on stability, and how each of these coefficients "balance" one another and/or the applied electric/magnetic field and thereby establish a complete picture of stability across the material's entire parameter space. Such principles may also be tentatively applied across a range of temperatures at which the given material exhibits its SmA phase, though one would have to look beyond this isothermal framework for a realistic study regarding this matter. As has already been mentioned, full characterisation of the stability properties of a complex material such as this can only be hoped for by analysis of the nonlinear system, and it is only by appeal to more sophisticated method that one can hope to fully describe the transition to instability and what may happen thereafter. It is hoped that the material in this chapter will provide a starting point from which such considerations and many more will naturally follow.





(b) $\kappa_1 = 0.07 \, \text{Pas.}$

Figure 3.5: Variation of the quantity p_1 with modulus q of the wave vector when $\psi = 0$. The threshold value of q which determines the onset of instability is increased by increasing the value of κ_1 : see Fig. 3.13. Note that for these plots, and for all others that follow unless otherwise stated, $\kappa_2 = \kappa_3 = \kappa_6 = -0.1 \text{ Pa} \text{ s}$, $\kappa_4 = \kappa_5 = 0.1 \text{ Pa} \text{ s}$.


(b) $\kappa_1 = 0.07 \, \text{Pas.}$

Figure 3.6: As in Fig. 3.5 with $\psi = \pi/8$. In this case, increasing the value of κ_1 has led to the instability no longer being visible for comparable and even significantly higher values of q.



(b) $\kappa_1 = 0.07 \, \text{Pas.}$

Figure 3.7: As in Fig. 3.5 with $\psi = \pi/4$. Altering the direction of the wave vector leads to no violation of the first Routh-Hurwitz criterion for values of q at which instability was previously realisable.



(b) $\kappa_1 = 0.07 \, \text{Pas.}$

Figure 3.8: As in Fig. 3.5 with $\psi = 3\pi/8$.



(b) $\kappa_1 = 0.07 \, \text{Pas.}$

Figure 3.9: Variation of the quantity p_3 with modulus q of the wave vector when $\psi = 0$.



(b) $\kappa_1 = 0.07 \, \text{Pas.}$

Figure 3.10: Variation of the quantity p_3 with modulus q of the wave vector when $\psi = \pi/4$.



(b) $\kappa_1 = 0.07 \,\mathrm{Pa\,s.}$

Figure 3.11: Variation of the quantity $p_1p_2 - p_3$ with modulus q of the wave vector when $\psi = \pi/8$.



(b) $\kappa_1 = 0.07 \, \text{Pas.}$

Figure 3.12: Variation of the quantity $p_1p_2 - p_3$ with modulus q of the wave vector when $\psi = \pi/4$.

Figure 3.13: The variation of p_1 against all permissible values of κ_1 for values of q increasing from $1-5 \times 10^6 \text{ m}^{-1}$; $\psi = \pi/2$.







Figure 3.15: (From previous page.) The variation of p_3 against all permissible values of κ_1 for various values of q.





(c) $q = 10^6 \,\mathrm{m}^{-1}$.

Figure 3.17: (From previous page.) The variation of $p_1p_2 - p_3$ against all permissible values of κ_1 for various values of q.

Chapter 4

A Two-Dimensional Lubrication Approximation

In this chapter, a preliminary investigation regarding a lubrication theory for SmA liquid crystals will be presented. In Section 4.1, we introduce dimensionless variables and thereby derive a system of lubrication equations, allowing for the approximation of equations (3.6.1)–(3.6.5) on omitting terms of sufficiently small magnitude. However, it will be shown in Section 4.2 that the process of truncation is somewhat more involved than in classical lubrication theory for both Newtonian and non-Newtonian fluids, with the nature of the leading-order system being intricately dependent upon the values of the many dimensionless combinations of physical parameters governing the system, in addition to the length and velocity scales characterising the problem. The ideas outlined here will then be demonstrated in Section 4.3, in which our simplified system is applied to the example of flow past a finite obstacle considered above in Section 3.3, enabling us to determine expressions for the director profile and layer displacement at leading order, as well as allowing for more in-depth considerations of the stability properties of the observed configuration by examining the higher-order systems of equations. The chapter will close with some concluding remarks and potential applications amenable to further deployment of this system, as well as ways in which it might be extended, in Section 4.4.

4.1 Non-Dimensionalisation of the Equations

Recall equations (3.6.1)–(3.6.5), restated here for ease of reference:

$$v_{x,x} + v_{z,z} = 0, (3.6.1)$$

$$\rho v_{x,t} + \tilde{p}_{,x} = \eta_1 v_{x,xx} + \eta_2 v_{x,zz} + \nu_1 \theta_{,tz}, \qquad (3.6.2)$$

$$\rho v_{z,t} + \tilde{p}_{,z} = \eta_3 v_{z,xx} + \eta_4 v_{z,zz} + \nu_2 \theta_{,tx}$$

$$V_{,t}^{a} + P_{,tx} + P_$$

$$-K_1^a u_{,xxxx} + B_0 u_{,zz} + B_1(\theta_{,x} + u_{,xx}), \qquad (3.6.3)$$

$$K_1^n \theta_{,xx} = B_1(\theta + u_{,x}) - (\gamma_1 \theta_{,t} + \nu_1 v_{x,z} + \nu_2 v_{z,x}), \qquad (3.6.4)$$

$$v_z - u_t = \lambda_p \{ K_1^a u_{,xxxx} - B_0 u_{,zz} - B_1 (\theta_{,x} + u_{,xx}) \}, \qquad (3.6.5)$$

Dimensionless quantities are introduced as follows:

$$x = Lx',$$
 $z = hz',$ $v_x = v_0 v_{x'},$ $v_z = \frac{v_0 h v_{z'}}{L}$ (4.1.1)

$$\tilde{p} = \frac{\eta_2 v_0 L}{h^2} p', \qquad t = \frac{Lt'}{v_0}, \qquad S = \frac{L}{\delta_3}, \qquad u = Lu', \qquad (4.1.2)$$

where L and h are characteristic length scales in the x-direction and z-direction, respectively, and are taken to satisfy

$$\varepsilon = \frac{h}{L} \ll 1 \tag{4.1.3}$$

(though see comments in the following section), and δ is a length scale given by

$$\delta_3 = \sqrt{\lambda_p \eta_3}.\tag{4.1.4}$$

Finally, we introduce the quantity β as

$$\beta = \frac{B_0}{B_1}.\tag{4.1.5}$$

With these scalings, equation (3.6.1) is readily shown to reduce to

$$v_{x,x} + v_{z,z},$$
 (4.1.6)

where the primes have been immediately dropped for convenience. The dimensionless form of equation (3.6.2) reads

$$\frac{\rho v_0^2}{L} v_{x,t} = \frac{\eta_1 v_0}{L^2} v_{x,xx} + \frac{\eta_2 v_0}{h^2} v_{x,zz} - \frac{\eta_2 v_0}{h^2} p_{,x} + \frac{\nu_1 v_0}{hL} \theta_{,tz}, \qquad (4.1.7)$$

i.e.,

$$\mathcal{R}_{e}^{(2)}\varepsilon^{2}v_{x,t} + p_{,x} = \frac{\eta_{1}}{\eta_{2}}\varepsilon^{2}v_{x,xx} + v_{x,zz} + \frac{\nu_{1}}{\eta_{2}}\varepsilon\theta_{,tz}, \qquad (4.1.8)$$

where we have identified

$$\mathcal{R}_e^{(2)} = \frac{\rho v_0 L}{\eta_2} \tag{4.1.9}$$

as a Reynolds number for the flow. The magnitude of $\mathcal{R}_e^{(2)}$ will determine whether we are in a strongly or weakly time-dependent flow regime, the latter case corresponding to approximately steady flow.

In a similar manner, the z-component of linear momentum balance given by equation (3.6.3) may, after non-dimensionalisation and some algebraic manipulation, be written

$$\mathcal{R}_{e}^{(3)}\varepsilon^{3}v_{z,t} + p_{,z} = \varepsilon S^{2}(u_{,t} - \varepsilon v_{z}) + \varepsilon^{2}\left(\varepsilon^{2}v_{z,xx} + \frac{\eta_{4}}{\eta_{3}}v_{z,zz} + \frac{\nu_{2}}{\eta_{3}}\varepsilon\theta_{,tx}\right), \quad (4.1.10)$$

where

$$\mathcal{R}_{e}^{(3)} = \frac{\rho v_0 h}{\eta_3}.$$
(4.1.11)

The balance of angular momentum equation transforms to give

$$\varepsilon^2 \theta_{,xx} = \frac{B_1 h^2}{K_1^n} (\theta + u_{,x}) + \mathcal{E}_r \left(\varepsilon \theta_{,t} + \frac{\nu_1}{\gamma_1} v_{x,z} + \frac{\nu_2}{\gamma_1} \varepsilon^2 v_{z,x} \right), \tag{4.1.12}$$

where

$$\mathcal{E}_r = \frac{\gamma_1 v_0 h}{K_1^n} \tag{4.1.13}$$

is an Ericksen number [68, Section 5.6.1], a dimensionless quantity which determines the ratio of viscous to elastic forces. Finally, the dimensionless permeation equation is found to be of the form

$$\frac{Lv_0}{\lambda_p B_0} \varepsilon^2 (u_{,t} - \varepsilon v_z) = \frac{\varepsilon^2}{\beta} (\theta_{,x} + u_{,xx}) - \frac{\lambda_a^2}{L^2} \varepsilon^2 u_{,xxxx} + u_{,zz}, \qquad (4.1.14)$$

where $\lambda_a^2 = K_1^a / B_0$.

4.2 General Remarks on Truncation and Applicability

In summary, the dimensionless system of dynamic equations reads

$$v_{x,x} + v_{z,z} = 0, (4.1.6)$$

$$\mathcal{R}_e^{(2)}\varepsilon^2 v_{x,t} + p_{,x} = \frac{\eta_1}{\eta_2}\varepsilon^2 v_{x,xx} + v_{x,zz} + \frac{\nu_1}{\eta_2}\varepsilon\theta_{,tz},\tag{4.1.8}$$

$$\mathcal{R}_{e}^{(3)}\varepsilon^{3}v_{z,t} + p_{,z} = \varepsilon S^{2}(u_{,t} - \varepsilon v_{z}) + \varepsilon^{2}\left(\varepsilon^{2}v_{z,xx} + \frac{\eta_{4}}{\eta_{3}}v_{z,zz} + \frac{\nu_{2}}{\eta_{3}}\varepsilon\theta_{,tx}\right), \quad (4.1.10)$$

$$\varepsilon^2 \theta_{,xx} = \frac{B_1 h^2}{K_1^n} (\theta + u_{,x}) + \mathcal{E}_r \left(\varepsilon \theta_{,t} + \frac{\nu_1}{\gamma_1} v_{x,z} + \frac{\nu_2}{\gamma_1} \varepsilon^2 v_{z,x} \right), \quad (4.1.12)$$

$$\frac{Lv_0}{\lambda_p B_0} \varepsilon^2 (u_{,t} - \varepsilon v_z) = \frac{\varepsilon^2}{\beta} (\theta_{,x} + u_{,xx}) - \frac{\lambda_a^2}{L^2} \varepsilon^2 u_{,xxxx} + u_{,zz}.$$
(4.1.14)

Given the number of dimensionless quantities present in this system, it is immediately apparent that the best means of truncating and thereby obtaining a more tractable system in the spirit of "classical" lubrication theory depends very much upon

- 1. the values of the various physical constants characterising the particular SmA material under consideration;
- 2. the velocity, pressure, and spatial gradients thereof, as well as inertial forces to which the sample is subjected. In general, the directions in which these are applied have the potential to significantly influence the resultant flow.
- 3. The characteristic length scales and geometry of the problem, generally as determined by the sample's container.

Referring to standard lubrication theory, it is generally assumed that $\varepsilon \ll 1$ and that $v_x \gg v_z$, though in the case of smectics this is somewhat more limiting given the anisotropy. This particular system of equations follows from assuming that the layers lie parallel to the x-axis, and thus the flow is always predominantly in the plane of the layers. Should one wish to consider the case in which $v_x \ll v_z$, that is, flow directed primarily perpendicular to this plane, it makes more sense to impose the requirement $\varepsilon \gg 1$. It should be noted, however, that this may lead to our linear system not being valid on the grounds that significant layer distortion may occur in this case. Of course, a nonlinear or quasi-linear modification may prove of use in this instance; such considerations fall outwith the scope of the present work, however, and will form the basis of future investigations.

As a demonstration of these ideas, consider first equation (4.1.8). Given that $\varepsilon \ll 1$, it follows that, unless inertial forces are sufficiently high that $\mathcal{R}_e^{(2)} = \mathcal{O}(1/\varepsilon^2)$, we may disregard all terms of $\mathcal{O}(\varepsilon^2)$ and write this equation in the approximate form

$$p_{,x} = v_{x,zz} + \frac{\nu_1}{\eta_2} \varepsilon \theta_{,tz}.$$

Now, if $\nu_1 = \eta_2 \mathcal{O}(\varepsilon)$, the latter term on the right-hand side of this relation is also discarded; if, however, $\nu_1 = \eta_2 \mathcal{O}(1/\varepsilon)$, it must be retained. It follows that the magnitude of the ratio ν_1/η_2 , as well as the aspect ratio ε , play an important role in determining the behaviour of leading-order solutions to this balance law.

Let us now turn to relation (4.1.10): it is tempting to apply the same approach to the previous equation and erroneously conclude that the leading order behaviour in all cases is described by

$$p_{,z} = \varepsilon S^2 u_{,t},$$

or, in the case of steady flow and/or when $S^2 = \mathcal{O}(\varepsilon)$,

$$p_{,z} = 0.$$

However, noting that $S = L/\delta_3$, it follows that, for physically relevant values of δ_3 (see Section 4.3.1 below), $S^2 \gg 1/\varepsilon^2$. On physical grounds, then, a more realistic truncated form of equation (4.1.10) is

$$p_{,z} = \varepsilon S^2(u_{,t} - \varepsilon v_z),$$

in spite of the presence of the factor of ε^2 multiplying v_z . In fact, for S sufficiently large relative to the pressure gradient normal to the layers, a more accurate approximation may be given by

$$u_{,t} = \varepsilon v_z.$$

In this case, the value of the permeation coefficient λ_p , as well as the viscosity coefficient η_3 and the characteristic lengths of the problem serve to significantly affect the dominant behaviour of solutions v_z as well as the layer displacement u and pressure p. Of course, for much smaller values of S and/or significantly higher values of any or all of the terms $\mathcal{R}_e^{(3)}$, η_4/η_3 and ν_2/η_3 , the governing equations and resultant solutions would start to look entirely different at leading order. However, such considerations may be of limited interest in terms of their physical relevance given the anticipated values of these parameters, as will be seen in the example of Section 4.3 below.

The angular momentum balance law as stated in equation (4.1.12) features several parameters. Discarding terms of $\mathcal{O}(\varepsilon^2)$ leads to

$$B_1h(\theta + u_x) + \gamma_1 v_0 \left(\varepsilon \theta_{,t} + \frac{\nu_1}{\gamma_1} v_{x,z}\right) = 0.$$

Three regimes present themselves:

1. $B_1 h \gg \gamma_1 v_0$. In this case, it immediately follows that

$$\theta + u_{,x} = 0,$$

unless ν_1/γ_1 is of a large magnitude, which may be deemed physically unreasonable.

- 2. $B_1h/\gamma_1v_0 = \mathcal{O}(1)$. Here, several possibilities present themselves. First, if $\varepsilon \ll 1$ is sufficiently small that the term $\varepsilon \theta_{,t}$ is also negligible, it may be discarded. Further, if $\nu_1/\gamma_1 = \mathcal{O}(\varepsilon)$, case 1 above is recovered. Alternatively, for ε sufficiently large that terms of $\mathcal{O}(\varepsilon)$ must be retained, we must either work with the full equation or, if $\nu_1 = \gamma_1 \mathcal{O}(\varepsilon^2)$, drop the final term and retain $\varepsilon \theta_{,t}$.
- 3. $B_1h \ll \gamma_1 v_0$. In the case where $\nu_1/\gamma_1 = \mathcal{O}(\varepsilon)$, the equation reads

$$\gamma_1 v_0 \left(\varepsilon \theta_{,t} + \frac{\nu_1}{\gamma_1} v_{x,z} \right) = 0.$$

Moreover, if ε is sufficiently large, this will also be the case for $\nu_1/\gamma_1 = \mathcal{O}(\varepsilon^2)$ or $\nu_1/\gamma_1 = \mathcal{O}(1)$. For ε very small, we have $v_{x,z} = 0$; this is also the case for $\nu_1/\gamma_1 = \mathcal{O}(1/\varepsilon^2)$. Finally, if $\nu_1/\gamma_1 = \mathcal{O}(\varepsilon^2)$, we have $\theta_{,t} = 0$.

It readily follows that the leading order behaviour of this equation has a subtle dependence upon the material coefficients γ_1 and B_0 , in addition to the sample dimensions and the characteristic velocity to which it is subjected.

Finally the permeation equation (4.1.14) admits many possibilities. First, naïvely discarding all terms featuring ε^2 leads to the simple relation

$$u_{,zz}=0.$$

Of course, on supposing that that β , λ_a/L and $Lv_0/\lambda_p v_0$ are all $\mathcal{O}(1)$, this is indeed the case. However, while $\lambda_a^2 \varepsilon^2/L^2$ may be assumed negligibly small for all systems of practical interest, this is not necessarily so for β and $Lv_0/\lambda_p v_0$. We therefore see a whole host of possibilities for the leading order behaviour, which is determined by the terms B_0 , B_1 and λ_p for the given SmA sample, as well as the container's dimensions and the velocity applied to the sample.

These ideas will be made more concrete in the following section, in which we revisit the problem of flow past a finite obstacle as outlined in Section 3.3 above.

4.3 Application: Flow Past a Finite Obstacle Revisited

In this section, we apply the lubrication equations (4.1.6), (4.1.8), (4.1.10), (4.1.12) and (4.1.14) to the obstacle problem considered above in Section 3.3, with the aim of gaining further insight into the resultant flow pattern and its influence on the behaviour of the SmA, as well as illustrating the principles discussed in the preceding section. First, in Subsection 4.3.1, we determine the magnitudes of the various dimensionless parameters within the equations by appeal to various values quoted in the literature, allowing us to pick out the dominant behaviour, which is then outlined in Subsection 4.3.2. The subsequent order of approximation is then presented in Subsection 4.3.3.

