

Defects in Liquid Crystals: Mathematical and Experimental Studies



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Abstract

Nematic liquid crystals are mesogenic materials that are popular working materials for optical displays. There has been an increased interest in bistable liquid crystal devices which support two optically distinct stable equilibria. These devices typically exploit a complex geometry or anchoring conditions, which often induces defects in the equilibria. There remains a great deal to be understood about the structure of the defects and how they stabilize multiple equilibria in modern devices.

This thesis focuses on four problems: the first three explore the effect of confinement and defects on nematic equilibria in simple geometries, with the aim of exploring multistability in these geometries; the fourth problem concerns the fine structure of point defects, essential for future modelling of nematic equilibria in more complex geometries. Firstly, we study nematic liquid crystals confined to two-dimensional rectangular wells using the Oseen-Frank theory. Secondly, we study equilibria within a semi-infinite rectangular domain with weak tangential anchoring on the surfaces. Thirdly, we study nematic equilibria within two-dimensional annuli. We derive explicit expressions for the director fields and free energies of equilibria within these geometries and discuss the stability of the predicted states. These three problems are motivated by the experimental work on colloidal nematic liquid crystals, which we interpret in the context of our results. Finally, we study the fine structure and stability of the radial hedgehog defect in the Landau-de Gennes theory with a sixth order bulk potential, relevant to the observability of global biaxial phases in a model with higher order potential terms.

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Chapter 1

Introduction

1.1 What are Liquid Crystals?

Liquid crystals are examples of mesophases, states of matter which have physical properties intermediate between crystalline states and isotropic liquid states [1, 2]. To understand how liquid crystals differ from the more widely understood crystals and liquids, it is useful to recap the basic structure and properties of both states. The constitutive particles of a substance in a crystal state have a regular structure, with their positions fixed in a three-dimensional lattice with a repeating pattern [1]. This fixed lattice structure ensures that the substance cannot flow and typically will not be easily deformed by external forces. If the crystal is translucent and the lattice is anisotropic, the crystal will be optically birefringent [3]. In a liquid state, the constitutive particles have no long range ordering. The particles diffuse freely and the substance flows under external forces. As a consequence of the lack of long range positional ordering in a liquid, the optical properties and response to external forces will be directionally isotropic. Liquid crystals are states of matter that are able to flow similarly to liquids, but have some positional or orientational ordering in at least one dimension [1]. This ordering occurs for materials comprised of strongly anisotropic particles, such as particles shaped like rods [4], disks [5] or boards [6]. In Figure 1.1, we show sketches of the ordering of rod-like molecules in a solid, liquid crystal and

liquid phase. In Figure 1.1b, we see that this anisotropy leads to the particles aligning approximately parallel, causing orientational ordering.

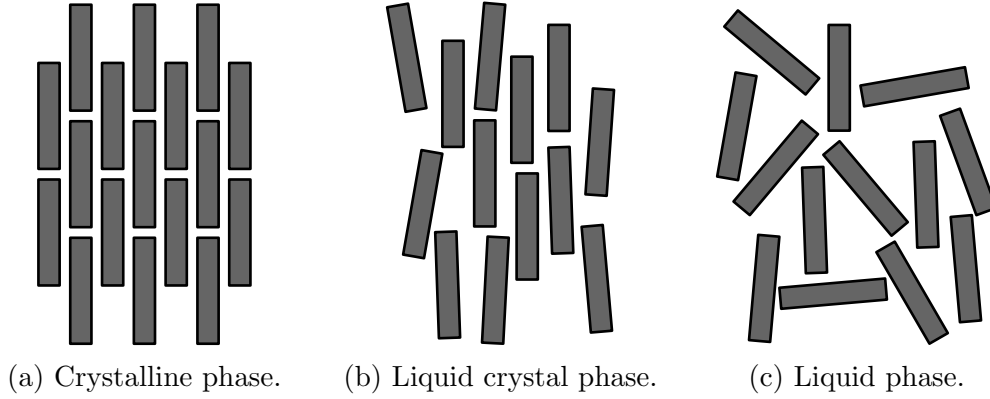


Figure 1.1: Sketches of rod-like particles in crystalline, liquid crystal and isotropic liquid phases.

The discovery of the first recorded liquid crystal phase is attributed to Friederich Reinitzer in 1888 [2]. Heating cholesteryl benzoate, a solid at room temperature, Reinitzer observed two melting points. At 145.5°C the solid melted into cloudy liquid phase, and at 178.5°C the cloudy liquid melted again, this time forming a clear fluid [7]. Further investigation showed the cloudy liquid phase exhibited many of the properties of a solid, including birefringence, and is now understood to be a liquid crystal phase. Liquid crystals which occur in the transition from solid to liquid due to changes in temperature, such as cholesteryl benzoate, are referred to as thermotropic. Thermotropic liquid crystals are normally comprised of small elongated molecules [1], such as the *p*-azoxyanisole (PAA) and *N*-(4-Methoxybenzylidene)-4-butylniline (MBBA) molecules shown in Figures 1.2a and 1.2b. These molecules have dimensions on the order of a few nanometres.

Liquid crystal phases also occur for larger particles suspended in a solvent [8], such as DNA [9], the Tobacco Mosaic Virus [10] and the *fd*-virus [11] (shown in Figure 1.2c). These particles are typically much larger than thermotropic liquid crystal molecules; for example, the tobacco mosaic virus has a length of 300 nm [1]. For these systems,

the transition to a liquid crystal phase is driven by the concentration of particles instead of the temperature, and are referred to as lyotropic liquid crystals.