4.3.1 Some Order-of-Magnitude Calculations

Assuming a constant pressure gradient applied in the *x*-direction, we may take 20 Pa to be a representative value of the pressure difference across the sample [53]; following references [75, 82], we take $L = 1.5 \times 10^{-3}$ m, $h = 10^{-4}$ m. It is then readily shown that

$$\varepsilon = 1/15 \tag{4.3.1}$$

and

$$p_{,x} \simeq \frac{4}{3} \times 10^4 \,\mathrm{Pa}\,\mathrm{m}^{-1}.$$

Note that this value of ε is such that dropping terms of $\mathcal{O}(\varepsilon)$ in a particular equation would lead to a poor approximation of the leading-order behaviour, though terms of $\mathcal{O}(\varepsilon^2)$ may be considered negligible when compared with those of $\mathcal{O}(1)$. In order to estimate the viscosity combinations η_i , $i \in \{1, 2, 3, 4\}$ and ν_j , j = 1, 2, we once again appeal to inequalities (3.6.44)–(3.6.49) and assume that the parameter values as stated above in Table 3.1 are representative of the sample under consideration. It then readily follows that

$$-0.0397 \operatorname{Pas} \le \eta_2 \le 0.3153 \operatorname{Pas}, \tag{4.3.2}$$

so that we may select $\eta_2 = 0.1500 \text{ Pa} \text{ s}$, discarding the possibility of a negative viscosity combination. Selecting $\nu_1 = 0.0600 \text{ Pa} \text{ s}$ implies that $\kappa_1 = 0.0636 \text{ Pa} \text{ s}$ and thus $\nu_2 = -0.0176 \text{ Pa} \text{ s}$; then $\eta_3 = \eta_2 + \nu_1 + \nu_2 = 0.0024 \text{ Pa} \text{ s}$. Finally, it is necessary to obtain an estimate for the velocity ν_0 . The steady-state version of equation (4.1.8) is given by

$$p_{,x} = v_{x,zz} + \mathcal{O}(\varepsilon^2),$$

from which

$$\frac{\Delta p}{L} \simeq \frac{\eta_2 v_0}{h^2} \implies v_0 \simeq \frac{8}{9} \times 10^{-3} \,\mathrm{m \, s^{-1}}.$$
 (4.3.3)

We are now in a position to calculate the orders of magnitude of the parameter combinations involved in the dimensionless governing equations above. These are

$$\mathcal{R}_e^{(2)} \simeq \frac{8}{9} \times 10^{-4}, \qquad \mathcal{R}_e^{(3)} \simeq 4.68 \times 10^{-4}, \qquad \mathcal{E}_r \simeq \frac{7}{5} \times 10^3, \qquad (4.3.4)$$

$$S^2 \simeq \frac{5}{3} \times 10^8, \qquad \frac{B_1 h^2}{K_1^n} \simeq \frac{4}{5} \times 10^{11}, \qquad \frac{v_0 L}{\lambda_p B_0} \simeq 148.$$
 (4.3.5)

4.3.2 The Leading-Order Equations

Retaining only the dominant terms as a first approximation, the system of equations (4.1.6), (4.1.7), (4.1.10), (4.1.12) and (4.1.14) may be written in the approximate forms

$$v_{x,x} + v_{z,z} = 0, (4.1.6)$$

$$p_{,x} = v_{x,zz},\tag{4.3.6}$$

$$\eta_2 p_{,z} = \eta_3 \varepsilon S^2 (u_{,t} - \varepsilon v_z), \qquad (4.3.7)$$

$$\theta + u_{,x} = 0, \tag{4.3.8}$$

$$u_{,zz} = \frac{v_0 L}{\lambda_p B_0} \varepsilon^2 \left(u_{,t} - \varepsilon v_z \right).$$
(4.3.9)

Returning to dimensional variables, the incompressibility condition reads as in equation (3.2.8). Equation (4.3.6) takes the form

$$p_{,x} = \eta_2 v_{x,zz},\tag{4.3.10}$$

while equation (4.3.7) is equivalent to

$$p_{,z} = \frac{u_{,t} - v_z}{\lambda_p},\tag{4.3.11}$$

the term $u_{,t}$ vanishing in the case of steady flow. Equation (4.3.8) looks identical in dimensional variables, and simply tells us that $\mathbf{n} = \mathbf{a}$ at this order of approximation (c.f., equations (3.4.3) and (3.4.5)). Finally, rewriting equation (4.3.9) in terms of dimensional variables yields

$$u_{,t} - \lambda_p B_0 u_{,zz} = v_z, \tag{4.3.12}$$

where, as above, the term $u_{,t}$ vanishes in the case of steady flow.

Steady Flow

Our time-independent leading-order equations take the form

$$v_{x,x} + v_{z,z} = 0,$$
 $p_{,x} = \eta_2 v_{x,zz},$ $p_{,z} = -v_z/\lambda_p,$ (4.3.13)

$$\theta + u_{,x} = 0, \qquad v_z = -\lambda_p B_0 u_{,zz}.$$
 (4.3.14)

Note that equations (4.3.13) are identical in form to those due to Walton *et al.* [82] (c.f. equations (3.3.1)–(3.3.3) with $\nu_2 \rightarrow \eta_3$), with boundary conditions on the velocity as above, viz.,

$$v_x(0,z) = \begin{cases} 0 & \text{when } |z| < 1/2, \\ v_0 & \text{when } |z| > 1/2, \end{cases} \qquad v_z(0,z) = 0.$$
(3.3.4)

The velocity is then given by

$$v_x = v_0 + \frac{v_0}{2} \left\{ \operatorname{erf}\left(\frac{2z+1}{4\sqrt{\delta_2|x|}}\right) - \operatorname{erf}\left(\frac{2z-1}{4\sqrt{\delta_2|x|}}\right) \right\},$$
(4.3.15)

$$v_z = \pm \frac{v_0 \sqrt{\delta_2}}{\sqrt{\pi |x|}} \sinh\left(\frac{z}{4\delta_2 |x|}\right) \exp\left(-\frac{4z^2 + 1}{16\delta_2 |x|}\right),\tag{4.3.16}$$

where the upper (lower) sign corresponds to z < 0 (z > 0) as before, and we have introduced the notation

$$\delta_2 = \sqrt{\lambda_p \eta_2} \tag{4.3.17}$$

in analogy with equation (4.1.4). The second of equations (4.3.14) may then be integrated twice with respect to z, yielding

$$u = \pm \frac{v_0 \delta_2}{2\lambda_p B_0} \left\{ \left(z + \frac{1}{2}\right) \operatorname{erf}\left(\frac{2z+1}{4\sqrt{\delta_2 |x|}}\right) + \left(\frac{1}{2} - z\right) \operatorname{erf}\left(\frac{2z-1}{4\sqrt{\delta_2 |x|}}\right) - \sqrt{\frac{\delta_2 |x|}{\pi}} \operatorname{sinh}\left(\frac{z}{4\delta_2 |x|}\right) \operatorname{exp}\left(-\frac{4z^2+1}{16\delta_2 |x|}\right) \right\} + z\alpha(x) + \beta(x).$$
(4.3.18)

Then, making use of equation $(4.3.14)_1$, we obtain for the director profile

$$\theta(x,z) = \pm \frac{v_0 \operatorname{sgn}(x)}{4\lambda_p B_0} \sqrt{\frac{\delta_2}{\pi |x|}} \left\{ \frac{(2z+1)^2}{4|x|} \exp\left[-\frac{(2z+1)^2}{16\delta_2 |x|}\right] - \frac{(2z-1)^2}{4|x|} \exp\left[-\frac{(2z-1)^2}{16\delta_2 |x|}\right] + \delta_2 \left[\left(1 + \frac{4z^2+1}{8\delta_2 |x|}\right) \sinh\left(\frac{z}{4\delta_2 |x|}\right) - \frac{z}{2\delta_2 |x|} \cosh\left(\frac{z}{4\delta_2 |x|}\right)\right] \exp\left(-\frac{4z^2+1}{16\delta_2 |x|}\right) \right\} - z\alpha'(x) - \beta'(x), \quad (4.3.19)$$

where sgn(x) denotes the sign function (or signum function), defined as

$$\frac{d}{dx}(|x|) = \operatorname{sgn}(x) = \begin{cases} -1 & \text{when } x < 0, \\ 0 & \text{when } x = 0, \\ 1 & \text{when } x > 0. \end{cases}$$
(4.3.20)

By imposing the requirements that θ is an odd function of z and that it is zero at the boundary of the sample, it readily follows that $\alpha' = \beta' = 0$, yielding an exact solution for the director profile and defining the layer displacement u to within an arbitrary constant.

Unsteady Flow: Linear Stability of the Leading-Order System

Our equations are

$$v_{x,x} + v_{z,z} = 0,$$
 $p_{,x} = \eta_2 v_{x,zz},$ $p_{,z} = (u_{,t} - v_z)/\lambda_p,$ (4.3.21)

$$\theta + u_{,x} = 0,$$
 $v_z = u_{,t} - \lambda_p B_0 u_{,zz}.$ (4.3.22)

Rather than immediately seeking solutions to these equations, let us assume small perturbations to the terms v_x , v_z , p, θ and u in the same form as those given above in equations (3.6.8)–(3.6.12). One readily finds that non-trivial solutions to this system of equations exist if and only if

$$\omega = -\frac{B_0(q_x^2 + \delta_2^2 q_z^4)}{\eta_2 q_z^2} < 0, \qquad (q_z \neq 0), \tag{4.3.23}$$

from which it follows that the flow pattern is stable at leading order, as may be expected on recalling the result of Section 3.3.

4.3.3 Truncation at Higher Order

Taking the lubrication equations to the next order of approximation, i.e., discarding terms at $\mathcal{O}(\varepsilon^3)$ and above, the dimensionless equations read

$$v_{x,x} + v_{z,z} = 0, (4.1.6)$$

$$p_{,x} = \frac{\eta_1}{\eta_2} \varepsilon^2 v_{x,xx} + v_{x,zz} + \frac{\nu_1}{\eta_2} \varepsilon \theta_{,tz}, \qquad (4.3.24)$$

$$\eta_2 p_{,z} = \eta_3 \varepsilon S^2 (u_{,t} - \varepsilon v_z), \qquad (4.3.25)$$

$$\theta + u_{,x} = 0,$$
 (4.3.26)

$$\frac{v_0 L}{\lambda_p B_0} \varepsilon^2 \left(u_{,t} - \varepsilon v_z \right) = \frac{\varepsilon^2}{\beta} (\theta_{,x} + u_{,xx}) + u_{,zz}, \qquad (4.3.27)$$

the first term on the right-hand side of (4.3.27) vanishing by virtue of (4.3.26). These are almost identical to the leading order equations, bar the addition of the first and third terms on the right-hand side of equation (4.3.24). To see why none of the other equations is modified by additional terms, one need only look at the order-of-magnitude calculations presented above in Subsection 4.3.1: the factors εS^2 and $B_1 h^2/K_1^n$ are so large in magnitude that the terms containing them significantly dwarf the other terms in the equations in which they appear and, similarly, the coefficients ε^2/β and λ_a^2/L^2 are substantially smaller in magnitude than the dominant terms of the equations in which they feature.

As to the question of whether the inclusion of this extra term alters the stability result outlined in Section 4.3.2, we simply assume oscillatory perturbations as above to find the following requirement for non-trivial solutions:

$$\nu_1 q_x \omega^2 + i \left(\eta_1 q_x^2 + \eta_2 q_z^2 \right) \omega + i B_0 \left\{ q_x^2 + \lambda_p q_z^2 \left(\eta_1 q_x^2 + \eta_2 q_z^2 \right) \right\} = 0, \qquad (4.3.28)$$

from which

$$\omega = \frac{\pm \sqrt{-(\eta_1 q_x^2 + \eta_2 q_z^2)^2 + 4i\nu_1 B_0 q_x \{q_x^2 + \lambda_p q_z^2 (\eta_1 q_x^2 + \eta_2 q_z^2)\}}}{2\nu_1 q_x} - \frac{i(\eta_1 q_x^2 + \eta_2 q_z^2)}{2\nu_1 q_x}, \tag{4.3.29}$$

and thus it follows that we can always expect one value of ω with a positive real part provided ν_1 and q_z are non-zero. It is evident from the form of equation (4.3.28) that the presence of the term $\nu_1\theta_{,tz}$ leads to the destabilisation of the system at this order of approximation. Of course, we could continue to work to higher order, eventually building up to the full system as considered in Sections 3.4 and 3.6 and leading to the rather involved expressions which show a somewhat more subtle dependence of the system's behaviour upon the value of ν_1 ; however, the simpler analysis presented herein has led us to an account of the dominant behaviour for this particular example. Time will tell whether this approach yields similar insight for the stability properties of other model systems, which we will leave as topics for further research.

4.4 Discussion and Further Considerations

This chapter has presented the results of a preliminary investigation regarding the possibility of applying a lubrication approximation to the study of flow phenomena in SmA liquid crystals. After deriving the model from the two-dimensional system and discussing in general terms various limiting cases for each of the equations, we showed how the framework can be applied to the problem of flow past a finite obstacle, obtaining exact solutions for all the relevant physical quantities to leading order and examining in-depth the stability properties at the subsequent higher order of approximation, in effect enabling us to determine which physical parameters play dominant roles in the onset of instability.

We have but scratched the surface: it is hoped that analytical progress on a range of flow problems satisfying the criteria required for the validity of this approach will be the subject of much future work. For example, bearing-type situations involving a range of geometries as well as squeeze-film flows (examples of such for both Newtonian and non-Newtonian fluids may be found in [74]), would make for interesting problems in terms of solving for the physical quantities of interest, as well as potentially providing a suitable means of comparison of experimental results with predictions made by the theory. Another "classical" fluid mechanics problem which could realistically be extended to SmA is that of thinfilm flow down an inclined plane with a free surface; the theory would of course require slight modifications to account for body forces (i.e., gravity) and surface tension due to the presence of a free surface; these should not prove difficult to implement. In all cases, comparison with similar studies in Newtonian and other non-Newtonian fluids as well as recent work on thin-film flows in nematics [42] would no doubt prove fruitful.

Some further generalisations could be made, such as working in three spatial dimensions or introducing nonlinearities to account for defects or boundary-layer flows. Further, as alluded to in Chapter 3, one might employ a nonlinear system in the region of some defect, the edge dislocation to be considered in Chapter 6, for instance, while working with the linear system in regions sufficiently far from the defect "core" and employing some form of matching condition between the boundary and far-field regions.

Chapter 5

Behaviour of a Shear Wave at a Solid-Smectic Interface

5.1 Introduction

The analysis presented herein will consider a perturbation to a sample of bookshelfaligned SmA induced by a shear wave incident at the plane interface between the smectic and an isotropic elastic solid such that the wave first propagates through the solid then undergoes a reflection and refraction on contact with the interface, as shown in Fig. 5.1. Section 5.2 will present the analysis for a sample of bookshelf-aligned SmA with the director \boldsymbol{n} strongly anchored to lie parallel to the interface. On utilising the method of normal modes [34], we will derive dispersion relations governing the behaviour of the anticipated perturbations to the director and layer normal, as well as the velocity of the refracted wave within the smectic. Two possibilities for director motion will be considered, though it will be shown that one of these leads to an inconsistency. Using these and the interfacial conditions, expressions will then be obtained for the refracted wave number and the amplitudes of both reflected and refracted waves in terms of the problem's physical parameters. In Section 5.3 we will summarise the analogous problem, first studied by Gill & Leslie [25], in which the region occupied by the SmA is instead occupied by a sample of SmC, similarly anchored in such a way that nlies parallel to the interface, which will then be extended to provide expressions for the reflected and refracted wave amplitudes in an analogous fashion to those presented in Section 5.2 in terms of the relevant parameters. Section 5.4 features plots which demonstrate how the amplitudes of the reflected and refracted waves vary with the angular frequency and angle of incidence of the initial disturbance, and Section 5.5 will close the chapter with some concluding remarks.



Figure 5.1: On contact with the interface, the incident wave is both reflected and refracted. The region z < 0 is occupied by an isotropic elastic solid, while the region z > 0 contains bookshelf-aligned SmA.



Figure 5.2: Problem set-up for bookshelf SmA.

5.2 The "Bookshelf" SmA Case

In a configuration analogous to that set forth by Gill & Leslie [25], consider a plane interface between an isotropic elastic solid and a smectic A liquid crystal, as depicted in Fig. 5.2, with the interface taken to lie along the *y*-axis, and the smectic taken to be initially undistorted, so that the director \boldsymbol{n} is parallel to the interface. In this unperturbed state, \boldsymbol{n} coincides with the unit layer normal \boldsymbol{a} . Following [25], it is assumed that both solid and smectic are unbounded, as any other boundaries involved in the set up are expected to bear no relevance to the problem to be considered. With respect to the Cartesian reference frame as depicted in Fig. 5.1,

$$\boldsymbol{n} = \boldsymbol{n_0} = (0, 1, 0), \ \boldsymbol{\Phi} = \boldsymbol{\Phi}_0 = y,$$
 (5.2.1)

and the incident wave displacement $\boldsymbol{u} = (u_x, u_y, u_z)$ takes the form

$$u_x = A \exp\{i[\omega t - k(y\sin\phi + z\cos\phi)]\}, \ u_y = u_z = 0,$$
 (5.2.2)

where A is the constant amplitude of the wave, which may be assumed to be a real number without any loss of generality, and ϕ the constant angle of incidence (to the interface's normal); ω and k denote the constant incident frequency and wave number, respectively. As each of these constants would be prescribed according to the experimental set up, they will be assumed known in the analysis that follows. This displacement must satisfy the wave equation for an isotropic solid [36, p. 87]; noting that \boldsymbol{u} as given in equation (5.2.2) is divergence-free, this leads to

$$\rho_s \boldsymbol{u}_{,tt} = \mu_s \nabla^2 \boldsymbol{u}, \tag{5.2.3}$$

where ρ_s and μ_s denote, respectively, the mass density and shear modulus (or bulk modulus) of the solid. It then follows from (5.2.2) that

$$\rho_s \omega^2 = \mu_s k^2. \tag{5.2.4}$$

It is natural to suppose that the displacement of the reflected wave $u^r = (u^r_x, u^r_y, u^r_z)$ takes the form

$$u_x^r = B \exp\{i[\omega t - k(y\sin\phi - z\cos\phi)]\}, \ u_y^r = u_z^r = 0,$$
(5.2.5)

with B a constant amplitude which will be shown to depend upon the prescribed parameters discussed above.

It is expected that the incident wave will induce a perturbation to the smectic, and we anticipate that this disturbance may cause small changes to the alignment of the constituent molecules (that is, to the director) and to the layer normal; further, as discussed in Section 2.3, a potential separation of \boldsymbol{a} and \boldsymbol{n} will be allowed for on employing the dynamic theory of Stewart [69].

The velocity $\boldsymbol{v} = (v_x, v_y, v_z)$ in the smectic is assumed to take the form

$$v_x = v \exp\{i[\omega t - k(y\sin\phi + qz)]\}, \ v_y = v_z = 0,$$
(5.2.6)

with v and q to be determined. Note that this form of v automatically satisfies the condition of incompressibility $v_{i,i} = 0$. The scalar Φ will be given by

$$\Phi = y - u(y, z, t), \ u \ll 1, \tag{5.2.7}$$

for small perturbations $u = \hat{u} \exp\{i[\omega t - k(y\sin\phi + qz)]\}$ such that $|\hat{u}| \ll 1$. Then

$$\boldsymbol{a} = \frac{\nabla\Phi}{|\nabla\Phi|} = (0, 1, -u_z) \tag{5.2.8}$$

to first order in u and derivatives thereof.