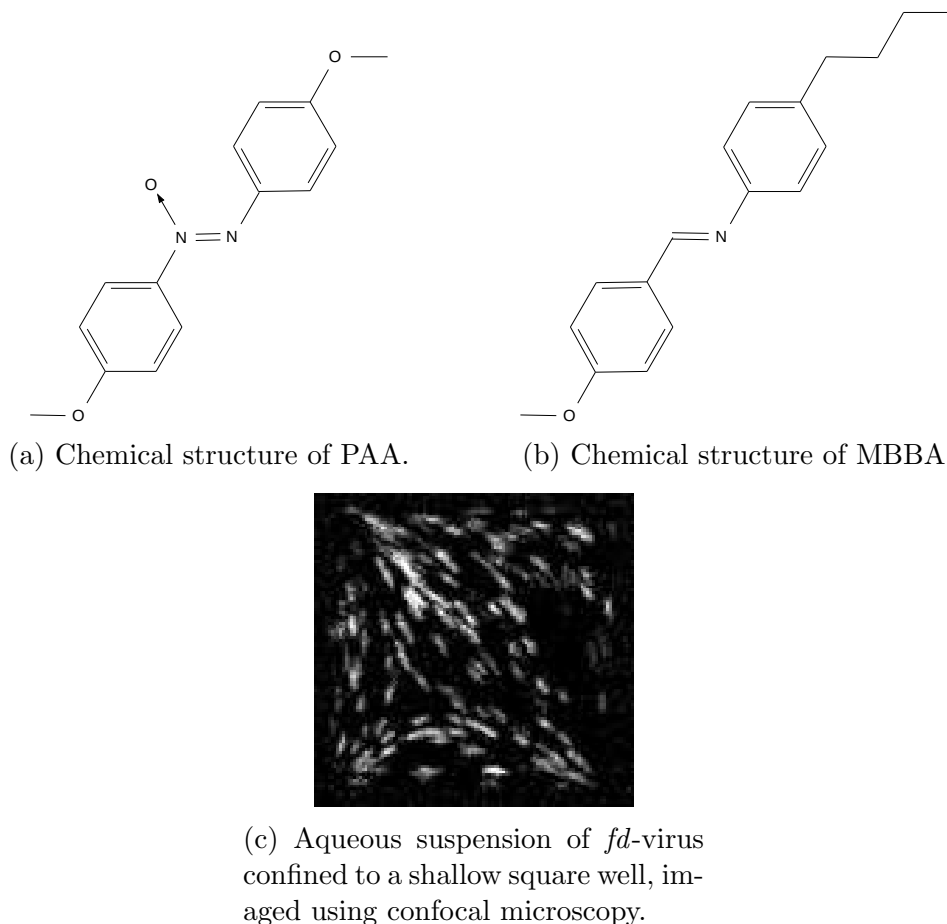


Figure 1.2: Examples of mesogenic materials. *Figure 1.2c adapted from Ref. [12] with permission from the Royal Society of Chemistry.*

There are a number of possible liquid crystal phases, each with distinct structural characteristics [1, 8]. We briefly summarize the major classes of liquid crystal phases:

- Nematic liquid crystals are the simplest liquid crystal phase, with long-range orientational ordering caused by the constituent molecules aligning approximately parallel to each other, as shown in Figure 1.3a. Nematics can be uniaxial, with a single direction of orientation, or biaxial, with discernible orientation in two distinct directions [13].

- Cholesteric liquid crystal phases exhibit orientational ordering similar to nematic liquid crystals, however, they occur for molecules with a chiral structure such as cholesteryl benzoate [2]. This chiral structure causes the preferred direction of alignment to rotate with some fixed pitch about a helical axis, as depicted in Figure 1.3b.
- Smectic liquid crystal phases feature positional ordering in one dimension as well as the orientational ordering exhibited by nematics and cholesterics. The molecules are aligned in regularly spaced layers, inside which the molecules exhibit orientational ordering. There are a number of distinct smectic phases [14]. We show two in Figures 1.3c and 1.3d. In the Smectic A phase, the preferred direction of molecular alignment is normal to the layers, while in the Smectic C phase, this preferred direction is offset at some constant angle.
- Columnar liquid crystal phases have positional ordering in two dimensions, and physically appear as regular arrays of liquid columns [15], as shown in Figure 1.3e. This phase is most commonly associated with disk-shaped particles.

Materials may exhibit multiple liquid crystal phases depending on their temperature or concentration. For example, the *fd*-virus in aqueous suspension displays cholesteric, smectic and columnar phases with increasing concentration [16].

Nematic liquid crystals have received a significant amount of attention, in part due to their industrial application as part of optical displays. A combination of the physical properties of nematic liquid crystals make them suitably for use in a class of optical displays, referred to as liquid crystal displays (LCDs). We briefly illustrate these properties with the aid of a model LCD shown in Figure 1.4. On a surface, such as a glass plate, the liquid crystal molecules can be made to align in a fixed direction by suitable treatment of the surface [1]. Between the two plates, the liquid crystal molecules will align so as to minimize their distortion. Applying an electric

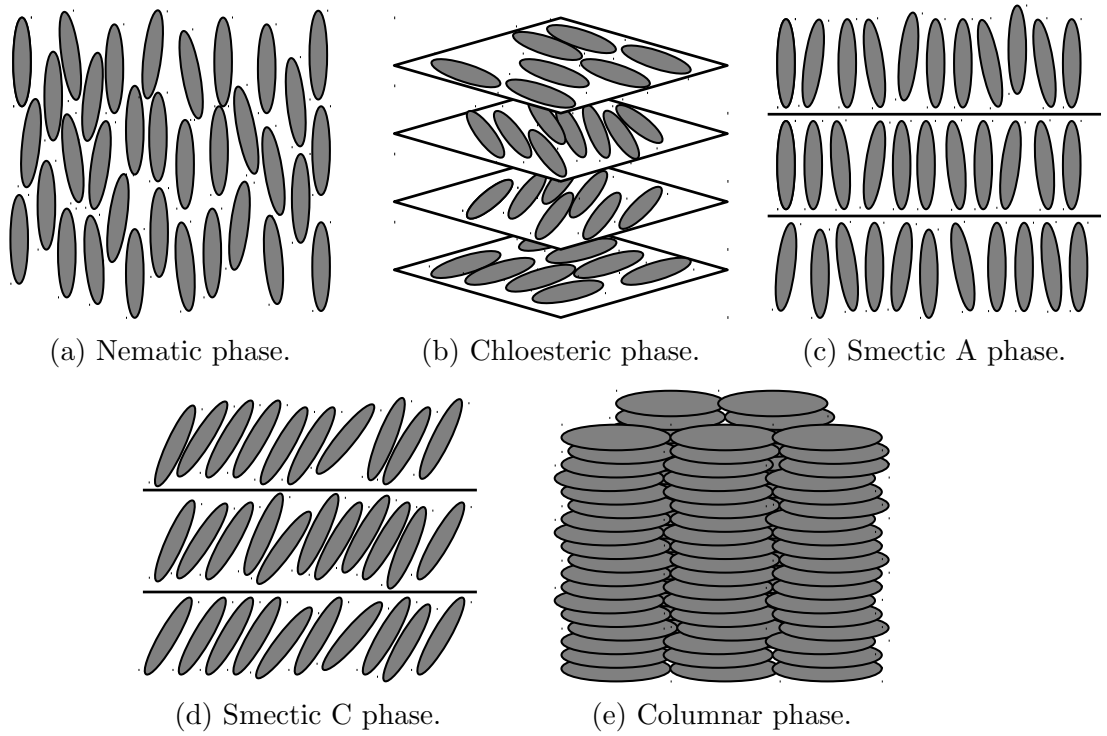


Figure 1.3: Sketches of the major liquid crystal phases for rod or disk shaped particles.