While Gill and Leslie considered only one form of disturbance to their director c, a small perturbation in the x-direction, it is necessary to consider two possibilities here for our director n:

- 1. a disturbance in the x-direction corresponding to the director moving out of the yz-plane;
- 2. a disturbance in the z-direction, corresponding to a change in the angle by which the director n tilts with respect to the y-axis.

This follows as a consequence of the fact that, on fixing the smectic cone angle θ for the problem considered in [25], Gill and Leslie removed a degree of freedom in the set up of their problem. In general, it is necessary to consider, along with the out-of-plane disturbance already studied, the possibility of there being an oscillation of n in the yz-plane.

5.2.1 Ansatz 1

The director $\boldsymbol{n} = (n_x, n_y, n_z)$ is perturbed so that

$$n_x = n \exp\{i[\omega t - k(y\sin\phi + qz)]\}, \ n_y = 1, \ n_z = 0, \qquad n \ll 1.$$
 (5.2.9)

There are no body forces, and linearisation allows for the elimination of the terms $\tilde{g}_i n_{j,i}$, so that the balance of linear momentum equation (2.3.33) reduces to

$$\rho \dot{v}_i = -\tilde{p}_{,i} + |\nabla \phi| a_i J_{j,j} + \tilde{t}_{ij,j}.$$

$$(5.2.10)$$

Calculations reveal that

$$\boldsymbol{J} = (B_1 n_x, B_0 u_{,yy}, B_1 u_{,z} - K_1^a u_{,zzz}), \qquad (5.2.11)$$

$$\implies J_{i,i} = B_0 u_{,yy} + B_1 u_{,zz} - K_1^a u_{,zzzz}, \qquad (5.2.12)$$

so that, to first order,

$$|\nabla \Phi| \boldsymbol{a} J_{i,i} = (0, B_0 u_{,yy} + B_1 u_{,zz} - K_1^a u_{,zzzz}, 0).$$
 (5.2.13)

The divergence of the stress tensor has only one non-zero component:

$$\tilde{t}_{xj,j} = \frac{1}{2}k^2 v_x \left(\eta \sin^2 \phi - \alpha_4 q^2\right) + \omega k n_x (\alpha_2 + \kappa_1) \sin \phi, \qquad (5.2.14)$$

where

$$\eta = \alpha_2 - \alpha_4 - \alpha_5 - \tau_2 + 2(\kappa_1 - \kappa_6).$$
(5.2.15)

The balance of linear momentum equations (5.2.10) then read

$$i\rho\omega v_x = -\tilde{p}_{,x} + \frac{1}{2}k^2 v_x \left(\eta \sin^2 \phi - \alpha_4 q^2\right) + \omega k n_x (\alpha_2 + \kappa_1) \sin \phi, \qquad (5.2.16)$$

$$0 = -\tilde{p}_{,y} + B_0 u_{,yy} + B_1 u_{,zz} - K_1^a u_{,zzzz}, \qquad (5.2.17)$$

$$0 = -\tilde{p}_{,z}.$$
 (5.2.18)

The last of these clearly requires \tilde{p} to be a function of x, y and t only. Now, v_x and n_x are functions of y, z and t, so that (5.2.16) is only satisfied if $\tilde{p}_{,x} = 0$; similarly, (5.2.17) contains derivatives of u, a function of y, z and t, so $\tilde{p}_{,y}$ must also be zero. We therefore conclude that $\tilde{p} = \tilde{p}(t)$, an arbitrary function of time t. It then follows that we need only consider the equations

$$i\rho\omega v_x = \frac{1}{2}k^2 v_x \left(\eta \sin^2 \phi - \alpha_4 q^2\right) + \omega k n_x (\alpha_2 + \kappa_1) \sin \phi, \qquad (5.2.19)$$

$$0 = B_0 u_{,yy} + B_1 u_{,zz} - K_1^a u_{,zzzz}.$$
(5.2.20)

The balance of angular momentum equations may similarly be reduced to

$$\left(\frac{\partial w_{\rm A}}{\partial n_{i,j}}\right)_{,j} - \frac{\partial w_{\rm A}}{\partial n_i} + \tilde{g}_i = \lambda n_i.$$
(5.2.21)

Recalling the expressions given in Section 2.3 for the derivatives of the free energy density, the linearised component equations are

$$i\{(\alpha_2 + \kappa_1)kv_x \sin \phi + (\alpha_2 - \alpha_3)\omega n_x\} = \lambda n_x, \qquad (5.2.22)$$

$$B_1 = \lambda, \qquad (5.2.23)$$

$$-B_1 u_{,z} = 0, (5.2.24)$$

so that, on combining the first two of these, one may write

$$i\{(\alpha_2 + \kappa_1)kv_x \sin \phi + (\alpha_2 - \alpha_3)\omega n_x\} = B_1 n_x, \qquad (5.2.25)$$

$$u = 0.$$
 (5.2.26)

Noting that $\dot{\Phi} = -u_{,t} = 0$ by equation (5.2.26) above, the permeation equation is simply $J_{i,i} = 0$, so that

$$J_{i,i} = B_0 u_{,yy} + B_1 u_{,zz} - K_1^a u_{,zzzz} = 0, (5.2.27)$$

in agreement with equation (5.2.20). Cancelling exponentials in equations (5.2.19) and (5.2.25) gives the dispersion relations

$$\{2i\rho\omega + k^2 \left(\alpha_4 q^2 - \eta \sin^2 \phi\right)\} v - 2\omega k(\alpha_2 + \kappa_1) n \sin \phi = 0, \qquad (5.2.28)$$

$$(\alpha_2 + \kappa_1) kv \sin \phi + \{(\alpha_2 - \alpha_3)\omega - B_1\} n = 0.$$
 (5.2.29)

Equations (5.2.28) and (5.2.29) provide non-trivial solutions for v and n provided that the determinant of the 2×2 matrix

$$\begin{bmatrix} 2i\rho\omega + k^2(\alpha_4 q^2 - \eta \sin^2 \phi) & -2\omega k(\alpha_2 + \kappa_1) \sin \phi \\ (\alpha_2 + \kappa_1)k \sin \phi & (\alpha_2 - \alpha_3)\omega - B_1 \end{bmatrix}$$

is zero; thus

$$\{2i\rho\omega + k^2(\alpha_4 q^2 - \eta \sin^2 \phi)\} \{(\alpha_2 - \alpha_3)\omega - B_1\}$$

+ 2\omega k^2(\alpha_2 + \kappa_1)^2 \sin^2 \phi = 0. (5.2.30)

Rearranging this gives an expression for q^2 in the form

$$q^2 = \beta_1 - 2i\beta_2, \tag{5.2.31}$$

where β_1 and $-2\beta_2$ are the real and imaginary parts of q^2 , respectively, given by

$$\beta_1 = \left\{ \eta + \frac{2\omega(\alpha_2 + \kappa_1)^2}{B_1 + \gamma_1 \omega} \right\} \sin^2 \phi, \qquad \beta_2 = \frac{\rho\xi}{\alpha_4}, \qquad (5.2.32)$$

in which the notation

$$\xi = \omega/k^2 \tag{5.2.33}$$

has been introduced for later comparison with Gill & Leslie's work [25], which features the same parameter, and $\gamma_1 \equiv \alpha_3 - \alpha_2$. It then follows that

$$q = \chi - i\psi, \ \psi > 0,$$
 (5.2.34)

where

$$\chi = \frac{\beta_2}{\psi}, \qquad \psi = \sqrt{\frac{1}{2} \left(\sqrt{\beta_1^2 + 4\beta_2^2} - \beta_1\right)},$$
(5.2.35)

Note that the requirement $\psi > 0$ in (5.2.34) is to ensure that the solution for q is physically meaningful [25]; since the imaginary part of q corresponds to the shear attenuation of the refracted wave, the case $\psi < 0$ in (5.2.34) would lead to an unbounded solution, as is readily seen on substitution back into (5.2.6) and (5.2.9). Note that normal incidence corresponds to

$$q = \frac{\beta_2}{\psi} - i\sqrt{\beta_2} = (1-i)\sqrt{\frac{\rho\xi}{\alpha_4}}.$$
 (5.2.36)

The penetration depth, that is the analogue of the Stokes boundary layer thickness in an isotropic Newtonian fluid [37, p.84], is given by

$$\delta = 1/k\psi, \tag{5.2.37}$$

which, at normal incidence, reduces to

$$\delta|_{\phi=0} = \frac{1}{k} \sqrt{\frac{\alpha_4}{\rho\xi}} = \sqrt{\frac{\alpha_4}{\rho\omega}},\tag{5.2.38}$$

which is exactly the Stokes layer for an isotropic Newtonian fluid (recall from Section 2.3 that $\alpha_4 = 2\mu$, μ denoting the viscosity of such a fluid), and is identical to the Stokes layer that occurs in oscillatory flow of SmA [49].

Boundary Conditions

Following the arguments set forth by Gill & Leslie [25], continuity of velocity and surface traction are imposed at the interface between the solid and the smectic. With the displacements of the incident and reflected waves as given above in equations (5.2.2) and (5.2.5), respectively, and the refracted wave velocity taking the form in (5.2.6), continuity of velocity at the interface reads

$$i\omega(A+B) = v. \tag{5.2.39}$$

In the solid, the surface traction t is required to satisfy the constitutive equations for isotropic elasticity [66, p.115], so that

$$\mathbf{t}|_{z=0} = (ik\mu_s(B-A)e^{i(\omega t - ky\sin\phi)}\cos\phi, \, 0, \, 0).$$
 (5.2.40)

Calculating the same for the smectic and imposing the requirement of continuity leads to the condition

$$2\mu_s(A-B)\cos\phi = \alpha_4 qv. \tag{5.2.41}$$

5.2.2 Ansatz 2

The other possible form of the director is

$$n_x = 0, \qquad n_y = 1, \qquad n_z = n \exp\{i[\omega t - k(y\sin\phi + qz)]\}.$$
 (5.2.42)

In this instance, calculations analogous to those used to obtain equations (5.2.11)–(5.2.14) give the components of the balance of linear momentum equation as

$$i\rho\omega v_x = -\tilde{p}_{,x} + \frac{1}{2}k^2 v_x \left(\eta \sin^2\phi - \alpha_4 q^2\right),$$
 (5.2.43)

$$0 = -\tilde{p}_{,y} + (\alpha_3 + \kappa_1)\omega kqn_z + B_0 u_{,yy} + B_1(u_{,zz} - ikqn_z) - K_1^a u_{,zzzz},$$
(5.2.44)

$$0 = -\tilde{p}_{,z} + (\alpha_2 + \kappa_1)\omega kn_z \sin\phi. \qquad (5.2.45)$$

Equation (5.2.43) implies that $\tilde{p}_{,x}$ is a function of y, z and t, so that

$$\tilde{p} = x\tilde{p}_{,x} + p_1(y,z,t);$$

by (5.2.44) and (5.2.45), however, $\tilde{p}_{,y}$ and $\tilde{p}_{,z}$ are functions of y, z and t, suggesting that

$$\tilde{p}_{,y} = x\tilde{p}_{,xy} + p_{1,y}, \qquad \qquad \tilde{p}_{,z} = x\tilde{p}_{,xz} + p_{1,z},$$

which means these derivatives must be functions of x also, in direct contradiction of equations (5.2.44) and (5.2.45) unless $\tilde{p}_{,x} = 0$. We can therefore re-write equation (5.2.43) as

$$\left\{i\rho\omega - \frac{1}{2}k^2\left(\eta\sin^2\phi - \alpha_4 q^2\right)\right\}v_x = 0.$$
 (5.2.46)

and assume a solution for the pressure of the form

$$\tilde{p} = p_0 + \hat{p} \exp\{i[\omega t - k(y\sin\phi + qz)]\}, \qquad (5.2.47)$$

where p_0 and \hat{p} are constants such that $|\hat{p}| \ll 1$.

The angular momentum equations are

$$i(\alpha_2 + \kappa_1)kv_x \sin \phi = 0; \qquad (5.2.48)$$

$$-K_1^n k^2 q n_z \sin \phi + B_1 = \lambda; \tag{5.2.49}$$

$$-K_1^n k^2 q^2 n_z - B_1 u_{,z} + i(\alpha_2 - \alpha_3)\omega n_z = \lambda n_z, \qquad (5.2.50)$$

and the permeation equation yields the relation

$$u_{t} = \lambda_p \{ B_0 u_{yy} - K_1^a u_{zzz} + B_1 (u_{zz} - ikqn_z) \}.$$
 (5.2.51)

Clearly, the only way to simultaneously satisfy (5.2.46) and (5.2.48) is to have v = 0. This means that, to first order, we may discard the possibility of perturbations to the director in the z-direction in the case of bookshelf geometry.

5.2.3 Expressions for the Wave Amplitudes

Having eliminated the second ansatz as inconsistent when working to first order, we may therefore return to ansatz 1, as outlined in Section 5.2.1 as our only possibility. Having established dispersion relations and thereby obtained the wave number and penetration depth for the refracted wave, in addition to establishing boundary conditions at the interface, we may now utilise these to progress further. Recalling expressions (5.2.39), (5.2.41), it follows that

$$2\mu_s(A-B)\cos\phi = i\omega\alpha_4q(A+B),$$

which leads to

$$B = A \left(\frac{2\rho_s \xi \cos \phi + i\alpha_4 q}{2\rho_s \xi \cos \phi - i\alpha_4 q} \right)$$

= $A \left\{ \frac{4\rho_s^2 \xi^2 \cos^2 \phi - \alpha_4^2 (\chi^2 + \psi^2) - 4i\alpha_4 \chi \rho_s \xi \cos \phi}{4\rho_s^2 \xi^2 \cos^2 \phi + \alpha_4^2 (\chi^2 + \psi^2) + 4\alpha_4 \psi \rho_s \xi \cos \phi} \right\},$ (5.2.52)

on making use of equations (5.2.4) and (5.2.34). At normal incidence, equation (5.2.52) reduces to

$$B|_{\phi=0} = A\left(\frac{2\rho_s^2\xi - \rho\alpha_4 - 2i\rho_s\sqrt{\rho\xi\alpha_4}}{2\rho_s^2\xi + \rho\alpha_4 + 2\rho_s\sqrt{\rho\xi\alpha_4}}\right).$$
 (5.2.53)

On making further use of (5.2.41), it is readily seen that

$$v = i\omega A \left\{ 1 + \frac{4\rho_s^2 \xi^2 \cos^2 \phi - \alpha_4^2 (\chi^2 + \psi^2) - 4i\alpha_4 \chi \rho_s \xi \cos \phi}{4\rho_s^2 \xi^2 \cos^2 \phi + \alpha_4^2 (\chi^2 + \psi^2) + 4\alpha_4 \psi \rho_s \xi \cos \phi} \right\}$$

= $4A\omega \rho_s \xi \cos \phi \left\{ \frac{2i\rho_s \xi \cos \phi + \alpha_4 (\chi + i\psi)}{4\rho_s^2 \xi^2 \cos^2 \phi + \alpha_4^2 (\chi^2 + \psi^2) + 4\alpha_4 \psi \rho_s \xi \cos \phi} \right\},$ (5.2.54)

and, at normal incidence

$$v|_{\phi=0} = 2A\rho_s \omega \left\{ \frac{2i\rho_s \xi + (1+i)\sqrt{\rho\xi\alpha_4}}{2\rho_s^2 \xi + \rho\alpha_4 + 2\rho_s\sqrt{\rho\xi\alpha_4}} \right\}.$$
 (5.2.55)

Taking moduli of the complex amplitudes given in equations (5.2.52) - (5.2.55) gives the measurable amplitudes of the reflected and refracted waves. (Note that their argument corresponds to a phase shift and therefore plays no part in our analysis.)

$$|B| = \frac{A\sqrt{16\rho_s^2\xi^4\cos^4\phi + \alpha_4^4(\chi^2 + \psi^2)^2 + 8\rho_s^2\xi^2\alpha_4^2(\chi^2 - \psi^2)\cos^2\phi}}{4\rho_s^2\xi^2\cos^2\phi + \alpha_4^2(\chi^2 + \psi^2) + 4\alpha_4\psi\rho_s\xi\cos\phi}, \quad (5.2.56)$$

$$\implies |B|_{\phi=0} = \frac{A\sqrt{4\rho_s^4\xi^2 + \rho^2\alpha_4^2}}{2\rho_s^2\xi + \rho\alpha_4 + 2\rho_s\sqrt{\rho\xi\alpha_4}},\tag{5.2.57}$$

and

$$|v| = \frac{4A\omega\rho_s\xi\omega\cos\phi}{\sqrt{4\rho_s^2\xi^2\cos^2\phi + \alpha_4^2(\chi^2 + \psi^2) + 4\alpha_4\psi\rho_s\xi\cos\phi}},$$
 (5.2.58)

$$\implies |v|_{\phi=0} = \frac{2A\rho_s\omega\sqrt{2\xi}}{\sqrt{2\rho_s^2\xi + \rho\alpha_4 + 2\rho_s\sqrt{\rho\xi\alpha_4}}}.$$
(5.2.59)

Then, for a refracted wave displacement of the form

$$\boldsymbol{u}^{s} = (C \exp\{i[\omega t - k(y\sin\phi + qz)]\}, 0, 0), \qquad (5.2.60)$$

|C| is given by

$$|C| = \frac{4A\rho_s\xi\cos\phi}{\sqrt{4\rho_s^2\xi^2\cos^2\phi + \alpha_4^2(\chi^2 + \psi^2) + 4\alpha_4\psi\rho_s\xi\cos\phi}},$$
(5.2.61)

from which

$$|C|_{\phi=0} = \frac{2A\rho_s\sqrt{2\xi}}{\sqrt{2\rho_s^2\xi + \rho\alpha_4 + 2\rho_s\sqrt{\rho\xi\alpha_4}}}.$$
 (5.2.62)

The moduli of these amplitudes as stated above will be plotted in Section 5.4 below, in which their dependencies on a selection of the problem's parameters will be examined in detail.

5.3 The SmC Case

In this section, a review of Gill & Leslie's results [25] for Smectic C will be presented, followed by extensions to their work by the present author analogous to those carried out in Section 5.2.3. For brevity, full details of the calculations will not be presented here; instead, the reader may consult references [24, 25].

5.3.1 Dispersion Relations and Interfacial Conditions



Figure 5.3: Schematic depiction of the SmC case contained in [25].