field will induce the liquid crystal molecules to align with the direction of the field [17], altering the internal orientation of the liquid crystal molecules away from the surfaces. Altering the orientation of the liquid crystal molecules will necessarily alter the optical axis of the liquid crystal. By placing suitably orientated polarising filters on both glass plates, we have a device which transmits polarized light when there is no electrical field applied, and prevents light being transmitted when the electrical field is applied. There are a number of commercially used devices which work on this principle, including the twisted nematic device [18] and the in-plane switching device [19].

Conventional LCDs require a constant electrical field in order to maintain one of the optically contrasting states. Recently, there has been increased interest in liquid crystal devices that feature multiple optically distinct stable liquid crystal equilibria, referred to as bistable or multistable devices. These devices typically take

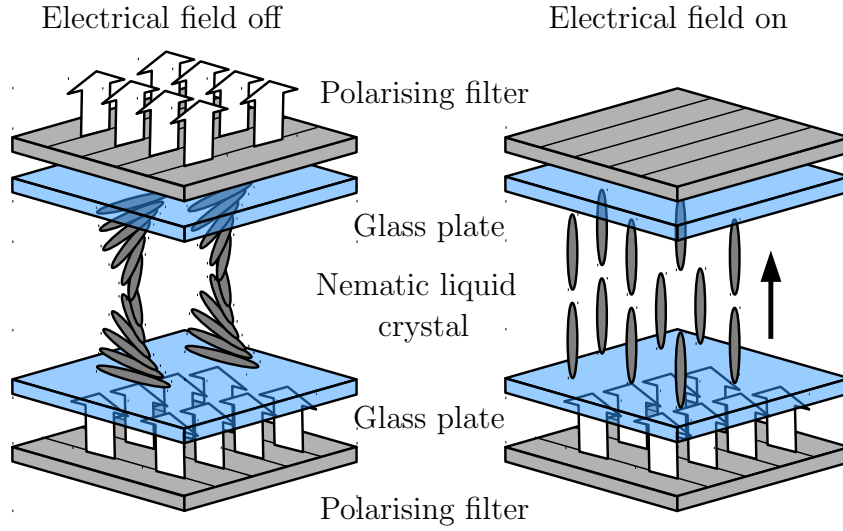


Figure 1.4: The twisted nematic device, with no electrical field (left) and a vertically aligned electrical field (right). Polarized light direction is indicated by the white arrows. *Adapted from [17]. Copyright 2004 from The Static and Dynamic Continuum Theory of Liquid Crystals: A Mathematical Introduction by I.W. Stewart. Reproduced by permission of Taylor and Francis Group, LLC, a division of Informa plc.*

advantage of a complex geometry that supports multiple stable nematic equilibria. Switching between these equilibria can be accomplished by a brief application of an electrical field [20], which offers considerable improvements in energy efficiency over conventional devices. Some examples of bistable devices include the post-aligned bistable nematic device, which features an array of posts on one wall of the device [21, 22], and the zenithal bistable nematic device, with a sinusoidal texture on one surface of the device [23, 24]. The use of these complex domains and anchoring conditions induces defects in many of these equilibria. The presence of the defects distort the surrounding liquid crystal molecules, and stabilize the optically contrasting stable states required for bistable devices.

1.2 Modelling of Nematic Liquid Crystals

There are a number of approaches for modelling nematic liquid crystals, which can be broadly divided into continuum models and statistical models. In this thesis, we

work with the continuum Oseen-Frank and Landau-de Gennes theories. Here, we provide an introduction to these models, as well as the Ericksen continuum model which serves as a bridge between the Oseen-Frank and Landau-de Gennes models.

Nematic liquid crystals are characterized by some ordering in the orientation of the constitutive molecules [1, 13]. The simplest nematic liquid crystal is the uniaxial phase, with a single preferred direction of local orientation. This locally preferred direction, referred to as the director, is mathematically represented by a unit vector field $\mathbf{n} \in \mathbb{R}^3$. In Figure 1.5, we show the director for systems of rod-like and discotic particles. For systems of rod-like molecules, the director is the average direction of the long axes of the rods [1]. For discotic systems, the director is the local average of the normal to the discs. Since liquid crystal molecules typically have no preferred polarity, the vectors $\mathbf{n}$ and $-\mathbf{n}$ are indistinguishable.

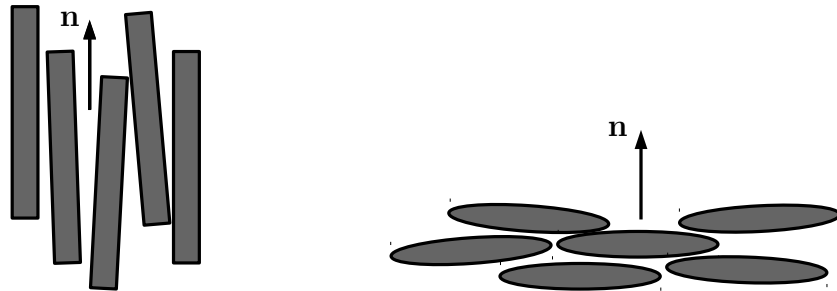


Figure 1.5: The director for uniaxial systems of rod-like particles (left) and discotic particles (right).

It is also useful to consider the degree of ordering about the director $\mathbf{n}$ at the point $\mathbf{x} \in \mathbb{R}^3$. This is measured by the order parameter, an average of the particle orientation relative to the director, defined to be

$$s = \frac{1}{2} \langle 3 \cos^2(\theta) - 1 \rangle \equiv \frac{1}{2} \int_0^\pi (3 \cos^2(\theta) - 1) f(\theta) d\theta, \quad (1.1)$$

where θ is the angle between the long axis of a molecule and the director, and $f(\theta)$ is a statistical distribution function governing the probability of finding a molecule with

orientation θ in the ball $\mathcal{B}$ centred at the point $\mathbf{x}$ [13]. If the liquid crystal particles align perfectly with the director, then $\theta = 0$ and $s = 1$. If the liquid crystal particles are all perpendicular to the director, for example the discotic particles in Figure 1.5, then $s = -\frac{1}{2}$. In an isotropic phase, the particles will be orientated randomly and $s = 0$.

In a biaxial nematic phase, liquid crystal molecules have two distinguished directions of alignment [13], which are typically denoted by the unit vectors $\mathbf{n}$ and $\mathbf{m} \in \mathbb{R}^3$. Associated with each director $\mathbf{n}$ and $\mathbf{m}$ is a scalar order parameter measuring the degree of orientational ordering, usually denoted s and r respectively.

1.2.1 The Oseen-Frank Model

The Oseen-Frank model is the simplest continuum theory for nematic liquid crystals, developed by C. W. Oseen in [25] and then further by F. C. Frank in [26]. The liquid crystal is assumed to be uniaxial with a constant order parameter, so the state of the liquid crystal is described by the director $\mathbf{n}$.

The Oseen-Frank energy is the free energy due to distortions to the director $\mathbf{n}$ away from a uniform alignment within a domain Ω . The free energy density is derived by considering a Taylor expansion in terms of $\nabla\mathbf{n}$ of the elastic Helmholtz free energy, subject to the conditions that the energy density is an even function of $\mathbf{n}$ and $\nabla\mathbf{n}$ (since $\mathbf{n} \equiv -\mathbf{n}$) and is frame invariant [1, 17]. These conditions require that there are no terms of order $\nabla\mathbf{n}$, and the smallest remaining terms are order $(\nabla\mathbf{n})^2$. By considering all terms of $(\nabla\mathbf{n})^2$ and applying the evenness and frame invariant conditions, the Oseen-Frank energy is defined to be the functional

$$E[\mathbf{n}] := \iiint_{\Omega} \frac{1}{2} (K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2) + \frac{1}{2} (K_2 + K_4) (\nabla \cdot [(\mathbf{n} \cdot \nabla)\mathbf{n} - (\nabla \cdot \mathbf{n})\mathbf{n}]) \, d\Omega, \quad (1.2)$$

where each term in the energy density corresponds to a type of distortion to the director. The deformations associated with coefficients K_1 , K_2 and K_3 are shown in Figure 1.6. The final term, with coefficient $(K_2 + K_4)$, is the saddle-splay term. By applying the divergence theorem, we see that the saddle-splay term can be converted to a surface term. The director is subject to the constraint $|\mathbf{n}| = 1$, which can be enforced by the use of a Lagrange multiplier, or by expressing $\mathbf{n}$ as

$$\mathbf{n} = (\cos(\theta) \sin(\phi), \sin(\theta) \sin(\phi), \cos(\phi)), \quad (1.3)$$

and rewriting (1.2) in terms of functions in terms of azimuthal angle θ and polar angle ϕ . The energy can be considerably simplified for systems with no variation in the z -axis and with ϕ constant, as both the twist and saddle-splay terms are equal to zero. Stable equilibria correspond to minimizers of (1.2). The existence and partial regularity of these minimizers is proved in [27]. Additional effects such as electrical fields can be modelled by including additional terms in (1.2).

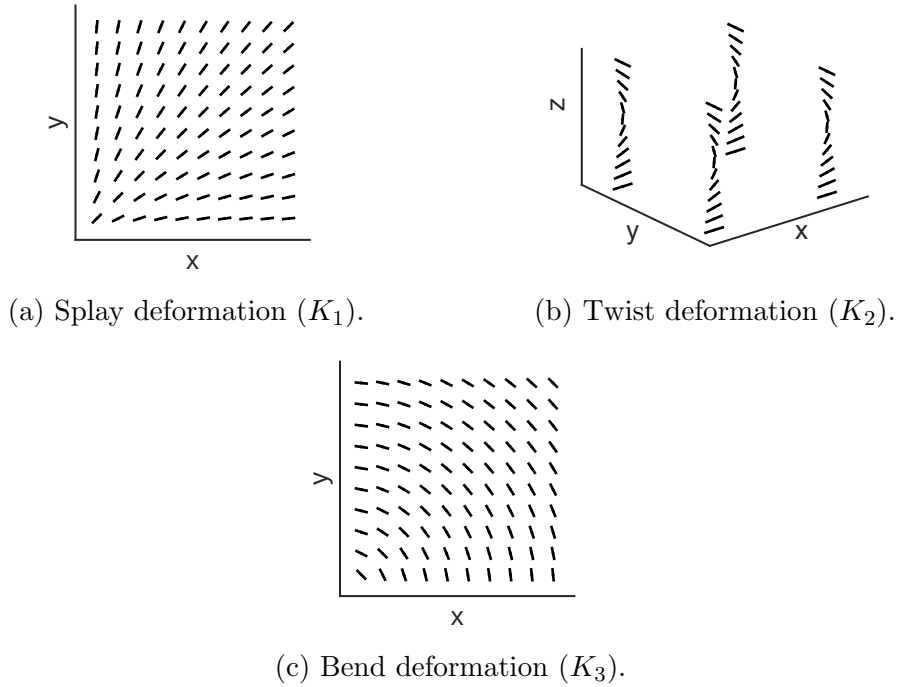


Figure 1.6: The three types of deformation to the director (dashed lines).