Consider Fig. 5.3, which depicts a plane interface between an isotropic solid and a sample of SmC material. For an incident wave of the form given in equation (5.2.2), the relation

$$\rho_s \omega^2 = \mu_s k^2 \tag{5.3.1}$$

still holds in the isotropic solid. The reflected wave displacement is exactly as given in (5.2.5), while the refracted wave velocity is the same as above in equation (5.2.6). Gill & Leslie's analysis also allows for perturbations in the vector \boldsymbol{c} as introduced in Section 2.2 of a similar form, viz.,

$$c_x = c \exp\{i[\omega t - k(y\sin\phi + qz)]\}, \qquad c_y = \sin\theta, \qquad c_z = -\cos\theta, \qquad (5.3.2)$$

where θ denotes the usual smectic cone angle. (Note that $c \neq |\mathbf{c}|$.) Insertion of these perturbations into the balance laws for linear and angular momentum at

(2.2.39) and (2.2.38), respectively, yields the two dispersion relations

$$\{2i\rho\omega + k^2\eta(q)\}v - 2\omega k\nu(q)c = 0,$$
(5.3.3)

$$ik\nu(q)v - \{2i\lambda_5\omega + k^2\sigma(q)\}c = 0,$$
 (5.3.4)

from which we obtain the following analogue of the determinant condition contained in equation (5.2.30):

$$\{\eta(q) + 2i\rho\xi\}\{\sigma(q) + 2i\lambda_5\xi\} - 2i\xi\nu^2(q) = 0.$$
(5.3.5)

In the above, $\eta(q)$ and $\nu(q)$ denote the somewhat unwieldy combinations of SmC viscosities

$$\eta(q) = \eta_1 q^2 + \eta_2 q \sin \phi + \eta_3 \sin^2 \phi, \qquad (5.3.6)$$

where

$$\eta_{1} = \eta_{11} \sin^{2} \theta + \eta_{12} \sin(2\theta) + \eta_{13} \cos^{2} \theta,$$

$$\eta_{2} = 2\eta_{12} \cos(2\theta) + (\eta_{11} - \eta_{13}) \sin(2\theta),$$

$$\eta_{3} = \eta_{11} \cos^{2} \theta - \eta_{12} \sin(2\theta) + \eta_{13} \sin^{2} \theta,$$

(5.3.7)

with

$$\eta_{11} = \mu_0 + \mu_2 - 2\lambda_1 + \lambda_4,$$

$$\eta_{12} = \tau_1 + \tau_2 - \tau_5 - \kappa_1,$$

$$\eta_{13} = \mu_0 + \mu_4 - 2\lambda_2 + \lambda_5,$$

(5.3.8)

and

$$\nu(q) = \nu_1 q + \nu_2 \sin \phi, \tag{5.3.9}$$

where

$$\nu_1 = (\tau_1 - \tau_5) \sin \theta - (\lambda_2 - \lambda_5) \cos \theta,$$

$$\nu_2 = (\tau_1 - \tau_5) \cos \theta + (\lambda_2 - \lambda_5) \sin \theta.$$
(5.3.10)

The term $\sigma(q)$, meanwhile, denotes a similar combination of SmC elastic constants, and is given by

$$\sigma(q) = \sigma_1 q^2 + \sigma_2 q \sin \phi + \sigma_3 \sin^2 \phi, \qquad (5.3.11)$$
where (in the notation of Stewart [68, equations (6.15), (6.34), and (6.25)]),

$$\sigma_{1} = K_{4} \sin^{2} \theta + K_{7} \sin(2\theta) + K_{3} \cos^{2} \theta,$$

$$\sigma_{2} = 2K_{7} \cos(2\theta) + (K_{4} - K_{3}) \sin(2\theta),$$

$$\sigma_{3} = K_{4} \cos^{2} \theta - K_{7} \sin(2\theta) + K_{3} \sin^{2} \theta.$$

(5.3.12)

Notice that (5.3.5) is a quartic in q, so that there are four solutions for q; as discussed in Section 5.2.1 above, only those solutions q with a negative imaginary part are of physical relevance. These are [24]

$$q_1 = (1-i)\sqrt{\frac{\xi\Gamma_1}{\eta_1\sigma_1}}, \qquad q_2 = \varepsilon - i\zeta, \qquad \zeta > 0, \qquad (5.3.13)$$

where

$$\varepsilon = \frac{b_2}{\zeta} - \frac{\Gamma_2 \sin \phi}{2\Gamma_1}, \qquad \qquad \zeta = \sqrt{\frac{1}{2} \left(\sqrt{b_1^2 + 4b_2^2} - b_1\right)}, \qquad (5.3.14)$$

$$b_1 = \left(\frac{\Gamma_2^2}{4\Gamma_1^2} - \frac{\Gamma_3}{\Gamma_1}\right)\sin^2\phi, \qquad b_2 = \frac{\rho\xi\lambda_5}{\Gamma_1},\tag{5.3.15}$$

on setting

$$\Gamma_1 = \lambda_5 \eta_1 - \nu_1^2, \qquad \Gamma_2 = \lambda_5 \eta_2 - 2\nu_1 \nu_2, \qquad \Gamma_3 = \lambda_5 \eta_3 - \nu_2^2, \qquad (5.3.16)$$

and making use of certain approximations, for instance $\rho\sigma_1 \ll \Gamma_1$ [25]. At normal incidence, we have

$$q_1 = (1-i)\sqrt{\frac{\xi\Gamma_1}{\eta_1\sigma_1}}, \qquad q_2 = (1-i)\sqrt{\frac{\rho\xi\lambda_5}{\Gamma_1}},$$
 (5.3.17)

from which the Stokes layer for mode 1 and mode 2 are, respectively,

$$\delta_1 = \sqrt{\frac{\eta_1 \sigma_1}{\omega \Gamma_1}}, \qquad \delta_2 = \frac{1}{k\zeta}, \tag{5.3.18}$$

the second of these reducing at normal incidence to

$$\delta_2|_{\phi=0} = \sqrt{\frac{\Gamma_1}{\rho\omega\lambda_5}}.$$
(5.3.19)

As remarked by Gill [24], the dependence of q_1 on the elastic constants leads to it

being regarded as an orientational mode relating to attenuation of reorientation of the *c*-director, while mode 2 is a hydrodynamic mode, characterising attenuation due to the diffusion of a vorticity. Note that the corresponding dependence of δ_1 on σ_1 leads to the conclusion that $\delta_1 \ll \delta_2$, and thus mode 2 will be dominant after a depth $\sim \delta_1$ into the smectic.

In what follows, it is the behaviour of mode 2 which will be of interest, since it is this mode which is analogous to the SmA solution for q at (5.2.34) in SmA. Recall that, in this case, the depth of the Stokes layer is given by equation (5.2.37), or (5.2.38) in the case of normal incidence.

Interfacial Conditions

Recalling that there are two modes to be considered, a slight modification of the interfacial conditions (5.2.39) and (5.2.41) in Section 5.2.1 is required. Specifically, we have continuity of velocity

$$i\omega(A+B) = v_1 + v_2 \tag{5.3.20}$$

and traction

$$2\mu_s(A-B)\cos\phi = \eta_1(q_1v_1 + q_2v_2) + \frac{1}{2}\eta_2(v_1 + v_2)\sin\phi, \qquad (5.3.21)$$

the latter reducing at normal incidence to

$$2\mu_s(A-B) = \eta_1(q_1v_1 + q_2v_2). \tag{5.3.22}$$

Further, strong anchoring at the boundary requires that

$$c_1 + c_2 = 0. \tag{5.3.23}$$

5.3.2 Expressions for the Amplitudes

In a similar manner to the calculations carried out to obtain the results in Section 5.2.3 for SmA, we obtain for the SmC (where we will henceforth, when required, denote any physical quantities relevant to SmA or SmC with subscript A or C, respectively):

$$B_{\rm c} = \frac{A\{f^+f^- - g^2 - ig(f^+ + f^-)\}}{(f^+)^2 + g^2},$$
(5.3.24)

where, for convenience, we have defined

$$f^{\pm} = 4\rho_s \xi \lambda_5 \cos \phi \pm 2\Gamma_1 \zeta, \qquad (5.3.25)$$

$$g = 2\Gamma_1 \varepsilon + \Gamma_2 \sin \phi. \tag{5.3.26}$$

It then follows that

$$|B_{\rm c}| = \frac{A\sqrt{(f^+f^- - g^2)^2 + g^2(f^+ + f^-)^2}}{(f^+)^2 + g^2},$$
(5.3.27)

and the corresponding quantities at normal incidence are

$$B_{\rm C}|_{\phi=0} = A \left\{ \frac{2\rho_s^2 \xi \lambda_5 - \rho \Gamma_1 - 2i\rho_s \sqrt{\rho \xi \lambda_5 \Gamma_1}}{2\rho_s^2 \xi \lambda_5 + \rho \Gamma_1 + 2\rho_s \sqrt{\rho \xi \lambda_5 \Gamma_1}} \right\}$$
(5.3.28)

and

$$|B_{\rm c}|_{\phi=0} = \frac{A\sqrt{4\rho_s^4\xi^2\lambda_5^2 + \rho^2\Gamma_1^2}}{2\rho_s^2\xi\lambda_5 + \rho\Gamma_1 + 2\rho_s\sqrt{\rho\xi\lambda_5\Gamma_1}}.$$
 (5.3.29)

In order to solve for the refracted wave velocity amplitudes $v_{1,2}$, it proves necessary to solve for the *c*-director; making use of the strong anchoring condition above at (5.3.23) and [25, eqs. (5.6), (4.3)], one obtains

$$c_{2} = -c_{1} = \frac{Ak(f^{+} + f^{-}) \{f^{+}l_{2} + gl_{1} + i(f^{+}l_{1} - gl_{2})\}}{2\lambda_{5} \{(f^{+})^{2} + g^{2}\}}$$
(5.3.30)

in which

$$l_1 = \nu_1 \varepsilon + \nu_2 \sin \phi, \qquad l_2 = \nu_1 \zeta.$$
 (5.3.31)

We record that, for mode one, the velocity amplitude is given by

$$v_1 = \frac{Ak\nu_1(f^+ + f^-)}{2\lambda_5} \sqrt{\frac{\omega\sigma_1}{\eta_1\Gamma_1}} \left\{ \frac{f^+h^- + gl + i(f^+l - gh^+)}{(f^+)^2 + g^2} \right\},$$
 (5.3.32)

where

$$h^{\pm} = \pm \{\nu_1(\varepsilon - \zeta) + \nu_2 \sin \phi\}$$
 (5.3.33)

and $l = l_1 + l_2$ as given in (5.3.31). As for the second mode, it is tedious but relatively straightforward to find that

$$v_2 = \frac{A\omega(f^+ + f^-)(g + if^+)}{(f^+)^2 + g^2},$$
(5.3.34)

and the modulus is simply

$$|v_2| = \frac{A\omega(f^+ + f^-)}{\sqrt{(f^+)^2 + g^2}}.$$
(5.3.35)

At normal incidence, it follows that these quantities are given by

$$v_2|_{\phi=0} = 2A\rho_s\omega \left\{ \frac{2i\rho_s\xi\lambda_5 + (1+i)\sqrt{\rho\xi\lambda_5\Gamma_1}}{2\rho_s^2\xi\lambda_5 + \rho\Gamma_1 + 2\rho_s\sqrt{\rho\xi\lambda_5\Gamma_1}} \right\},\tag{5.3.36}$$

$$|v_2|_{\phi=0} = \frac{2A\rho_s\omega\sqrt{2\xi\lambda_5}}{2\rho_s^2\xi\lambda_5 + \rho\Gamma_1 + 2\rho_s\sqrt{\rho\xi\lambda_5\Gamma_1}}.$$
(5.3.37)

We therefore obtain the analogous quantities to those given in equations (5.2.61) and (5.2.62) (recalling that we are seeking the hydrodynamic modes in each of the smectics):

$$|C_{\rm c}| = \frac{A(f^+ + f^-)}{\sqrt{g^2 + (f^+)^2}},\tag{5.3.38}$$

with normal incidence easily following from (5.3.36), viz.,

$$|C_{\rm c}|_{\phi=0} = \frac{2A\rho_s\sqrt{2\xi\lambda_5}}{\sqrt{2\rho_s^2\xi\lambda_5 + \rho\Gamma_1 + 2\rho_s\sqrt{\rho\xi\lambda_5\Gamma_1}}}.$$
(5.3.39)

5.4 Comparison of the Responses of Smectics A and C

In this section we present some numerical examples demonstrating the response of both smectics A and C for a set of physical parameters typical of these materials. The values for SmA may be found above in Table 3.1, while the SmC parameters used are tabulated in Table 5.1.

Parameter	Value [68, p. 301] (Pas)
η_{11}	0.0377
η_{12}	-0.0366
η_{13}	0.0533
$\lambda_5 - \lambda_2$	0.0325
$ au_5 - au_1$	0.0273

Table 5.1: Values of the SmC viscosity coefficients used in the plots to follow.

5.4.1 Normal Incidence

The graphs presented in Figs. 5.4 and 5.5 compare the behaviour of both the reflected and refracted wave amplitudes in smectics A and C at normal incidence. From the two graphs contained in Fig. 5.5, it is readily observed that the behaviour of each of these expressions in (5.2.62) and (5.3.38) is qualitatively the same, and we deduce that, until $\omega \sim 10^{10}$ Hz,

$$|C_{\rm A}|_{\phi=0} \sim \left(2 - 1.01 \times 10^{-6} \sqrt{\omega}\right) A,$$
 (5.4.1)

$$|C_{\rm c}|_{\phi=0} \sim \left(2 - 4.12 \times 10^{-7} \sqrt{\omega}\right) A,$$
 (5.4.2)

from which it is evident that $|C_A|_{\phi=0} \doteq 1.9A$ and $|C_C|_{\phi=0} \doteq 1.96A$ when $\omega = 10^{10}$ Hz, both showing comparatively little change over the range $0 \le \omega \le 10^{10}$ Hz. Thereafter, the refracted wave amplitudes begin to fall off more noticeably, and by $\omega = 10^{14}$ Hz, $|C_A|_{\phi=0}$ is just over one tenth of its initial value, while $|C_C|_{\phi=0}$ is somewhat below thirty percent of its initial value.

5.4.2 Oblique Incidence

The plots contained in Figs. 5.6 and 5.7 demonstrate the variation of angle of incidence of the shear wave upon the amplitudes of the reflected and refracted wave amplitudes, respectively. In Figs. 5.6 (a),(b), one sees different qualitative behaviour of the reflected wave amplitude as a function of ϕ for values of ω above 10^{10} Hz: in the SmC case, the angle of incidence has little apparent effect upon the value of this amplitude, while in the case of SmA, increasing the value of ϕ from 0 to ~1 rad leads to a significant increase in the value of this amplitude.

In an analogous fashion, Figs. 5.7 (a),(b) show that, while the SmC refracted wave amplitude does not show an especially strong dependence on ϕ for a given value of ω , the SmA refracted wave amplitude varies in a striking nonlinear manner as ϕ is increased for values of ω above 10¹¹, first increasing slightly, then falling off rapidly.



Figure 5.4: The amplitudes $|B_A|_{\phi=0}$ and $|B_C|_{\phi=0}$ of the reflected waves at normal incidence with (a) a linear scale and (b) a logarithmic scale for the horizontal axis. See Table 3.1 and Table 5.1 for material parameter values. Note that for all plots we have normalised by setting A = 1



(a)

Figure 5.5: The amplitudes $|C_A|_{\phi=0}$ and $|C_C|_{\phi=0}$ of the refracted waves at normal incidence with (a) a linear scale and (b) a logarithmic scale for the horizontal axis.



(b)

Figure 5.6: The variation of the amplitudes (a) $|B_A|$ and (b) $|B_C|$ of the reflected waves with angle of incidence ϕ for selected values of ω .



(b)

Figure 5.7: The variation of the amplitudes (a) $|C_A|$ and (b) $|C_C|$ of the refracted waves with angle of incidence ϕ .

5.5 Discussion and Possibilities for Further Work

Results have been presented regarding the behaviour of a shear wave at a plane interface between an isotropic elastic solid and a semi-infinite sample of SmA, fully establishing the behaviour of the reflected and refracted waves in terms of the problem's physical parameters. In particular, the refracted wave number q, which characterises the attenuation of the wave in the SmA case, was provided in terms of the parameters characterising the solid and the smectic by equation (5.2.34). Further, expressions for the amplitudes of both the reflected and refracted waves have been derived in terms of the incident wave amplitude and these parameters, where the general case of oblique incidence is as stated above in equations (5.2.56), (5.2.61). For the purpose of a qualitative comparison, we derived analogous terms via the results of Gill and Leslie [25], who performed calculations for the identical experiment for a sample of SmC, utilising the LSN theory for this phase. It is readily seen that, at normal incidence, the behaviour of the two phases is qualitatively the same, with the refracted wave amplitudes showing a departure in behaviour from the approximate expressions given in equations (5.4.1) and (5.4.2) as ω attains values ~ 10¹⁰Hz and above. Before ω attains this value, the aforementioned expressions provide a very accurate approximation to the respective solutions for the refracted wave amplitudes given in (5.2.62) and (5.3.38).

In the case of oblique incidence, we see an interesting difference in the behaviours of the two types of smectic, with varying angle of incidence having a significant effect on the both the reflected and refracted wave amplitudes in the SmA case while barely changing the analogous quantities in the SmC case. This may come as something of a surprise: one might expect that the amplitude of oscillations would depend upon the angle of incidence for both phases, given their anisotropy and not entirely dissimilar molecular structure. It remains unclear to the author as to why this is the case.

It could be argued that the comparison of the behaviour of the two smectics considered in this chapter is not quite a fair one: as previously mentioned, the SmA dynamic theory of Stewart allows for both permeation between the smectic layers and variability of the layers themselves, while the LSN theory for SmC accounts for neither. Nevertheless, the linear analysis outlined in this chapter requires that the layer displacement of the SmA is treated as zero (recalling equation (5.2.26)) and thus the phenomenon of permeation plays no role; it stands to reason that we would expect the same to be true for SmC.

The assumption of spatially semi-infinite samples is valid when the sample

depth is greater than the penetration depth of the relevant smectic. It may prove instructive to consider a smectic confined to a region with at least one of its boundary lengths less than that of these penetration depths and investigate the effects of sample boundaries in this case. Further, the stability of the material's layered structure to perturbations will presumably be valid for sufficiently small amplitudes of incident wave; just how sensitive this structure is to disturbances of higher amplitude and what exactly the threshold for the onset of damage might be are matters for further investigation. For the latter case, however, it is worth noting that a linear analysis may not be able to capture fully the behaviour of the SmA: at the very least, permeation of molecules between the layers may prove a non-negligible effect. This being the case, one would need to look beyond LSN theory for SmC to a model allowing for flexible layers and permeation.

Finally, it is worth noting that both the SmA and SmC cases could be generalised further to account for arbitrary tilts of the layer normal and/or director alignment with respect to the solid/smectic interface, weaker anchoring constraints on the director at the boundary, or considering a curved interface separating the solid and smectic. In each case, especially the latter, the mathematical work may be significantly more involved.

Chapter 6

Edge Dislocations in Smectic A Liquid Crystals

6.1 Introduction

This chapter is concerned with the problem of determining the configuration of the layer normal and director profile of a sample of SmA in the presence of an edge dislocation. Background material on the theory of edge dislocations in crystalline solid media may be found in references [30, 35, 36]; for information regarding dislocations in smectics, the reader may consult the latter two of these references or the book of de Gennes and Prost [23]. While previous works have derived expressions for the smectic layer displacement u in the presence of these defects, all the aforementioned references have failed to take into account any independent distortion of the director field, assuming that it always coincides with layer normal. Moreover, the authors have predominantly operated under the assumption that the energy density associated with deformations caused by the edge dislocation is quadratic in spatial derivatives of the layer displacement, thus leading to linearity of the resultant Euler-Lagrange equation whose solution determines the layer displacement which minimises the energy cost associated with the presence of the dislocation.

More recent work due to Brener and Marchenko [9] deals with an energy density which contains an extra term, which is quartic in a spatial derivative of u. A summary of their work, which will be shown to arise as a special case of the considerations to follow, will be given in Section 6.2 below. As before, however, the authors still operate under the assumption that the layer normal and director profile are always coincident, and are therefore confined to an energy with only two material constants.



Figure 6.1: Schematic representation of the configuration of the smectic layers in the presence of an edge dislocation. The Burgers vector in this case is $\boldsymbol{b} = d\boldsymbol{e}_z$, where d denotes the smectic interlayer distance.

In this chapter, the problem will be revisited under the framework of the De Vita-Stewart energy for non-polarisable SmA, as outlined above in Subsection 2.3.2 and recalled here for ease of reference:

$$w_{\rm DS} = \frac{1}{2} K_1^a (\nabla \cdot \boldsymbol{a})^2 + \frac{1}{2} K_1^n (\nabla \cdot \boldsymbol{n} - s_0)^2 + \frac{1}{2} K_2 \nabla \cdot [(\boldsymbol{n} \cdot \nabla) \boldsymbol{n} - (\nabla \cdot \boldsymbol{n}) \boldsymbol{n}] + \frac{1}{2} B_0 |\nabla \Phi|^{-2} (1 - |\nabla \Phi|)^2 + \frac{1}{2} B_1 [1 - (\boldsymbol{n} \cdot \boldsymbol{a})^2] + B_2 (\nabla \cdot \boldsymbol{n}) (1 - |\nabla \Phi|^{-1}), \qquad (2.3.11)$$

First, Section 6.2 provides a derivation of the energy density under the assumption of small deviations of both director and layer normal from the unstrained planar configuration n = a = (0, 0, 1). Section 6.3 presents the case where n and a are constrained to coincide, allowing for the recovery of the above noted results of previous investigations, as well as considering small time-independent perturbations to the layer displacement. In Section 6.4, we allow for separation of the director and layer normal. Taking the energy density to quadratic order allows us to formulate and solve the equilibrium equations, obtaining exact solutions for both the layer normal and director to this order of approximation. Tentative calculations in the direction of obtaining solutions to fourth order are outlined in Section 6.5, and we close the chapter with a summary of the results obtained and a discussion of potential further explorations in Section 6.6.

6.2 Calculating the Energy Density to Fourth Order

Consider a sample of SmA subject to an edge dislocation such that the Burgers vector of the dislocation, which will be taken to have magnitude b, and the dislocation axis are parallel to the z- and y- axes, respectively. We wish to measure the deviation of the configuration of the SmA away from that of the corresponding "relaxed" reference configuration, described by

$$n = n_0 \equiv (0, 0, 1), \qquad \Phi = \Phi_0 \equiv z.$$
 (6.2.1)

The imposed dislocation will then lead to a director profile of the form

$$\boldsymbol{n} = (\sin\theta, 0, \cos\theta), \tag{6.2.2}$$

while the function Φ is modified to read

$$\Phi = z - u(x, z). \tag{6.2.3}$$

From the latter equation, it readily follows that $\nabla \Phi = (-u_x, 0, 1 - u_z)$, and thus

$$\boldsymbol{a} = \frac{(-u_x, 0, 1 - u_z)}{\sqrt{1 - 2u_z + u_x^2 + u_z^2}},\tag{6.2.4}$$

where, for the remainder of this chapter, we employ the convention that a variable appearing in a subscript denotes partial differentiation with respect to that variable for ease of notation. Given the somewhat unwieldy form of equation (6.2.4) for \boldsymbol{a} , it makes sense as a first step to follow previous work [9, 36] and assume that only small deviations away from the reference configuration are anticipated, and that such deformations occur sufficiently slowly that we need only take into account terms to quartic order in a Taylor series of the various terms involved when computing the energy density. In spite of the lengthiness of some of the resultant expressions, working to fourth order allows for the possibility of capturing behaviour which could be missed on only retaining only lower-order terms. (Note, however, that numerical methods probably provide the best route for determining this given the intractable nature of the expressions which arise; these are not pursued in this thesis.) Further, it follows that all results in the aforementioned previous work should be readily attained by truncation of at the appropriate lower order.

Equation (6.2.2) may be approximated by

$$\boldsymbol{n} = \left(\theta - \frac{1}{6}\theta^3, 0, 1 - \frac{1}{2}\theta^2 + \frac{1}{24}\theta^4\right), \qquad (6.2.5)$$

from which it is readily deduced that $\mathbf{n} \cdot \mathbf{n} = 1 + \mathcal{O}(\theta^6)$. Further, on noting that, for $v \ll 1$

$$\sqrt{1+v} = 1 + \frac{1}{2}v - \frac{1}{8}v^2 + \frac{1}{16}v^3 - \frac{5}{128}v^4 + \mathcal{O}(v^5),$$
$$\frac{1}{\sqrt{1+v}} = 1 - \frac{1}{2}v + \frac{3}{8}v^2 - \frac{5}{16}v^3 + \frac{35}{128}v^4 + \mathcal{O}(v^5),$$

it is easy to show that the approximations

$$|\nabla\Phi| = 1 - u_z + \frac{1}{2}u_x^2 + \frac{1}{2}u_x^2u_z - \frac{1}{8}u_x^4 + \frac{1}{2}u_x^2u_z^2, \qquad (6.2.6)$$

$$|\nabla\Phi|^{-1} = 1 + u_z - \frac{1}{2}u_x^2 + u_z^2 + u_z^3 - \frac{3}{2}u_x^2u_z + \frac{3}{8}u_x^4 + u_z^4 - 3u_x^2u_z^2, \qquad (6.2.7)$$

hold to fourth order, and thus we may approximate \boldsymbol{a} as

$$\boldsymbol{a} = \left(-u_x - u_x u_z + \frac{1}{2}u_x^3 - u_x u_z^2(1+u_z) + \frac{3}{2}u_x^3 u_z, \\ 0, \ 1 - \frac{1}{2}u_x^2 - u_x^2 u_z + \frac{3}{8}u_x^4 - \frac{3}{2}u_x^2 u_z^2\right).$$
(6.2.8)

It readily follows that a is also a unit vector to fourth order. We may now use equations (6.2.5) and (6.2.6)–(6.2.8) to compute the terms comprising w_{DS} . Firstly, a simple calculation yields

$$(\nabla \cdot \boldsymbol{a})^2 = u_{xx}^2 + 2u_{xx}^2 u_z + 4u_x u_{xx} u_{xz} + 3u_{xx}^2 u_z^2 + 4u_x^2 u_{xz}^2 - 3u_x^2 u_{xx}^2 + 2u_x^2 u_{xx} u_{zz} + 12u_x u_{xx} u_z u_{xz}, \qquad (6.2.9)$$

while

$$(\nabla \cdot \boldsymbol{n} - s_0)^2 = \theta_x^2 - 2\theta \theta_x \theta_z + \theta^2 (\theta_z^2 - \theta_x^2) + s_0 \left(s_0 - 2\theta_x + 2\theta \theta_z + \theta^2 \theta_z - \frac{1}{3} \theta^3 \theta_z \right).$$
(6.2.10)

Tedious but straightforward calculations allow us to conclude that

$$(\boldsymbol{n} \cdot \nabla)\boldsymbol{n} - (\nabla \cdot \boldsymbol{n})\boldsymbol{n} = (\theta_z, 0, -\theta_x),$$

$$\implies \nabla \cdot \{(\boldsymbol{n} \cdot \nabla)\boldsymbol{n} - (\nabla \cdot \boldsymbol{n})\boldsymbol{n}\} = 0, \qquad (6.2.11)$$

where it is assumed that partial derivatives of θ commute. Squaring both sides of equation (6.2.7) leads to

$$|\nabla\Phi|^{-2} = 1 + 2u_z - u_x^2 + 3u_z^2 + 4u_z^3 - 4u_x^2u_z + u_x^4 + 5u_z^4 - 10u_x^2u_z^2, \quad (6.2.12)$$

which, taken in conjunction with (6.2.6), allows us to conclude

$$|\nabla\Phi|^{-2} \left(1 - |\nabla\Phi|\right)^2 = u_z^2 + 2u_z^3 - u_x^2 u_z + \frac{1}{4}u_x^4 + 3u_z^4 - 4u_x^2 u_z^2.$$
(6.2.13)

Taken together, equations (6.2.5) and (6.2.8) yield

$$\boldsymbol{n} \cdot \boldsymbol{a} = 1 - \theta u_x - \frac{1}{2}\theta^2 - u_x^2 u_z + \frac{1}{2}\theta u_x^3 - \theta u_x u_z^2 + \frac{1}{6}\theta^3 u_x + \frac{3}{8}u_x^4 - \frac{3}{2}u_x^2 u_z^2 + \frac{1}{24}\theta^4 + \frac{1}{4}\theta^2 u_x^2,$$
(6.2.14)

from which

$$1 - (\boldsymbol{n} \cdot \boldsymbol{a})^2 = \theta^2 + u_x^2 + 2\theta u_x + 2u_x^2 u_z + 2\theta u_x u_z - \frac{1}{3}\theta^4 - u_x^4 - 2\theta u_x^3 - \frac{4}{3}\theta^3 u_x - 2\theta^2 u_x^2 + 2\theta u_x u_z^2 + 3u_x^2 u_z^2.$$
(6.2.15)

Finally, since

$$\nabla \cdot \boldsymbol{n} = \theta_x - \theta \theta_z - \frac{1}{2} \theta^2 \theta_x - \frac{1}{6} \theta^3 \theta_z, \qquad (6.2.16)$$

it may be deduced by further appeal to equation (6.2.7) that

$$(\nabla \cdot \boldsymbol{n}) \left(1 - |\nabla \Phi|^{-1} \right) = -\theta_x u_z + \frac{1}{2} \theta_x u_x^2 - \theta_x u_z^2 + \theta \theta_z u_z - \theta_x u_z^3 + \frac{3}{2} \theta_x u_x^2 u_z - \frac{1}{2} \theta \theta_z u_x^2 + \theta \theta_z u_z^2 + \frac{1}{2} \theta^2 \theta_x u_z.$$
(6.2.17)

Putting all this together, the energy density $w_{\scriptscriptstyle\rm DS}$ may be expressed to fourth order in the form

$$w_{\rm DS} = \frac{1}{2} K_1^a (u_{xx}^2 + 2u_{xx}^2 u_z + 4u_x u_{xx} u_{xz} + 3u_{xx}^2 u_z^2 + 4u_x^2 u_{xz}^2 - 3u_x^2 u_{xx}^2 + 2u_x^2 u_{xx} u_{zz} + 12u_x u_{xx} u_z u_{xz}) + \frac{1}{2} K_1^n \left\{ \theta_x^2 - 2\theta \theta_x \theta_z + \theta^2 (\theta_z^2 - \theta_x^2) + s_0 \left(s_0 - 2\theta_x + 2\theta \theta_z + \theta^2 \theta_z - \frac{1}{3} \theta^3 \theta_z \right) \right\} + \frac{1}{2} B_0 \left(u_z^2 + 2u_z^3 - u_x^2 u_z + \frac{1}{4} u_x^4 + 3u_z^4 - 4u_x^2 u_z^2 \right) + \frac{1}{2} B_1 \left(\theta^2 + u_x^2 + 2\theta u_x + 2u_x^2 u_z + 2\theta u_x u_z - \frac{1}{3} \theta^4 - u_x^4 - 2\theta u_x^3 - \frac{4}{3} \theta^3 u_x - 2\theta^2 u_x^2 + 2\theta u_x u_z^2 + 3u_x^2 u_z^2 \right) + B_2 \left(-\theta_x u_z + \frac{1}{2} \theta_x u_x^2 - \theta_x u_z^2 + \theta \theta_z u_z - \theta_x u_z^3 + \frac{3}{2} \theta_x u_x^2 u_z - \frac{1}{2} \theta \theta_z u_x^2 + \theta \theta_z u_z^2 + \frac{1}{2} \theta^2 \theta_x u_z \right).$$
(6.2.18)

As stated in Subsection 2.3.2, the energy density w_A for samples of SmA consisting of non-polarisable molecules is recovered when $s_0 = K_2 = B_0 = 0$.

6.3 Director and Layer Normal Coincident

In this section, we impose the requirement that the director and layer normal show no decoupling, thus enabling us to recover the results of the aforementioned previous work. In this instance, the energy density simplifies further still, viz.,

$$w_{\rm A} = \frac{1}{2} (K_1^a + K_1^n) (\nabla \cdot \boldsymbol{a})^2 + \frac{1}{2} B_0 |\nabla \Phi|^{-2} (1 - \nabla |\Phi|)^2$$

= $\frac{1}{2} (B_0 w_0 + K_1 w_1^a),$ (6.3.1)

where $K_1 = K_1^a + K_1^n$ and

$$w_{0} = \left(u_{z} - \frac{1}{2}u_{x}^{2}\right)^{2} + u_{z}^{3}(2 + 3u_{z}) - 4u_{x}^{2}u_{z}^{2}, \qquad (6.3.2)$$

$$w_{1}^{a} = u_{xx}^{2} + 2u_{xx}^{2}u_{z} + 4u_{x}u_{xx}u_{xz} + 3u_{xx}^{2}u_{z}^{2} + 4u_{x}^{2}u_{xz}^{2} - 3u_{x}^{2}u_{xx}^{2} + 2u_{x}^{2}u_{xx}u_{zz} + 12u_{x}u_{xx}u_{z}u_{xz}. \qquad (6.3.3)$$

In order to obtain an expression for the layer displacement u, we require the minimum of the energy per unit length in the y-direction, which may be written

$$W = \int_D w_{\rm A} \, dA, \tag{6.3.4}$$

where D denotes the two-dimensional domain occupied by the SmA sample, which in this chapter is taken to be all of \mathbb{R}^2 . This necessitates an appeal to standard methods of the calculus of variations, a cursory overview of which is presented in Appendix C. For an overview of the methods to be utilised here, the reader may also consult reference [11]. Let us calculate the first variation of the energy δW , defined for admissible variations h (see Appendix C) by

$$\delta W = \frac{d}{dt} \iint_{\mathbb{R}^2} \eta \, dx dz \bigg|_{t=0} = \iint_{\mathbb{R}^2} \left\{ \partial_t (\eta_0 + \eta_1^a) \right\} \big|_{t=0} \, dx dz, \tag{6.3.5}$$

where we have set

$$\eta_0 = w_0(u+th) - w_0(u), \qquad \eta_1^a = w_1^a(u+th) - w_1^a(u), \qquad (6.3.6)$$

and

$$\eta = \eta_0 + \eta_1^a = w_A(u + th) - w_A(u).$$
(6.3.7)

It is a tedious but simple matter to compute the following:

$$\eta_{0} = t \left\{ h_{x}(u_{x}^{3} - 2u_{x}u_{z} - 8u_{x}u_{z}^{2}) + h_{z}(2u_{z} + 6u_{z}^{2} - u_{x}^{2} + 12u_{z}^{3} - 8u_{x}^{2}u_{z}) \right\} + \mathcal{O}(t^{2}), \qquad (6.3.8)$$
$$\eta_{1}^{a} = t \left\{ h_{xx}(2u_{xx} + 4u_{xx}u_{z} + 4u_{x}uxz + 6u_{xx}u_{z}^{2} - 6u_{x}^{2}u_{xx} + 2u_{x}^{2}u_{zz} + 12u_{x}u_{z}u_{xz}) + h_{xz}(4u_{x}u_{xx} + 8u_{x}^{2}u_{xz} + 12u_{x}u_{xx}u_{z}) + 2h_{zz}u_{x}^{2}u_{xx} + h_{x}(4u_{xx}u_{xz} + 8u_{x}u_{xz}^{2} - 6u_{x}u_{xx}^{2} + 4u_{x}u_{xx}u_{zz} + 12u_{xx}u_{z}u_{xz}) + h_{z}(2u_{xx}^{2} + 6u_{xx}^{2}u_{z} + 12u_{z}u_{xx}u_{xz}) \right\} + \mathcal{O}(t^{2}), \qquad (6.3.9)$$

from which it readily follows that the integrand of δW is simply the sum of the terms enclosed in curly brackets within equations (6.3.8) and (6.3.9). Writing $\delta W = \delta W_0 + \delta W_1^a$, where

$$\delta W_0 = \frac{1}{2} B_0 \iint_{\mathbb{R}^2} (\partial_t \eta_0)|_{t=0} \, dx dz, \qquad \delta W_1^a = \frac{1}{2} K_1 \iint_{\mathbb{R}^2} (\partial_t \eta_1^a)|_{t=0} \, dx dz,$$

it follows that we may, on integrating by parts and requiring that any admissible h and spatial derivatives thereof vanish at the limits of integration, rewrite δW_0 and δW_1 in the respective forms

$$\delta W_0 = B_0 \iint_{\mathbb{R}^2} h \left\{ u_{xx} \left(4u_z^2 - \frac{3}{2}u_x^2 + u_z \right) + u_{zz} (4u_x^2 - 18u_z^2 - 6u_z - 1) + 2u_x u_{xz} (8u_z + 1) \right\} dxdz,$$
(6.3.10)

$$\delta W_1^a = K_1 \iiint_{\mathbb{R}^2} h \left\{ u_{xxxx} (3u_z^2 - 3u_x^2 + 2u_z + 1) + 4u_x u_{xxxz} (3u_z + 1) \right. \\ \left. + 6u_x^2 u_{xxzz} + 6u_{xxx} (3u_z u_{xz} - 2u_x u_{xx} + u_x u_{zz} + u_{xz}) \right. \\ \left. + 6u_{xxz} (3u_{xx} u_z + 5u_x u_{xz} + u_{xx}) + 12u_x u_{xx} u_{xzz} \right. \\ \left. + 3u_{xx} (u_{xx} u_{zz} - u_{xx}^2 + 6u_{xz}^2) \right\} dxdz.$$

$$(6.3.11)$$

The energy W is then minimised by setting $\delta W = \delta W_0 + \delta W_1^a = 0$ for all admissible variations h, which yields a highly nonlinear and intractable partial differential equation for u. Progress regarding solutions u to the full equation is probably best achieved by appeal to computational means, and this will not be considered here. However, assuming small layer displacements with sufficiently small spatial derivatives, analytical progress can be made in the following manner: according to both theoretical studies [23, Subsection 9.2.1] and experimental observations [32], the distortion of the layered structure is essentially confined to parabolic regions described by $x^2 = c\lambda z$ for some constant c, where $\lambda = \sqrt{K_1/B_0}$, which tells us

that this configuration relaxes back to planar layers rapidly along x but significantly more slowly along z. Thus, if one assumes that $u_x \sim u/\xi$ and $u_z \sim u/L$ for some characteristic length scales ξ and L of displacement in the x and z directions, respectively, with $\xi^2 = \mathcal{O}(\lambda L)$, it is apparent from equations (6.3.10) and (6.3.11) that, on regarding terms of magnitude smaller than $\sim 1/\xi^4$ as negligible, one immediately arrives at the truncated equilibrium equation

$$\lambda^2 u_{xxxx} + u_{xx} \left(u_z - \frac{3}{2} u_x^2 \right) - u_{zz} + 2u_x u_{xz} = 0, \qquad (6.3.12)$$

for the case z > 0; a similar equation is obtained in the case z < 0. This is exactly the PDE obtained by Brener and Marchenko [9, equation (4)], which is then non-dimensionalised by means of measuring all lengths in terms of λ ; the non-dimensional form reads

$$u_{xxxx} + u_{xx} \left(u_z - \frac{3}{2} u_x^2 \right) - u_{zz} + 2u_x u_{xz} = 0, \qquad (6.3.13)$$

which may be solved by first noting that solutions to this equation also solve a lower-order PDE and solving this latter equation by appeal to the similarity variable $v = x/\sqrt{z}$ (see Appendix D for an outline of the method) subject to the condition

$$\lim_{v \to \infty} u(v) - \lim_{v \to -\infty} u(v) = \frac{b}{2}$$

to give

$$u = 2\lambda \ln\left\{\frac{1}{2}\left[1 + e^{b/4\lambda} + (e^{b/4\lambda} - 1)\operatorname{erf}\left(\frac{x}{2\sqrt{\lambda z}}\right)\right]\right\},\tag{6.3.14}$$

on returning to dimensional form. In the limit where $b \ll \lambda$, it is simple to show that $e^{b/4\lambda} \sim 1 + b/4\lambda$, which leads to

$$u \sim 2\lambda \ln \left\{ 1 + \frac{b}{8\lambda} \left[1 + \operatorname{erf} \left(\frac{x}{2\sqrt{\lambda z}} \right) \right] \right\}$$
$$\sim \frac{b}{4} \left\{ 1 + \operatorname{erf} \left(\frac{x}{2\sqrt{\lambda z}} \right) \right\}, \qquad (6.3.15)$$

this being exactly the result derived in the classical case [35, 36], which may also be obtained by only considering terms to quadratic order in u and its derivatives in the energy density.