The elastic constants K_i ($i = 1, 2, 3$) have been measured experimentally for some liquid crystal materials, examples for thermotropic liquid crystals are given in Table 1.1. The elastic constants are all the same order of magnitude, and therefore it is not uncommon to make the one-constant approximation [1, 17], where $K_1 = K_2 = K_3 \equiv K$ and $K_4 = 0$. Under this assumption, the Oseen-Frank energy reduces to the Dirichlet energy,

$$E[\mathbf{n}] = \frac{K}{2} \iiint_{\Omega} |\nabla \mathbf{n}|^2 \, d\Omega, \quad (1.4)$$

plus surface terms. Minimizers of the Dirichlet energy are the widely studied harmonic maps, which are real analytic except at a finite number of points [2, 28].

Material	K_1	K_2	K_3
PAA at 120°C [1]	$5 \times 10^{-12} N$	$3.8 \times 10^{-12} N$	$10.1 \times 10^{-12} N$
MBBA at 22°C [29]	$6 \times 10^{-12} N$	$3.8 \times 10^{-12} N$	$7.5 \times 10^{-12} N$

Table 1.1: Values of the elastic constants for two thermotropic liquid crystals.

On the surface of a domain Ω , a preferred direction of alignment can be enforced on the liquid crystal molecules. This is modelled by considering one of two anchoring regimes.

If the surface forces acting on the liquid crystal molecules are sufficiently strong, then we assume that these forces will apply a fixed direction on the director $\mathbf{n}$ [1, 17]. This is referred to as strong anchoring. When minimizing the Oseen-Frank energy, $\mathbf{n}$ will be subject to the Dirichlet boundary condition $\mathbf{n} = \mathbf{n}_B$ on $\partial\Omega$, where the unit vector $\mathbf{n}_B \in \mathbb{R}^3$ is the preferred direction of alignment. This vector $\mathbf{n}_B$ may take any orientation with respect to the surface $\partial\Omega$. However, there are two main cases considered; homeotropic anchoring, where the director is at a normal direction to the surface, and planar anchoring, where the director is tangent to the surface. Homeotropic anchoring conditions can be enforced in experimental systems by treat-

ing a surface with chemicals or detergents [1]. For surfaces with planar anchoring, we can enforce a preferred in-plane orientation by rubbing the surface in a single direction, creating an ‘easy axis’ for the liquid crystal to align with. If there is no ‘easy axis’ then we have planar degenerate anchoring, in which the director can align in any direction as long it is tangent to the surface.

If the surface forces acting on the boundary are weak, then the director may not align perfectly with the preferred direction of alignment. The simplest surface potential is the Rapini-Papoular energy, originally considered in [30]. It is defined to be

$$E_S = \oint_{\partial\Omega} \frac{W}{2} (\mathbf{n} \cdot \mathbf{v})^2 dA, \quad (1.5)$$

where W is the anchoring strength and $\mathbf{v}$ is the outward unit normal to the surface $\partial\Omega$. This surface energy is minimized when $\mathbf{n}$ is tangent to the surface. We note that if $W \rightarrow \infty$, we recover the strong anchoring regime.

The important parameter which determines if surface anchoring or elasticity dominates the behaviour near the walls is the extrapolation length [1], which in the one-constant approximation is

$$\xi = \frac{K}{W}. \quad (1.6)$$

The anchoring strength W is on the order of $\frac{E_W}{d^2}$, where d is a molecular dimension and E_W is the interaction energy between a molecule and the surface [1]. The elastic constant is of the order $\frac{E}{d}$, where E is the interaction energy between two molecules. It therefore follows that

$$\xi \approx \frac{dE}{E_W}. \quad (1.7)$$

In the strong anchoring regime, surface effects will dominate ($E_W > E$) and ξ will be comparable to the molecular dimensions d . In the weak anchoring regime, elastic behaviour dominates ($E > E_W$) and ξ will larger than molecular dimensions.

1.2.2 The Ericksen Model

The Ericksen model for nematic liquid crystals describes the state of the liquid crystal in terms of the director $\mathbf{n}$ and the order parameter s [31]. The simplest form of the free energy, using the one-constant approximation, is

$$E[s, \mathbf{n}] = \iiint_{\Omega} (K|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2) + f_B(s) \, d\Omega, \quad (1.8)$$

where $f_B(s)$ is a temperature dependent bulk potential which enforces a preferred order parameter. Boundary conditions can be applied similarly to the Oseen-Frank model, either by applying a fixing condition on $\mathbf{n}$ and s , or introducing a surface potential. This theory allows phase transitions from isotropic to uniaxial nematics, but does not account for biaxial nematic phases.

1.2.3 The Landau-de Gennes Model

The Landau-de Gennes model is the most sophisticated continuum theory for nematic liquid crystals, which can account for isotropic, uniaxial or biaxial phases, as well as transitions between these states [13, 32]. The state of the liquid crystal is expressed in terms of the $\mathbf{Q}$ -tensor [1], a 3×3 symmetric, traceless matrix

$$\mathbf{Q} = \begin{pmatrix} q_1 & q_3 & q_4 \\ q_3 & q_2 & q_5 \\ q_4 & q_5 & -q_1 - q_2 \end{pmatrix}. \quad (1.9)$$

The phase of the liquid crystal can be determined by the number of distinct eigenvalues of $\mathbf{Q}$. Any 3×3 matrix can be expressed in terms of its eigenvalues, λ_i , and eigenvectors, $\mathbf{e}_i$,

$$\mathbf{Q} = \lambda_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + \lambda_2 \mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \otimes \mathbf{e}_3. \quad (1.10)$$

Since $\mathbf{Q}$ is traceless, we must have that $\lambda_1 + \lambda_2 + \lambda_3 = 0$. Together with the relation that $\sum_{i=1}^3 \mathbf{e}_i \otimes \mathbf{e}_i = \mathbf{I}_3$, where $\mathbf{I}_3$ is the 3×3 identity matrix,

$$\mathbf{Q} = (2\lambda_1 + \lambda_2)\mathbf{e}_1 \otimes \mathbf{e}_1 + (2\lambda_2 + \lambda_1)\mathbf{e}_2 \otimes \mathbf{e}_2 - (\lambda_1 + \lambda_2)\mathbf{I}_3. \quad (1.11)$$

Setting $s = (2\lambda_1 + \lambda_2)$, $r = (2\lambda_2 + \lambda_1)$, $\mathbf{n} = \mathbf{e}_1$ and $\mathbf{m} = \mathbf{e}_2$, the most general form of the $\mathbf{Q}$ -tensor is

$$\mathbf{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}_3}{3} \right) + r \left(\mathbf{m} \otimes \mathbf{m} - \frac{\mathbf{I}_3}{3} \right). \quad (1.12)$$

The $\mathbf{Q}$ -tensor in (1.12) represents a biaxial phase with two distinguished directions of alignment $\mathbf{n}$ and $\mathbf{m}$, and two order parameters s and r , and requires all three eigenvalues of $\mathbf{Q}$ to be distinct. If $\mathbf{Q}$ has two distinct eigenvalues, then (1.12) simplifies to

$$\mathbf{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}_3}{3} \right), \quad (1.13)$$

a uniaxial phase with director $\mathbf{n}$ and order parameter s . If there is a single distinct eigenvalue, then by the tracelessness condition, we must have $\lambda_i = 0$ for $i = 1, 2, 3$ and therefore

$$\mathbf{Q} = 0, \quad (1.14)$$

which corresponds to the isotropic phase.

The Landau-de Gennes free energy is defined to be

$$E[\mathbf{Q}] = \iiint_{\Omega} f_E(\mathbf{Q}) + f_B(\mathbf{Q}) \, d\Omega, \quad (1.15)$$

where $f_E(\mathbf{Q})$ is the elastic energy density, which penalizes spatial variations in $\mathbf{Q}$, and $f_B(\mathbf{Q})$ is the bulk potential, which determines the preferred phase.

The most general form of the elastic energy density is

$$f_E(\mathbf{Q}) := \sum_{i,j,k=1}^3 \left(\frac{L_1}{2} \left(\frac{\partial \mathbf{Q}_{ij}}{\partial x_k} \right)^2 + \frac{L_2}{2} \frac{\partial \mathbf{Q}_{ij}}{\partial x_j} \frac{\partial \mathbf{Q}_{ik}}{\partial x_k} + \frac{L_3}{2} \frac{\partial \mathbf{Q}_{ij}}{\partial x_k} \frac{\partial \mathbf{Q}_{ik}}{\partial x_j} \right), \quad (1.16)$$

where the elastic coefficients L_i are related to the Oseen-Frank elastic constants K_i by the following relations [33]:

$$L_1 = \frac{K_3 - K_1 + 3K_2}{6S_{\text{exp}}^2}, \quad L_2 = \frac{K_1 - K_2 - K_4}{S_{\text{exp}}^2}, \quad L_3 = \frac{K_4}{S_{\text{exp}}^2}. \quad (1.17)$$

Here S_{exp} denotes the experimentally measured order parameter. In the one-constant approximation, the elastic energy density reduces to

$$f_E(\mathbf{Q}) = \sum_{i,j,k=1}^3 \frac{L}{2} \left(\frac{\partial \mathbf{Q}_{ij}}{\partial x_k} \right)^2 \equiv \frac{L}{2} |\nabla \mathbf{Q}|^2, \quad (1.18)$$

where the elastic constant is $L = \frac{K}{2S_{\text{exp}}^2}$.

The bulk potential is a function of $\mathbf{Q}$ which determines the preferred phase and allows for a first-order isotropic to nematic phase transition [1]. It is assumed to be temperature dependent (or equivalently, pressure dependent for lyotropic liquid crystals). At high temperatures, isotropic states should be energetically preferable, and therefore $\mathbf{Q} = 0$ should be the global minimizer. At low temperatures uniaxial or biaxial states should be energetically preferable to the isotropic state. The bulk potential is expressed as a Taylor series expansion about the isotropic state $\mathbf{Q} = 0$ [1, 13].

The smallest expansion which allows for an isotropic-uniaxial transition is the fourth order expansion [1],

$$f_B(\mathbf{Q}) = F_0 + \frac{A}{2} \text{tr} \mathbf{Q}^2 + \frac{B}{3} \text{tr} \mathbf{Q}^3 + \frac{C}{4} (\text{tr} \mathbf{Q}^2)^2. \quad (1.19)$$

Here, F_0 is a constant term which is normally chosen so that $f_B \geq 0$. The second order coefficient, A , is assumed to be dependent on the temperature T , and the relationship is normally defined to be linear, i.e.

$$A = \alpha(T - T^*), \quad (1.20)$$

where $\alpha > 0$ and T^* is the critical temperature at which the isotropic state loses stability. The fourth order coefficient C must be positive, to have finite global minimizers. Typical values of the coefficients for the common liquid crystal MBBA are $\alpha = -0.042 \times 10^6 N/(Km^2)$, $B = -0.64 \times 10^6 N/m^2$ and $C = 0.35 \times 10^6 N/m^2$ [34]. Critical points of the fourth order bulk potential are uniaxial $\mathbf{Q}$ -tensors [32], with order parameters

$$s_{\pm} = \frac{-B \pm \sqrt{B^2 - 24AC}}{4C}, \quad (1.21)$$

and the isotropic state $\mathbf{Q} = 0$. It follows that the isotropic state ($s_0 = 0$) is unstable if $A < 0$, when we are below the critical temperature. If $B < 0$ and $A < 0$, then the global minimizer of (1.19) is a uniaxial tensor with positive order parameter s_+ [13]. Here, we see there is a discrepancy between the statistical definition of the order parameter given in Equation (1.1), where $s \in (-\frac{1}{2}, 1)$, and the order parameter using the $\mathbf{Q}$ -tensor, where $s \in \mathbb{R}$. This has motivated the development of new bulk potentials, for example see [35].

The fourth order potential does not allow for biaxial critical points [1, 36], and so any biaxial structures predicted using this potential occur due to the competition between the elastic and bulk energies. The smallest series expansion which allows for biaxial critical points, as well as uniaxial and isotropic critical points, is the sixth

order potential,

$$f_B(\mathbf{Q}) = F_0 + \frac{A}{2}\text{tr}\mathbf{Q}^2 + \frac{B}{3}\text{tr}\mathbf{Q}^3 + \frac{C}{4}(\text{tr}\mathbf{Q}^2)^2 + \frac{D}{5}(\text{tr}\mathbf{Q}^2)(\text{tr}\mathbf{Q}^3) + \frac{E}{6}(\text{tr}\mathbf{Q}^2)^3 + (F - E)(\text{tr}\mathbf{Q}^3)^2. \quad (1.22)$$

This potential is discussed in detail in Chapter 5.