As yet, the approach of Brener and Marchenko has not been found to be applicable when truncating the energy density at higher order, and the resultant equilibrium equations certainly do not admit solutions of the form $u(x/\sqrt{z})$. Moreover, given the unwieldy equations which arise from this higher order truncation, little is to be gained from an attempt at their analysis without appeal to computational means.

6.3.1 Perturbing Brener & Marchenko's Solution

In this subsection, we consider subjecting the solution for layer displacement of Brener and Marchenko, as stated in equation (6.3.14), to a small time-independent perturbation to in a bid to ascertain whether other equilibrium solutions may be found in the vicinity of that determined in reference [9]. Motivated by the work of Bogomol'nyi [8], the modified solution to the PDE (6.3.12) will be assumed to take the form

$$\hat{u} = u + \varepsilon(x, z), \tag{6.3.16}$$

with $|\varepsilon| \ll 1$. Substitution into the dimensionless equilibrium equation (6.3.13) leads to the requirement that ε approximately satisfies the PDE

$$\varepsilon_{xxxx} = \varepsilon_{zz} - 2(u_x\varepsilon_{xz} + u_{xz}\varepsilon_x) - u_{xx}\varepsilon_z - u_z\varepsilon_{xx} + \frac{3}{2}u_x^2\varepsilon_{xx} + 3u_xu_{xx}\varepsilon_x. \quad (6.3.17)$$

The solution \hat{u} is then a solution of equation (6.3.12) with the same energy as u for any ε satisfying this equation. Moreover, if ε is also a similarity solution of the form $\varepsilon(v)$ where $v = x/\sqrt{z}$, the PDE (6.3.17) may be rewritten to read

$$\psi''' = \frac{3}{4}v\psi + \frac{1}{4}v^2\psi' + 2\phi\psi + \frac{3}{2}v(\phi\psi)' + \frac{3}{2}(\phi^2\psi)', \qquad (6.3.18)$$

where $\phi = u'(v)$ and $\psi = \varepsilon'(v)$. For ease of reference, we record here that

$$\phi = \frac{2\left(e^{b/4} - 1\right)e^{-v^2/4}}{2\sqrt{\pi} + \left(e^{b/4} - 1\right)\int_{-\infty}^{v} e^{-t^2/4} dt} = \frac{2e^{-v^2/4}}{\sqrt{\pi}\left\{\coth(b/8) + \operatorname{erf}(v/2)\right\}}.$$
 (6.3.19)

The modified solution \hat{u} should satisfy the condition

$$\lim_{v \to \infty} \hat{u}(v) - \lim_{v \to -\infty} \hat{u}(v) = \frac{b}{2},$$

which leads to

$$\lim_{v \to \infty} \varepsilon(v) - \lim_{v \to -\infty} \varepsilon(v) = \int_{-\infty}^{\infty} \psi \, dv = 0.$$

Now, equation (6.3.18) may be written in the form

$$\psi''' = a(v)\psi' + b(v)\psi, \qquad (6.3.20)$$

where

$$a(v) = \frac{1}{4}v^2 + \frac{3}{2}\left(v\phi + \phi^2\right), \qquad b(v) = 2\phi + \frac{3}{2}\left\{v + v\phi' + \left(\phi^2\right)'\right\}.$$
(6.3.21)

From our expression for ϕ in equation (6.3.19), it follows that we may expand about an arbitrary point $v = v_0$ to obtain

$$\phi = \Gamma_0 - \Gamma_1 (v - v_0) + \Gamma_2 (v - v_0)^2 + \Gamma_3 (v - v_0)^3 + \mathcal{O}\left((v - v_0)^4 \right), \quad (6.3.22)$$

where

$$\Gamma_0 = \phi(v_0) = \frac{2e^{-v_0^2/4}}{\sqrt{\pi} \left\{ \coth(b/8) + \operatorname{erf}(v_0/2) \right\}},\tag{6.3.23}$$

$$\Gamma_1 = \phi'(v_0) = \frac{2e^{-v_0^2/2}}{\pi \left\{ \coth(b/8) + \operatorname{erf}(v/2) \right\}^2} + \frac{v_0 e^{-v_0^2/4}}{\sqrt{\pi} \left\{ \coth(b/8) + \operatorname{erf}(v/2) \right\}}, \quad (6.3.24)$$

$$\Gamma_{2} = \phi''(v_{0}) = \frac{2e^{-3v_{0}^{2}/4}}{\pi^{3/2} \left\{ \coth(b/8) + \operatorname{erf}(v/2) \right\}^{3}} + \frac{3v_{0}e^{-v_{0}^{2}/2}}{2\pi \left\{ \coth(b/8) + \operatorname{erf}(v/2) \right\}^{2}} + \frac{(v_{0}^{2} - 2) e^{-v_{0}^{2}/4}}{4\sqrt{\pi} \left\{ \coth(b/8) + \operatorname{erf}(v_{0}/2) \right\}}$$

$$(6.3.25)$$

$$\Gamma_{3} = \phi'''(v_{0}) = \frac{(6 - v_{0}^{2}) e^{-v_{0}^{2}/4}}{24\sqrt{\pi} \left\{ \coth(b/8) + \operatorname{erf}(v_{0}/2) \right\}} + \frac{(8 - 7v_{0}^{2}) e^{-v_{0}^{2}/2}}{12\pi \left\{ \coth(b/8) + \operatorname{erf}(v_{0}/2) \right\}^{2}} - \frac{2v_{0}e^{-3v_{0}^{2}/4}}{\pi^{3/2} \left\{ \coth(b/8) + \operatorname{erf}(v/2) \right\}^{3}} - \frac{2e^{-v_{0}^{2}}}{\pi^{2} \left\{ \coth(b/8) + \operatorname{erf}(v/2) \right\}^{4}}.$$
(6.3.26)

Note that, for a given value of v_0 , we have $x^2 = \lambda v_0^2 z$ (in dimensional variables): a parabola in the *xz*-plane with vertex at the origin and focus at $(x, z) = (0, \lambda v_0^2/4)$. The expansion (6.3.22) is thus an approximation to the behaviour of ϕ about this parabola. In the special case $v_0 = 0$, the approximation is valid about the straight line x = 0.

Using equation (6.3.22), we may deduce the following to quadratic order:

$$\phi^2 = \Gamma_0^2 - 2\Gamma_0\Gamma_1(v - v_0) + \left(\Gamma_1^2 + 2\Gamma_0\Gamma_2\right)(v - v_0)^2, \tag{6.3.27}$$

$$\phi' = -\Gamma_1 + 2\Gamma_2(v - v_0) + 3\Gamma_3(v - v_0)^2, \qquad (6.3.28)$$

$$\phi\phi' = -\Gamma_0\Gamma_1 + \left(\Gamma_1^2 + 2\Gamma_0\Gamma_2\right)(v - v_0) + 3\left(\Gamma_0\Gamma_3 - \Gamma_1\Gamma_2\right)(v - v_0)^2, \quad (6.3.29)$$

so that, on substitution into equations (6.3.21), we may write

$$a(v) = \frac{v^2}{4} + \frac{3}{2} \left\{ \left(\Gamma_2 v + \Gamma_1^2 + 2\Gamma_0 \Gamma_2 \right) (v - v_0)^2 - \Gamma_1 (v + 2\Gamma_2) (v - v_0) \right. \\ \left. + \Gamma_0 (v + \Gamma_0) \right\} + \mathcal{O} \left((v - v_0)^3 \right),$$
(6.3.30)

$$b(v) = \{2\Gamma_2 + 9(\Gamma_0\Gamma_3 - \Gamma_1\Gamma_2)\}(v - v_0)^2 + (3\Gamma_2v + 3\Gamma_1^2 + 6\Gamma_0\Gamma_2 - 2\Gamma_1)(v - v_0)$$

$$+\frac{3}{2}(1-\Gamma_1)v + \Gamma_0(2-3\Gamma_1) + \mathcal{O}\left((v-v_0)^3\right).$$
(6.3.31)

It follows that, if the layer displacement is modified by some small perturbation ε which may be expressed as a function of a similarity variable and which satisfies the ODE (6.3.18), then the function \hat{u} is a solution with approximately the same energy as the solution u due to Brener and Marchenko. In the neighbourhood of a given parabola $x^2 = \lambda v_0^2 z$, this ODE may be approximated by setting the coefficients a(v) and b(v) to the expressions stated in equations (6.3.30) and (6.3.31) above. Unfortunately no method attempted by the author led to an explicit solution ε to equation (6.3.18), though it is hoped that future work will enable progress in this direction.

6.4 Separation of Director and Layer Normal: Quadratic Order

In this section, we depart from the precedent set forth in previous work and allow n and a to separate. As a first step, we extend the most simple case by only retaining quadratic terms in u, θ and spatial derivatives thereof, obtaining exact solutions for both u and θ which we then compare with previous results via plots of their spatial variations for typical values of the constants appearing in the energy density.

6.4.1 Equilibrium Equations and Solution for the Layer Displacement

Recalling equation (6.2.18), it follows that the energy density w_A may be written to second order as

$$w_{\rm A} = \frac{1}{2} \left\{ K_1^a u_{xx}^2 + K_1^n \theta_x^2 + B_0 u_z^2 + B_1 (\theta + u_x)^2 \right\}.$$
 (6.4.1)

As above, we seek minimisers u and θ of the total energy per unit length in y, given above in (6.3.4), for which we require $\delta W = 0$. It is readily shown [11] that this requirement is equivalent to the following two PDEs

$$\frac{\partial^2}{\partial x^2} \left(\frac{\partial w_{\rm A}}{\partial u_{xx}} \right) = \frac{\partial}{\partial x} \left(\frac{\partial w_{\rm A}}{\partial u_x} \right) + \frac{\partial}{\partial z} \left(\frac{\partial w_{\rm A}}{\partial u_z} \right), \tag{6.4.2}$$

$$\frac{\partial}{\partial x} \left(\frac{\partial w_{\rm A}}{\partial \theta_x} \right) = \frac{\partial w_{\rm A}}{\partial \theta}.$$
(6.4.3)

Carrying out the required partial differentiation shows that these may be expressed in the forms

$$K_1^a u_{xxxx} = B_0 u_{zz} + B_1 (\theta_x + u_{xx}), (6.4.4)$$

$$K_1^n \theta_{xxx} = B_1(\theta_x + u_{xx}), \tag{6.4.5}$$

respectively. Note that requiring $\mathbf{n} = \mathbf{a}$ to second order gives $\theta + u_x = 0$ again, allowing for the recovery of the classical case provided we also set $K_1^n = 0$; we proceed with the general case $\mathbf{n} \neq \mathbf{a}$. Differentiating (6.4.5) twice with respect to x and rearranging gives

$$\theta_{xxx} = \frac{K_1^a}{B_1} u_{xxxxx} - \frac{B_0}{B_1} u_{zzxx} - u_{xxxx},$$

so that, on substitution into (6.4.5), it follows that

$$B_1(\theta_x + u_{xx}) = K_1^n \left(\frac{K_1^a}{B_1} u_{xxxxxx} - \frac{B_0}{B_1} u_{zxxx} - u_{xxxx} \right),$$

which may then be substituted into (6.4.4) to yield

$$\lambda_n^2 \left(u_{zzxx} - \lambda_a^2 u_{xxxxxx} \right) + \beta \left\{ \left(\lambda_a^2 + \lambda_n^2 \right) u_{xxxx} - u_{zz} \right\} = 0, \qquad (6.4.6)$$

where we have introduced the length scales

$$\lambda_a = \sqrt{K_1^a/B_0}, \qquad \lambda_n = \sqrt{K_1^n/B_0} \qquad (6.4.7)$$

to facilitate later comparisons with previously-established results, along with the dimensionless parameter β , given by

$$\beta = \frac{B_1}{B_0},\tag{6.4.8}$$

identical to the quantity introduced at equation (4.1.5) in Chapter 4 above.

Following the observation by Kleman and Lavrentovich [35] for the classical case, let us assume that the general solution to the PDE (6.4.6) in the region z > 0 may be expressed in the form

$$u(x,z) = \frac{b}{4} \left(1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{g(z)e^{i\sigma x}}{i\sigma} \, d\sigma \right). \tag{6.4.9}$$

Substitution into (6.4.6) readily yields the following ODE for g(z) in terms of the combination of parameters $\Gamma(\sigma)$:

$$g''(z) = \frac{\sigma^4 \left\{ \sigma^2 \lambda_a^2 \lambda_n^2 + \beta \left(\lambda_a^2 + \lambda_n^2 \right) \right\}}{\sigma^2 \lambda_n^2 + \beta} g(z) \equiv \Gamma^2(\sigma) g(z), \tag{6.4.10}$$

whose general solution is

$$g(z) = A(\sigma)e^{-\Gamma(\sigma)z} + B(\sigma)e^{\Gamma(\sigma)z}.$$

Since we require g(z) to be finite for all z > 0, it immediately follows that $B(\sigma) = 0$. Further, the boundary condition u(x, 0) = b/2 leads to the requirement

$$\int_{-\infty}^{\infty} \frac{A(\sigma)e^{i\sigma x}}{i\sigma} \, d\sigma = \pi. \tag{6.4.11}$$

Now, it may readily be shown by expanding $e^{i\vartheta} = \cos \vartheta + i \sin \vartheta$, substituting $x\sigma \to \tau$ and integrating along an appropriate contour in the complex plane that

$$\int_{-\infty}^{\infty} \frac{e^{i\sigma x}}{i\sigma} \, d\sigma = 2 \int_{0}^{\infty} \frac{\sin \tau}{\tau} \, d\tau = \pi,$$

from which it is evident that we may take $A(\sigma) \equiv 1$, and thus

$$u(x,z) = \frac{b}{4} \left(1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{i\sigma x - \Gamma(\sigma)z}}{i\sigma} \, d\sigma \right)$$
$$= \frac{b}{4} + \frac{b}{2\pi} \int_{0}^{\infty} \frac{e^{-\Gamma(\sigma)z} \sin(\sigma x)}{\sigma} \, d\sigma. \tag{6.4.12}$$

In Subsection 6.4.3 below we will go on to compute an exact solution for the director and compare its behaviour to that of the layer normal. First, however, we compare the behaviour of this solution u with its counterpart in the two-constant case as outlined by multiple authors [23, 35, 36].

6.4.2 Comparison with the Two-Constant Case

Let us denote the layer displacement in the classical case by v(x, z). This may be written in the form [35]

$$\upsilon(x,z) = \frac{b}{4} \left(1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{i\sigma x - \lambda_a \sigma^2 z}}{i\sigma} \, d\sigma \right)$$
$$= \frac{b}{4} + \frac{b}{2\pi} \int_{0}^{\infty} \frac{e^{-\lambda_a \sigma^2 z} \sin(\sigma x)}{\sigma} \, d\sigma, \qquad (6.4.13)$$

which is simply u(x, z) in the limit as either (or both) of λ_n , $\beta \to 0$. To facilitate graphical comparison of this displacement with that given above by equation (6.4.12), it proves convenient to write each of the expressions v and u above in terms of integrals over a finite domain. This is achieved by appeal to the substitution

$$\zeta = \frac{1}{1 + \lambda_a \sigma} \implies d\sigma = -\frac{d\zeta}{\lambda_a \zeta^2}, \tag{6.4.14}$$

so that equation (6.4.12) may, after appropriate substitution and rearrangement, be written in the form

$$u(x,z) = \frac{b}{4} + \frac{b}{2\pi} \int_0^1 g(\zeta) \, d\zeta, \qquad (6.4.15)$$

where

$$g(\zeta) = \frac{\exp\left\{-\Delta(\zeta)z\right\}\sin\left\{(\zeta^{-1} - 1)x/\lambda_a\right\}}{\zeta - \zeta^2},$$
(6.4.16)

with

$$\Delta(\zeta) = \frac{(1-\zeta)^2}{\lambda_a} \sqrt{\frac{\lambda_n^2 \left(\zeta^{-1} - 1\right)^2 + \beta \left(\lambda_a^2 + \lambda_n^2\right)}{\lambda_n^2 \left(\zeta - \zeta^2\right)^2 + \beta \lambda_a^2 \zeta^4}}.$$
 (6.4.17)

One readily deduces that

$$\Delta(\zeta) \to \infty \text{ as } \zeta \to 0^+, \quad \text{while} \quad \Delta(\zeta) \to 0 \text{ as } \zeta \to 1^-, \quad \text{from which}$$
$$g(\zeta) \to 0 \text{ as } \zeta \to 0^+ \quad \text{and} \quad g(\zeta) \to \frac{x}{\lambda_a} \text{ as } \zeta \to 1^-, \quad (6.4.18)$$

ensuring that the integral on the right-hand side of (6.4.15) does not diverge. Further, it is evident that the two displacements agree at the endpoints of integration by virtue of these limits being independent of both β and λ_n . Taking the appropriate limit in equation (6.4.12) shows that (6.4.13) is equivalent to

$$\upsilon(x,z) = \frac{b}{4} + \frac{b}{2\pi} \int_0^1 f(\zeta) \, d\zeta, \qquad (6.4.19)$$

where

$$f(\zeta) = \frac{\exp\left\{-\left(\zeta^{-1} - 1\right)^2 z/\lambda_a\right\} \sin\left\{\left(\zeta^{-1} - 1\right) x/\lambda_a\right\}}{\zeta - \zeta^2}.$$
 (6.4.20)

We note that the diffusion-like property of the spatial derivatives of v

$$\partial_z \upsilon = \lambda_a \partial_x^2 \upsilon, \tag{6.4.21}$$

does not hold for u when K_1^n and B_1 are non-zero; instead, the following generalised relationship holds:

$$\lambda_a \partial_x^2 u - \partial_z u = \frac{b}{2\pi} \int_0^\infty \left\{ \frac{\Gamma(\sigma)}{\sigma} - \lambda_a \sigma \right\} e^{-\Gamma(\sigma)z} \sin(\sigma x) \, d\sigma. \tag{6.4.22}$$

The properties stated in equations (6.4.18) allow for numerical integration of the expressions for v and u outlined in equations (6.4.15)–(6.4.17) and (6.4.19), (6.4.20), respectively, by defining the function $g(\zeta)$ in a piecewise manner over the interval [0, 1] and appealing to the *ApproximateInt* command in Maple [44]. From this, a range of plots has been generated for typical SmA parameter values.

Displayed in Figs. 6.2(a),(b), we see the displacements u and v due to the dislocation plotted as functions of z for varying orders of magnitude of the parameter β . Also shown is the difference between the two quantities in certain cases. Note that we have set $x = \lambda_a$, and the value $b = \lambda_a/2$ has been chosen to

ensure the validity of the quadratic energy density and the resultant linear equilibrium equations. A noticeable variation is observed across the different orders of magnitude of β ; while the case $\beta = 10$ may be deemed physically irrelevant [56], we nevertheless observe a difference of up to ~ 5% between the "far-field" limit of the displacement due to the dislocation in the cases $\beta = 0$ and $\beta = 1$.

Next, Figs. 6.3(a)–(c) show the effects of varying the constant K_1^n in the case $x = \lambda_a$ as before; plots are shown for $\lambda_n = \lambda_a/10$, λ_a , and $10\lambda_a$ with values of β as indicated in the relevant captions. Whilst clearly having an influence on the values of u, it is clear that increasing the value of β makes this influence far more pronounced.

6.4.3 Solution for Director Profile and Layer Normal

It still remains for us to derive an expression for θ . To this end, equation (6.4.5) is easily rearranged to yield

$$\theta_x = \lambda_a^2 u_{xxxx} - \beta u_{zz} - u_{xx}. \tag{6.4.23}$$

Carrying out the required differentiation leads to the following expressions for the spatial derivatives of u:

$$u_{xx} = -\frac{b}{2\pi} \int_0^\infty \sigma e^{-\Gamma(\sigma)z} \sin(\sigma x) \, d\sigma,$$
$$u_{xxxx} = \frac{b}{2\pi} \int_0^\infty \sigma^3 e^{-\Gamma(\sigma)z} \sin(\sigma x) \, d\sigma,$$
$$u_{zz} = \frac{b}{2\pi} \int_0^\infty \frac{\Gamma^2(\sigma) e^{-\Gamma(\sigma)z} \sin(\sigma x)}{\sigma} \, d\sigma,$$

so that

$$\theta_x = \frac{b}{2\pi} \int_0^\infty \left\{ \lambda_a^2 \sigma^3 + \sigma - \frac{\beta \Gamma^2(\sigma)}{\sigma} \right\} e^{-\Gamma(\sigma)z} \sin(\sigma x) \, d\sigma. \tag{6.4.24}$$

Integration of equation (6.4.24) with respect to x gives the general solution

$$\theta = \frac{b}{2\pi} \int_0^\infty \chi(\sigma) \left\{ \cos(\sigma x) + \tau(z) \right\} \, d\sigma, \tag{6.4.25}$$

where

$$\chi(\sigma) = \left\{ \frac{\beta \Gamma^2(\sigma)}{\sigma^2} - \lambda_a^2 \sigma^2 - 1 \right\} e^{-\Gamma(\sigma)z}, \qquad (6.4.26)$$



(b) The difference between the solution u as seen in equation (6.4.12) and the classical solution v stated in equation (6.4.13).



Figure 6.2: Effect of variation of β upon the layer displacement, plotted as a function of z for $x = \lambda_a = \lambda_n$.

Figure 6.3: The normalised layer displacements for various values of the parameters λ_n and β (continued on next page).



(b) $\beta = 1$.



(c) $\beta = 10$.

and $\tau(z)$ is an arbitrary function of z arising from the integration. On physical grounds, we must have $\theta(x, z) \to 0$ as $x \to \infty \forall z$; then, since $\chi(\sigma)$ has only a finite number of maxima and minima and no discontinuities for $\sigma \in [0, \infty)$, we may utilise [63, Section 3, Theorem 4] to determine that

$$\lim_{x \to \infty} \theta(x, z) = \frac{b}{2} \left\{ \lim_{x \to \infty} \int_0^\infty \chi(\sigma) \cos(\sigma x) \, d\sigma + \lim_{x \to \infty} \int_0^\infty \chi(\sigma) \tau(z) \, d\sigma \right\}$$
$$= \frac{b}{2} \left\{ 0 + \int_0^\infty \chi(\sigma) \tau(z) \, d\sigma \right\} = 0, \tag{6.4.27}$$

and hence

$$\theta(x,z) = \frac{b}{2\pi} \int_0^\infty \left\{ \frac{\beta \Gamma^2(\sigma)}{\sigma^2} - \lambda_a^2 \sigma^2 - 1 \right\} e^{-\Gamma(\sigma)z} \cos(\sigma x) \, d\sigma. \tag{6.4.28}$$

We have thus computed exact expressions for both the director profile and layer normal in the presence of an isolated edge dislocation.

Following the approach of the preceding section, let us write the expression (6.4.28) as an integral over the finite interval [0, 1]. Employing the substitution (6.4.14) once more, it follows that θ may be expressed in the equivalent form

$$\theta(x,z) = \frac{b}{2\pi\lambda_a} \int_0^1 h(\zeta) \, d\zeta, \qquad (6.4.29)$$

where

$$h(\zeta) = \left\{ \frac{\lambda_a^2 \beta \Delta^2(\zeta)}{(1-\zeta)^2} - \frac{(1-\zeta)^2 + \zeta^2}{\zeta^4} \right\} e^{-\Delta(\zeta)z} \cos\left\{ \left(\zeta^{-1} - 1\right) x / \lambda_a \right\}.$$
 (6.4.30)

It is readily deduced that, as $\zeta \to 0^+,$

$$|h(\zeta)| = \mathcal{O}\left(\frac{1}{\zeta^4}e^{-1/\zeta^2}\right),$$

and thus

 $h(\zeta) \to 0 \text{ as } \zeta \to 0^+, \qquad h(\zeta) \to -1 \text{ as } \zeta \to 1^-,$ (6.4.31)

and thus it is evident that the integral will not diverge. In order to directly compare the director profile with that of the layer normal, let us introduce the angle between a and the positive z-axis and agree to denote it by δ . It follows that the layer normal may be expressed in the form

$$\boldsymbol{a} = (\sin \delta, 0, \cos \delta) \approx \left(-u_x(1+u_z), 0, 1+u_z+u_z^2 - \frac{1}{2}u_x^2 \right),$$

from which it is evident that, to quadratic order,

$$\delta = \arcsin\{-u_x(1+u_z)\}.$$
(6.4.32)

Recalling equation (6.4.15), it is straightforward to conclude that

$$u_x = \frac{b}{2\pi\lambda_a} \int_0^1 \mu(\zeta) \, d\zeta, \qquad (6.4.33)$$

$$u_z = \frac{b}{2\pi} \int_0^1 \nu(\zeta) \, d\zeta, \tag{6.4.34}$$

where we have defined

$$\mu(\zeta) = \frac{e^{-\Delta(\zeta)z}\cos\{(\zeta^{-1} - 1)x\}}{\zeta},$$
(6.4.35)

$$\nu(\zeta) = \frac{\Delta(\zeta)e^{-\Delta(\zeta)z}\sin\{(\zeta^{-1} - 1)x\}}{\zeta - \zeta^2}.$$
 (6.4.36)

We record that

$$\mu(\zeta) \to 0 \text{ as } \zeta \to 0^+, \qquad \qquad \mu(\zeta) \to 1 \text{ as } \zeta \to 1^-, \qquad (6.4.37)$$

$$\nu(\zeta) \to 0 \text{ as } \zeta \to 0^+, \qquad \qquad \nu(\zeta) \to 0 \text{ as } \zeta \to 1^-.$$
 (6.4.38)

6.5 Separation of Director and Layer Normal: Preliminary Fourth Order Calculations

In the case where $K_1^n = 0$, the energy density w_A may be written in the form

$$w_{\rm A} = \frac{1}{2} \left(K_1^a w_1^a + B_0 w_0 + B_1 w_1 \right), \tag{6.5.1}$$

where w_0 and w_1^a are as given above by equations (6.3.2) and (6.3.3), respectively, while

$$w_{1} = (\theta + u_{x})^{2} + 2u_{x}u_{z}(\theta + u_{x}) - \frac{1}{3}\theta^{4} - u_{x}^{4} - 2\theta u_{x}^{3} - \frac{4}{3}\theta^{3}u_{x} - 2\theta^{2}u_{x}^{2} + 2\theta u_{x}u_{z}^{2} + 3u_{x}^{2}u_{z}^{2}.$$
(6.5.2)

The equilibrium equations are given by

$$\frac{\partial^2}{\partial x^2} \left(\frac{\partial w_{\rm A}}{\partial u_{xx}} \right) = \frac{\partial}{\partial x} \left(\frac{\partial w_{\rm A}}{\partial u_x} \right) + \frac{\partial}{\partial z} \left(\frac{\partial w_{\rm A}}{\partial u_z} \right), \tag{6.5.3}$$

$$\frac{\partial w_{\rm A}}{\partial \theta} = 0. \tag{6.5.4}$$

Carrying out the required differentiation and substitution gives the two equations as, respectively,

$$\lambda_a^2 u_{xxxx} = u_{zz} - 2u_x u_{xz} + u_{xx} \left(\frac{3}{2} u_x^2 - u_z \right) + \beta \left\{ 2u_{xz} (\theta + 2u_x) + \theta_z u_x + u_{xx} \left[1 + 2u_z - \theta u_x (1 + \theta) - 2\theta^2 \right] + \theta_x \left(1 + u_z - 3u_x^2 - 4\theta u_x \right) \right\},$$
(6.5.5)

$$0 = B_1 \left\{ (\theta + u_x)(1 - 2\theta u_x) + u_x u_z - \frac{2}{3}\theta^3 - u_x^3 \right\}.$$
 (6.5.6)

There are two possible means of approaching these equations: first, equation (6.5.6) could be solved for θ to yield three roots in terms of u_x and u_z , which may then be differentiated and substituted back into equation (6.5.5) to yield a messy equation for u. Alternatively, one could instead examine the case in which the coupling energy term is of a magnitude such that terms of sufficiently high order may be considered vanishingly small; for instance, assuming that terms of quartic order

in (6.2.15) may be discarded, equations (6.5.5) and (6.5.6) may be approximated by

$$K_1^a u_{xxxx} = B_0 \left\{ u_{zz} - 2u_x u_{xz} + u_{xx} \left(\frac{3}{2} u_x^2 - u_z \right) \right\} + B_1 (u_{xx} + \theta_x), \qquad (6.5.7)$$

$$\theta = -u_x(1+u_z). \tag{6.5.8}$$

Differentiation (6.5.8) with respect to x and substituting into (6.5.7) yields

$$\lambda_a^2 u_{xxxx} = u_{zz} - (2+\beta)u_x u_{xz} - (1+\beta)u_{xx}u_z + \frac{3}{2}u_x^2 u_{xx}, \qquad (6.5.9)$$

after dividing by B_0 . This is almost identical in form to the equation of Brener and Marchenko, equation (D.1) in Appendix D with a = 1/2, but with two somewhat modified coefficients incorporating the dimensionless parameter β . This modification of the coefficients unfortunately renders the method outlined in Appendix D of no use here, though it is hoped that this method may be generalised to be applicable to an equation of this type. It is worth remarking that, while a regular perturbation expansion approach may yield results in the case of small values of β , this has as yet not been investigated by the author; such an approach will be pursued in future work.

6.6 Conclusions and Discussion

This chapter has examined the effects of an isolated edge dislocation on the static behaviour of a SmA liquid crystal. After setting up the problem and deriving an expression for the energy density to fourth order, two cases were considered. First, working under the assumption that $n \equiv a$, the relevant equilibrium equation was obtained; while proving intractable, this allows for the recovery of results of previous investigations after truncating at the relevant order, provided the scaling property discussed in Section 6.3 holds. Next, it was shown that relaxation of the constraint that n must always coincide with a allows for the construction of exact solutions for both when the energy density is truncated at quadratic order. Moreover, the solution u for the layer displacement differs from the "classical" case in which n and a always coincide, as was demonstrated by the modified identity expressed in equation (6.4.22), as well as the plots contained in Figs. 6.2– 6.3 for various values of the relevant elasticity and energy terms. Finally, some tentative steps towards formulating equilibrium equations for the fourth order energy density in the particular case $K_1^n = 0$ have been presented; unfortunately no method attempted by the author has yielded solutions, and so this must be

made the goal of future investigations.

Many further avenues of investigation present themselves. Having explored the isolated edge dislocation case, it may be of interest to investigate configurations of multiple dislocations and ask what sort of distortion is to be anticipated and how different strengths and configurations of these defects would alter the smectic structure. It might also prove pertinent to examine the dynamics to which this would lead or, conversely, how the imposition of flow (for example by the application of a pressure gradient across the sample) might affect the configurations both as considered in this chapter and of various other configurations. Finally, it has been assumed throughout that the sample under consideration has infinite spatial extent: physically speaking, this corresponds to assuming that the sample boundaries are sufficiently far from the core of the defect so as to have no effect on the resultant configuration. It may prove worthwhile to examine the case of a dislocation near to a boundary under a variety of anchoring conditions. Such matters certainly warrant a great deal of further exploration.

Chapter 7

Concluding Remarks

7.1 Outline of Work Undertaken

This thesis is the result of a series of theoretical investigations into a range of phenomena in smectic A (SmA) liquid crystals employing the dynamic theory of Stewart [69] in conjunction with the energy density of De Vita and Stewart [13]. For convenience, a summary of the key findings is provided. In Chapter 3,

- a linearised two-dimensional version of the theory was derived, valid subject to suitable physical conditions;
- in particular, it has been shown that the theoretical framework of de Gennes [22] arises as a special case of the resultant system of equations, and that one can predict simple flow patterns and the corresponding alignment of the smectic using these.
- Moreover, a linear stability analysis served to establish regimes of expected stability and instability of solutions when subject to small oscillatory perturbations, as dictated by the relevant Routh-Hurwitz criteria, the satisfaction of which is ultimately determined by values of the various material parameters and perturbative wave numbers involved.

In Chapter 4,

- the system of equations derived in Chapter 3 was non-dimensionalised, allowing for the use of a lubrication approximation in the case of flows meeting the appropriate physical conditions.
- After discussing various regimes of leading-order behaviour on an equationby-equation basis, the approximation was utilised to determine the velocity

profile for pressure driven flow of SmA in agreement with previous work on the subject [82], as well as providing solutions for the director field and layer displacement to leading order.

• The leading-order theory predicts stability of the flow pattern, in agreement with the calculation using de Gennes' theory in Section 3.3. Stepping up to the next order of approximation, however, it was shown that instability is to be expected provided the component of the wave vector parallel to the plane of the layers and a particular viscosity coefficient are non-zero.

In Chapter 5, the behaviour of a shear wave incident at a plane boundary separating an isotropic elastic solid from a sample of SmA was established.

- After considering two possible ansätze for director motion in response to the wave-induced perturbation, it was determined that one leads to an inconsistency, while the other enables us to calculate the physical quantities of interest, namely the refracted wave number and penetration depth, as well as the reflected and refracted wave amplitudes, in terms of the problem's pre-determined quantities.
- Moreover, on extending the analogous investigation for a sample of smectic C (SmC) [25], we were able to compute expressions for the analogous quantities for this material, thereby enabling us to compare the responses of these two smectic phases.

Finally, Chapter 6 revisited the problem of determining the configuration of a sample of SmA in the presence of an edge dislocation.

- First, the energy density was calculated to fourth order in the director deflection and layer displacement, under the assumption that deformations are sufficiently small that such an approximation is valid.
- The case where director and layer normal are coincident was examined. After calculating the first variation of the energy density, we established that previous results for the layer displacement may be recovered on truncation of the resultant equilibrium equation; this equilibrium equation at third and fourth order is intractable, and no attempt was made at its solution.
- On allowing for separation of the director and layer normal, exact solutions for each of these were obtained in the case where deformations are
sufficiently small to allow for truncation at quadratic order. A quantitative comparison between the results obtained here with those found for the two-constant case was presented.

• Finally, preliminary investigations into higher order calculations have been carried out, with a "weak" decoupling case considered and the resultant equilibrium equation presented; as yet no method attempted has led to its solution.

7.2 Outlook

Many ideas for next steps in following up the work which constitutes this thesis have been presented within the concluding remarks of each chapter, and the reader's patience will not be tried by having them rehashed in this short afterword. As is so often the case, there remain many loose ends that remain to be tied up, but it is hoped that the studies undertaken as part of this thesis will provide some useful insights and play their role in furthering the community's understanding of the physical properties of the SmA phase, in addition to pointing out some useful mathematical approaches to the modelling of its behaviour.

Electric and magnetic field effects are known for their remarkable interactions with liquid crystals, giving rise to such phenomena as the Freedericksz transition in nematics and smectics [68, Sections 3.4, 5.9] and the Helfrich-Hurault effect found in smectics [23, Subsection 7.1.6], [68, p.286]. The study of such interactions is therefore conspicuous by its absence from the pages of this thesis. There is certainly scope for modification of the problems considered in Chapters 3–6 to include the presence of an electromagnetic field; this would no doubt serve to significantly alter the behaviour of the smectic. Also absent are any studies featuring free surfaces, in which surface tension effects would need to be taken into consideration for sufficiently small scales; examples include the modelling of thin films of SmA (for which a lubrication approach of the sort outlined in Chapter 4 may play a useful part) and the behaviour of small drops in various settings.

Generally speaking, the description of SmA as furnished by the dynamic theory of Stewart in conjunction with the energy density proposed by De Vita and Stewart presents a wealth of opportunities for studying features of its behaviour in these settings and many more, allowing novel descriptions of phenomena that may not be predicted by other models. Where possible, comparison with both predictions of previously-constructed theories in addition to experimental studies is key for those who wish to obtain a clear understanding of the behaviour of this phase and the mathematical approach to predictions thereof. It is certain that there is a great deal more work to be done in pursuit of this goal, and it is hoped that the studies contained within this thesis play their part, however small, in moving further towards that goal, both directly by means of the results obtained and indirectly via the further research directions to which they have led.