We see that the Ericksen and Oseen-Frank models can be viewed as simplifications of the Landau-de Gennes theory, by restricting $\mathbf{Q}$ to only admit solutions corresponding to uniaxial nematics and uniaxial nematics with constant order parameter respectively. The Landau-de Gennes theory continues to attract significant mathematical interest, particularly minimizers of the Landau-de Gennes energy [32] and the structure and behaviour of defects. Since solutions of the Euler-Lagrange equations are solutions of a system of 5 nonlinear coupled elliptic partial differential equations, modelling of liquid crystal devices in this framework relies on numerical simulations [37], and work on the design of efficient finite-element methods remains an active area of research [38, 39].

Similarly to the Oseen-Frank theory, conditions governing the behaviour of $\mathbf{Q}$ on surfaces are included in the Landau-de Gennes energy by considering the strong and weak anchoring regimes [13]. In the strong anchoring regime, we have a Dirichlet boundary condition of the form

$$\mathbf{Q} = \mathbf{Q}_B \quad \text{on } \partial\Omega, \quad (1.23)$$

where $\mathbf{Q}_B$ is a tensor which fixes the directors $\mathbf{n}$ and $\mathbf{m}$ and the order parameters s and r on the surface.

In the weak anchoring regime, we include a surface energy which enforces a preferred value of $\mathbf{Q}$ on the boundary of Ω . The generalization of Rapini-Papoular surface

energy to the Landau-de Gennes framework [40, 41] is

$$E_S[\mathbf{Q}] = \oint_{\partial\Omega} \frac{W \mathbf{v} \cdot \mathbf{Q} \mathbf{v}}{\sqrt{\text{tr} \mathbf{Q}^2}} dA, \quad (1.24)$$

where the vector $\mathbf{v}$ is the outward unit normal vector to $\partial\Omega$. In [42], the authors proposed an alternative surface energy of the form

$$E_S[\mathbf{Q}] = \oint_{\partial\Omega} W \text{tr} (\mathbf{Q} - \mathbf{Q}_B)^2 dA, \quad (1.25)$$

referred to as the Durand-Nobili surface energy. The Durand-Nobili surface energy offers several advantages over the Rapini-Papoular energy [40], in particular the Durand-Nobili energy converges to the strong anchoring limit as $W \rightarrow \infty$.

In two-dimensions, the $\mathbf{Q}$ -tensor is a 2×2 symmetric, traceless matrix of the form

$$\mathbf{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}_2}{2} \right), \quad (1.26)$$

or, expressed as a 3×3 matrix [43],

$$\mathbf{Q} = s (\mathbf{n} \otimes \mathbf{n} - \mathbf{m} \otimes \mathbf{m}) + \frac{1}{6} (\mathbf{n} \otimes \mathbf{n} - \mathbf{m} \otimes \mathbf{m}) - \frac{1}{3} (\mathbf{z} \otimes \mathbf{z}). \quad (1.27)$$

Using Equation (1.26), it follows that $\text{tr} \mathbf{Q}^3 = 0$, and therefore the one-constant Landau-de Gennes energy with a fourth order bulk potential simplifies to

$$E[\mathbf{Q}] = \iint_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + F_0 + \frac{A}{2} \text{tr} \mathbf{Q}^2 + \frac{C}{4} (\text{tr} \mathbf{Q}^2)^2 d\Omega. \quad (1.28)$$

Working below the critical temperature ($A < 0$), the bulk potential achieves its minimum at

$$\text{tr} \mathbf{Q}^2 = \frac{|A|}{C}. \quad (1.29)$$

Factorizing the bulk potential, the energy simplifies to

$$E[\mathbf{Q}] = \iint_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + \frac{C}{4} \left(|\mathbf{Q}|^2 - \frac{|A|}{C} \right)^2 d\Omega. \quad (1.30)$$

We introduce the rescaled tensor $\tilde{\mathbf{Q}}$, defined to be

$$\tilde{\mathbf{Q}}_{ij} = \sqrt{\frac{C}{|A|}} \mathbf{Q}_{ij}, \quad (1.31)$$

and the rescaled energy

$$\tilde{E}[\tilde{\mathbf{Q}}] = \frac{C}{L|A|} E[\mathbf{Q}] = \iint_{\Omega} \frac{1}{2} |\nabla \tilde{\mathbf{Q}}|^2 + \frac{1}{4\varepsilon^2} \left(|\tilde{\mathbf{Q}}|^2 - 1 \right)^2 d\Omega, \quad (1.32)$$

where $\varepsilon^2 = \frac{L}{|A|}$, which is the two-dimensional Ginzburg-Landau energy functional in superconductivity [44].

1.3 Defects in Nematic Liquid Crystals

Defects, or disclinations, are localized discontinuities in the director [2], which can occur as isolated points, lines or sheets. Sheet defects are unstable [1], and typically only point or line defects are observed experimentally. Defects are observable due to their effect on the ordering of the surrounding liquid crystal molecules, as the director varies about the discontinuity. This rotation creates distinctive distortion patterns, which can be detected by viewing the liquid crystal sample between polarising filters. In Figure 1.7, we show an optical texture of a thin nematic film containing two point defects, which are located at the centres of the two cross-shaped patterns.

Point defects in two-dimensions are isolated points where the director field becomes discontinuous. They are categorized by their ‘strength’ m , the winding number of the director on a closed path containing the defect [45, 46]. Since the director is

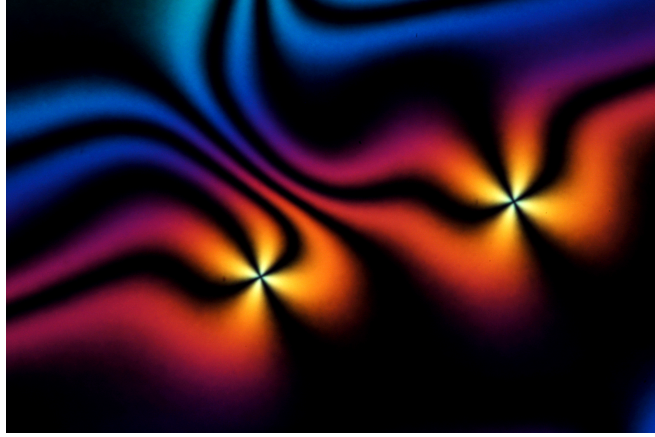


Figure 1.7: Schlieren texture of a nematic film with point defects. *Figure credit: Oleg Lavrentovich, Liquid Crystal Institute, Kent State University via the National Science Foundation, http://www.nsf.gov/news/mmg/mmg_disp.jsp?med_id=68656*

continuous on the closed path and satisfies $\mathbf{n} \equiv -\mathbf{n}$, the strength m is constrained to be either an integer or a half-integer [47]. Some examples of the director field surrounding point defects of strength $m = \pm\frac{1}{2}, \pm 1$ are shown in Figure 1.8. The defects shown in Figure 1.7 are strength ± 1 .