Appendix A

Index Notation and the Einstein Summation Convention

We follow the account set out by Stewart [69, Section 1.4]. Given the usual system of basis vectors $\{e_1, e_2, e_3\}$ in \mathbb{R}^3 , a vector \boldsymbol{x} may be expressed as

$$\boldsymbol{x} = x_1 \boldsymbol{e}_1 + x_2 \boldsymbol{e}_2 + x_3 \boldsymbol{e}_3 = \sum_{i=1}^n x_i \boldsymbol{e}_i.$$
 (A.1)

The terms x_i , $i \in \{1, 2, 3\}$, are the **components** of x. Employing the Einstein summation convention allows for equation (A.1) to be written in a more concise form. The convention is as follows: if an index i appears twice in a given term, the repetition of that index is taken to be a summation over all the contributions obtained by allowing the index to assume all its possible values. This is the case throughout the thesis unless an explicit statement is made to the contrary. In this way, equation (A.1) is equivalent to

$$\boldsymbol{x} = x_i \boldsymbol{e}_i, \qquad i = 1, 2, 3. \tag{A.2}$$

This convention is also applicable to tensors and matrices. Given two $n \times n$ matrices $A = [a_{ij}], B = [b_{ij}]$, their product $AB = C = [c_{ij}]$ has components as

$$c_{ij} = a_{ik}b_{kj},\tag{A.3}$$

where, again, the repeated index k is summed from 1 to n. The index k is referred to as a **dummy index**; a summation over a particular index is independent of the choice of letter, so that $a_{ik}b_{kj}$ is indistinguishable from $a_{im}b_{mj}$, $a_{it}b_{tj}$, etc. The **trace** of a matrix $A = [a_{ij}]$ is defined to be

$$\operatorname{Tr}(A) := a_{ii}.\tag{A.4}$$

It proves convenient to define, for $i, j, k \in \{1, 2, 3\}$ the **Kronecker delta** δ_{ij} by

$$\delta_{ij} := \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases}$$
(A.5)

and the **alternator** ε_{ijk}

$$\varepsilon_{ijk} := \begin{cases} 1 & \text{if } ijk \text{ is an even permutation of } \{1, 2, 3\}, \\ -1 & \text{if } ijk \text{ is an odd permutation of } \{1, 2, 3\}, \\ 0 & \text{if any of } i, j, k \text{ are equal.} \end{cases}$$
(A.6)

Two useful identities for alternators are the contraction rule

$$\varepsilon_{ijk}\varepsilon_{ipq} = \delta_{jp}\delta_{kq} - \delta_{jq}\delta_{kp},\tag{A.7}$$

and the determinant expression

$$\varepsilon_{ijk}\varepsilon_{pqr} = \begin{vmatrix} \delta_{ip} & \delta_{iq} & \delta_{ir} \\ \delta_{jp} & \delta_{jq} & \delta_{jr} \\ \delta_{kp} & \delta_{kq} & \delta_{kr} \end{vmatrix}.$$
 (A.8)

Note that equation (A.7) is simply a special case of (A.8).

The partial derivative of a given scalar quantity φ with respect to its *i*th variable is denoted by $\partial_i \varphi$ or $\varphi_{,i}$ for brevity. For example, the partial derivative of the scalar function $f(x_1, \ldots, x_n)$ with respect to its *i*th variable is $\partial f / \partial x_i = \partial_i f = f_{,i}$. Similarly, $a_{i,j} = \partial_j a_i$ denotes the partial derivative of the *i*th component of the vector **a** with respect to its *j*th variable. This may be extended in an obvious way to tensors of order two or higher.

The scalar product of two vectors $\boldsymbol{x} = (x_1, x_2, x_3)$ and $\boldsymbol{y} = (y_1, y_2, y_3)$, written $\boldsymbol{x} \cdot \boldsymbol{y}$, is defined as

$$\boldsymbol{x} \cdot \boldsymbol{y} := x_i y_i. \tag{A.9}$$

The magnitude of \boldsymbol{x} is $|\boldsymbol{x}| = \sqrt{x_i x_i}$. It is readily seen, then, that $\boldsymbol{x} \cdot \boldsymbol{x} = 0$ if and only if $\boldsymbol{x} = \boldsymbol{0}$. Two non-zero vectors \boldsymbol{x} and \boldsymbol{y} are **orthogonal** to one another if and only if $\boldsymbol{x} \cdot \boldsymbol{y} = 0$. The simple geometrical interpretation of this is that

 $\boldsymbol{x} \cdot \boldsymbol{y} = |\boldsymbol{x}||\boldsymbol{y}| \cos \theta$, where θ is the angle between \boldsymbol{x} and \boldsymbol{y} . If $\theta = \pi/2$, the two vectors are indeed orthogonal.

The *i*th component of the **vector product** $\boldsymbol{x} \times \boldsymbol{y}$ is given by

$$(\boldsymbol{x} \times \boldsymbol{y})_i := \varepsilon_{ijk} x_j y_k, \tag{A.10}$$

and the scalar triple product is defined as

$$\boldsymbol{x} \cdot (\boldsymbol{y} \times \boldsymbol{z}) = x_i \varepsilon_{ijk} y_j z_k. \tag{A.11}$$

The **tensor product** of two vectors is defined by its action on a third vector via the relation

$$(\boldsymbol{x} \otimes \boldsymbol{y})\boldsymbol{z} = (\boldsymbol{y} \cdot \boldsymbol{z})\boldsymbol{x}.$$
 (A.12)

The **gradient** of the scalar field f is

$$\nabla f = \boldsymbol{e}_i f_{,i}.\tag{A.13}$$

The **divergence** of a vector \boldsymbol{x} is given by

$$\nabla \cdot \boldsymbol{x} = x_{i,i},\tag{A.14}$$

and its **curl** is defined as

$$\nabla \times \boldsymbol{x} = \boldsymbol{e}_i \varepsilon_{ijk} \boldsymbol{x}_{k,j}.$$
 (A.15)

The divergence of a second order tensor with components t_{ij} has a divergence whose *i*th component is given by $t_{ij,j}$. Again, this extends in an obvious way to tensors of arbitrary order.

Appendix B

Two Useful Results Regarding the Roots of Polynomials

For convenience, two of the major results employed in Chapter 3 are presented.

Theorem B.1 (Descartes' rule of signs). If the terms of a single-variable polynomial with real coefficients are ordered by descending variable exponent, the number of positive roots is either equal to the number of sign differences between consecutive (non-zero) coefficients or is less than it by an even number. (Multiple roots of the same value are counted separately.)

The following theorem is an extension to the Routh-Hurwitz stability criteria [31, 57] for polynomials with complex coefficients.

Theorem B.2 (Frank [18]). Let p(z) be a complex polynomial of degree n of the form

$$p(z) := z^{n} + (a_{1} + ib_{1})z^{n-1} + \ldots + (a_{n-1} + ib_{n-1})z + a_{n} + ib_{n},$$
(B.1)

with $a_j, b_j \in \mathbb{R}$ (j = 1, ..., n). Then p(z) has all its zeros in the left half-plane if and only if the determinants $\Delta_k, k = 1, ..., n$, defined by

$$\Delta_1 := a_1, \tag{B.2}$$

$$\Delta_{k} := \begin{vmatrix} a_{1} & a_{3} & a_{5} & \cdots & a_{2k-1} & -b_{2} & -b_{4} & \cdots & -b_{2k-2} \\ 1 & a_{2} & a_{4} & \cdots & a_{2k-2} & -b_{1} & -b_{3} & \cdots & b_{2k-3} \\ \vdots & & \ddots & \vdots & & \ddots & \vdots \\ 0 & & \cdots & a_{k} & 0 & & \cdots & -b_{k-1} \\ 0 & b_{2} & b_{4} & \cdots & b_{2k-2} & a_{1} & a_{3} & a_{5} & a_{2k-3} \\ 0 & b_{1} & b_{3} & \cdots & b_{2k-3} & 1 & a_{2} & a_{2k-4} \\ \vdots & & \ddots & \vdots & & \ddots & \vdots \\ 0 & & \cdots & b_{k} & 0 & & \cdots & a_{k-1} \end{vmatrix}, \quad k \ge 2, \quad (B.3)$$

are all positive. (Note that a_j , $b_j = 0$ for all j > n.)

Proof. A proof of the result may be found in the paper by Frank [18]. \Box

As an example, let us consider an arbitrary polynomial of degree 2: $f(z) = z^2 + (a_1 + ib_1)z + a_2 + ib_2$. The roots of f lie in the left half-plane if and only if the inequalities

$$\Delta_1 = a_1 > 0, \qquad \Delta_2 = \begin{vmatrix} a_1 & 0 & -b_2 \\ 1 & a_2 & -b_1 \\ 0 & b_2 & a_1 \end{vmatrix} > 0 \tag{B.4}$$

are satisfied. We see that the latter of these inequalities simplifies to $a_2 > 0$ in the case where $b_1 = b_2 = 0$, thus reproducing the Routh-Hurwitz criteria for a quadratic polynomial with real coefficients. The case $a_1 = a_2 = 0$ is demonstrated above in Section 4.3.3.

Note that this is easily extended to a cubic polynomial of the form $g(z) = z^3 + (a_1 + ib_1)z^2 + (a_2 + ib_2)z + a_3 + ib_3$. Again, g(z) has its roots in the left half-plane if and only if

$$a_{1} > 0, \qquad \begin{vmatrix} a_{1} & a_{3} & -b_{2} \\ 1 & a_{2} & -b_{1} \\ 0 & b_{2} & a_{1} \end{vmatrix} > 0, \qquad \begin{vmatrix} a_{1} & a_{3} & 0 & -b_{2} & 0 \\ 1 & a_{2} & 0 & -b_{1} & -b_{3} \\ 0 & a_{1} & a_{3} & 0 & -b_{2} \\ 0 & b_{2} & 0 & a_{1} & a_{3} \\ 0 & b_{1} & b_{3} & 1 & a_{2} \end{vmatrix} > 0.$$
 (B.5)

It readily follows that, on setting $b_j = 0$ for $j \in \{1, 2, 3\}$, one obtains the usual Routh-Hurwitz criteria as employed above in Section 3.6, viz.,

$$a_1 > 0,$$
 $a_1 a_2 - a_3 > 0,$ $a_3 (a_1 a_2 - a_3)^2 > 0,$ i.e., $a_3 > 0.$ (B.6)

Appendix C

A Primer on Basic Variational Calculus

This appendix contains some essential definitions and techniques of the calculus of variations utilised in Chapter 6 above. For comprehensive introductory accounts to this vast topic and its powerful methods, the reader is directed to the books of Gel'fand & Fomin [20] and Sagan [59].

C.1 Differentiation of Functionals

Let $J : X \mapsto \mathbb{R}$ be a **functional**; that is, a mapping from the normed linear space X into the real numbers. The increment of J corresponding to an increment of $h \in X$ applied to the function $y \in X$ is given by

$$\Delta J(h) = J(y+h) - J(y), \qquad y \in X. \tag{C.1}$$

Definition C.1 (Fréchet Differential). The functional $J : X \mapsto \mathbb{R}$ is said to be **Fréchet differentiable** if

$$\Delta J(h) = d_f J(h) + \alpha(y, h), \qquad h \in X,$$

where $d_f J(h)$ is the **Fréchet differential** of J at y, a continuous linear functional of h, and

$$\lim_{\|h\|\to 0} \frac{\alpha(y,h)}{\|h\|} = 0,$$

that is $\alpha(y,h) = o(||h||)$ as $||h|| \to 0$.

Definition C.2 (Gâteaux Differential). The functional $J: X \to \mathbb{R}$ is said to be

Gâteaux differentiable if

$$\Delta J(h) = d_g J(h) + \alpha(y, h), \qquad h \in X,$$

where $d_g J(h)$ is the **Gâteaux differential** of J at y, a continuous linear functional of h, and

$$\lim_{t \to 0} \frac{\alpha(y, th)}{t} = 0,$$

i.e., $\alpha(y, th) = o(t)$ as $t \to \infty$.

Lemma C.3. Let $J : U \mapsto \mathbb{R}$ for some open subset U of X. If J is Fréchet differentiable then it is also Gâteaux differentiable. In this case, $d_f J(h) = d_g J(h)$.

Note that

- 1. the converse of Lemma C.3 is not true in general: there exist Gâteaux differentiable functions that are not Fréchet differentiable.
- 2. This Lemma holds in the particular case U = X.

Definition C.4. For $y, h \in X$ and $t \in \mathbb{R}$, define

$$\left. \frac{d}{dt} J(y+th) \right|_{t=0} := \lim_{t \to 0} \left\{ \frac{J(y+th) - J(y)}{t} \right\}.$$

Lemma C.5. If the functional $J : X \mapsto \mathbb{R}$ is Gâteaux differentiable,

$$\left. \frac{d}{dt} J(y+th) \right|_{t=0} = d_g J(h).$$

Definition C.6 (First Variation). The first variation (or Gâteaux variation) of J(y) at $y = y_0$, denoted by δJ , is defined by

$$\delta J := \left. \frac{d}{dt} J(y_0 + th) \right|_{t=0},\tag{C.2}$$

provided the right-hand side exists for all $h \in X$.

Note that if the right-hand side does not exist for all $h \in X$, the first variation is said not to exist.

C.2 Extrema

Suppose that $J: U \mapsto \mathbb{R}$ for some open subset U of the normed linear space X. On considering the difference J(y+h) - J(y), we must concern ourselves only with admissible functions: elements h such that, if $y \in U$, then $y + h \in U$ also. The functional J(y) is said to have a **relative extremum** at $\psi \in U$ if $J(\psi+h) - J(\psi)$ has the same sign for all admissible functions h in some neighbourhood of the origin in X. The function ψ for which J has an extremum is called an **extremal**.

Definition C.7. The functional J(y) is said to have a **weak extremum** at $y = \psi$ if there exists $\varepsilon > 0$ such that $J(\psi + h) - J(\psi)$ has the same sign for all admissible h such that $||h||_1 < \varepsilon$, where $||\cdot||_1$ denotes the norm in $C^1[a, b]$.

Definition C.8. The functional J(y) is said to have a **strong extremum** at $y = \psi$ if there exists $\varepsilon > 0$ such that $J(\psi + h) - J(\psi)$ has the same sign for all admissible h such that $||h|| < \varepsilon$, where $||\cdot||$ denotes the norm in C[a, b].

Theorem C.9. In order for a Fréchet differentiable functional $J : X \mapsto \mathbb{R}$ to have an extremal ψ , the Fréchet differential $d_f J(h)$ must satisfy the following property:

$$d_f J(h) = 0$$
 for all admissible h.

Moreover, we have

Theorem C.10. In order for a Fréchet differentiable functional $J : X \mapsto \mathbb{R}$ to have an extremal ψ , the Gâteaux differential $d_g J(h)$ must satisfy the following property:

$$d_g J(h) = 0$$
 for all admissible h ,

which implies a further necessary condition for J to have an extremal ψ is that

$$\delta J = 0$$
 for all admissible h.

C.3 The Euler Equation

Consider the integral

$$J(y) = \int_{a}^{b} f(x, y, y'(x)) \, dx.$$
 (C.1)

We outline the problem of determining an extremal $y = \psi(x)$ of this integral satisfying $\psi(a) = y_a$ and $\psi(b) = y_b$. While we only illustrate the method for one function of one independent variable, the approach readily generalises to multiple functions of multiple independent variables; see [11]. Denote the set of **admissible functions** by

$$\mathcal{F} := \left\{ y \in C^1[a, b] : y(a) = y_a \text{ and } y(b) = y_b \right\},\$$

and the set of **admissible variations** by

$$\mathcal{V} := \left\{ h \in C^1[a, b] : h(a) = h(b) = 0 \right\}.$$

Theorem C.11. Let J, as given in equation (C.1), be defined on the set \mathcal{F} and such that $f \in C^1(\mathbb{R})$. Then, if J has an extremum at $y = \psi(x)$, $\psi(x)$ must be a solution of **Euler's equation**

$$\frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) = \frac{\partial f}{\partial y}.$$
(C.2)

Proof. One readily computes the first variation of J as

$$\delta J = \left. \frac{d}{dt} J(y+th) \right|_{t=0} = \int_a^b \left(h \partial_y f + h' \partial_{y'} f \right) \, dx.$$

By Theorem C.10, a necessary condition for ψ to be an extremum of J is $\delta J(h) = 0$ at $y = \psi$ for all admissible h. Thus

$$\int_{a}^{b} (h\partial_{y}f + h'\partial_{y'}f) \, dx = 0, \qquad \forall h \in \mathcal{V}.$$

It then follows from an integration by parts of the second term in the integrand and [20, Section 3, Lemma 4] that

$$\frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) = \frac{\partial f}{\partial y}.$$

Appendix D

A Method for Solving a Class of Nonlinear PDE

Consider the nonlinear PDE

$$u_{xxxx} = 4a^2 \left(u_{zz} \pm u_{xx}u_z \pm 2u_x u_{xz} + \frac{3}{2}u_x^2 u_{xx} \right), \qquad (D.1)$$

where a is some real number. The case a = 1/2 with the lower signs chosen corresponds to equation (6.3.12) above; the case a = 1 with the upper signs chosen is the case considered by Nepomnyashchy and Pismen [51] for patternforming systems. It is readily checked via differentiation that a solution u(x, z)of the equation

$$u_{xx} = a \operatorname{sgn}(z) \left(2u_z \pm u_x^2 \right) \tag{D.2}$$

also solves equation (D.1). Further, if one introduces the similarity variable $v = x/\sqrt{z}$, the PDE (D.2) may be rewritten in the form

$$u'' = a \operatorname{sgn}(z) \left\{ \pm (u')^2 - vu' \right\}, \tag{D.3}$$

where $' \equiv d/dv$. To simplify notation, we will provide the general solution only for the case z > 0. To solve equation (D.3), we introduce the transformation

$$u' = \gamma(v)e^{-av^2/2}.$$

We may then express the ODE (D.3) in the form

$$\frac{d\gamma}{dv} = \pm a\gamma^2 e^{-av^2/2},\tag{D.4}$$

a first-order separable ODE which may be integrated with respect to v to yield

$$-\gamma = \left(c_1 \pm a \int_{-\infty}^{v} e^{-at^2/2} dt\right)^{-1},$$
 (D.5)

where c_1 is a constant of integration. The general solution for u is therefore

$$u(v) = \mp \frac{1}{a} \ln \left(\mp a \int_{-\infty}^{v} e^{-at^2/2} dt - c_1 \right) + c_2,$$
(D.6)

where the constants c_1 and c_2 are determined by appropriate boundary conditions on u. For instance, the solution (6.3.14) to the PDE (6.3.12) may be deduced from this by imposing the condition

$$\lim_{v \to \infty} u(v) - \lim_{v \to -\infty} u(v) = \frac{b}{2}$$

and applying the definition of the error function

$$\operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

It is straightforward to apply the same approach and thereby obtain the solution for z < 0.

It is readily deduced by substitution of a trial function of the form $u = u(xz^{\gamma})$ for some $\gamma \in \mathbb{R}$ into the PDE (D.1) that the only permitted value for a similarity solution is $\gamma = -1/2$.

Whether the approach outlined here can be generalised to apply to a wider class of PDE than that represented in equation (D.1) is a matter for further investigation.

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