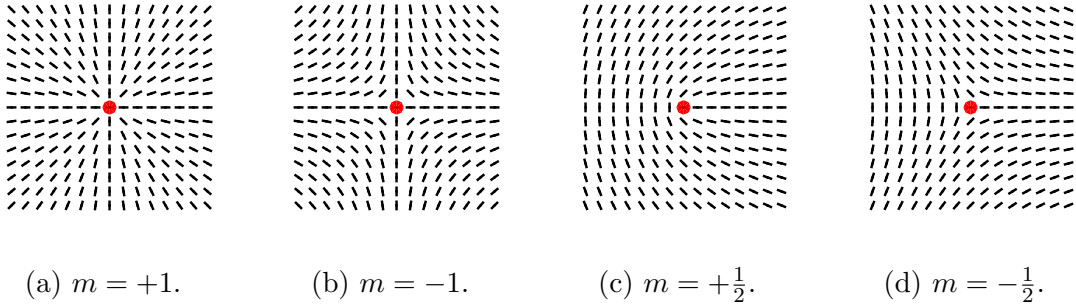


Figure 1.8: Examples of local behaviour of the director about two-dimensional point defects of strength m .

In three-dimensions, point defects are isolated discontinuities in the director. They can be categorized by a topological degree, [45, 48],

$$N = \frac{1}{4\pi} \iint_{\partial S} \mathbf{n} \cdot \left(\frac{\partial \mathbf{n}}{\partial \theta} \times \frac{\partial \mathbf{n}}{\partial \phi} \right) ds, \quad (1.33)$$

where S is a sphere containing the point defect. The degree must be an integer and only defects with degree $N = \pm 1$ are observed experimentally. Structurally, the $+1$ and -1 degree point defects resemble three-dimensional versions of the $+1$ and -1 strength point defects shown in Figures 1.8a and 1.8b respectively. Due to their structure, the $+1$ degree defect is referred to as the radial hedgehog and the -1 degree defect as the hyperbolic hedgehog.

Line defects are discontinuous lines in the director field. Like point defects in two-dimensions, the strength of a line defect is given by the winding number of the director on a closed path in the plane perpendicular to the axis of the line [17].

Both point and line defects can occur in a liquid crystal sample for a variety of reasons. Defects can occur during phase transitions, for example, when cooling from an isotropic phase, nematic regions form with different orientations. As these regions expand and meet, defects form due to the mismatch in orientations [49]. This defect formation process has been used as a model system to test theoretical predictions for cosmic strings in the early cooling of the universe [50]. Defects can also be used to initiate phase transitions from a nematic liquid crystal state to an isotropic phase, which also has the effect of lowering the temperature required to start the phase transition [51, 52]. Defects can be created manually, for example by the application of laser beams [53, 54] or electrical fields [55] to the sample. Creating defects in this manner can be used to switch between equilibria in bistable LCDs [21]. Finally, defects can occur due to constraints enforced by the geometry and surface anchoring behaviour of the domain containing nematic liquid crystals [48]. One of the simplest examples of this phenomenon is a nematic droplet, subject to homeotropic anchoring conditions on the surface of the droplet. The boundary conditions ensure that the droplet has topological degree $N = +1$, and therefore the droplet must contain a defect, typically a point defect of degree $+1$ or a closed disclination loop of strength $+\frac{1}{2}$. Defects can also occur at the boundary of domains, such as a geometry with

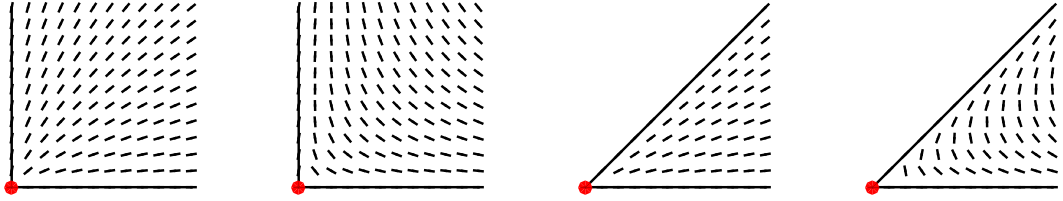
vertices and tangential anchoring on the surface. The discontinuity in the boundary conditions will induce the formation of defects in vertices. For example, consider a two-dimensional domain Ω with j vertices of vertex angle ϕ_i ($i = 1, \dots, j$) subject to strong tangential anchoring on the boundary $\partial\Omega$. Each vertex will induce a defect, some examples are shown in Figure 1.9. The strength of the boundary defect is

$$m = \frac{k}{2} - \frac{\phi_i}{2\pi}, \quad (1.34)$$

where $k \in \mathbb{Z}$. The total strength of the j boundary defects, as well as n interior defects is given by the relation in [49]:

$$\sum_{i=1}^j \left(m_i + \frac{\pi - \phi_i}{2\pi} \right) + \sum_{k=1}^n m_k = \chi, \quad (1.35)$$

where χ is the Euler characteristic of the domain Ω . Defects induced by a combination of surface anchoring conditions and geometry are commonly found in bistable devices, which serve to differentiate between the equilibria.



(a) $m = +\frac{1}{4}$, $\phi = \frac{\pi}{2}$. (b) $m = -\frac{1}{4}$, $\phi = \frac{\pi}{2}$. (c) $m = +\frac{1}{8}$, $\phi = \frac{\pi}{4}$. (d) $m = -\frac{1}{8}$, $\phi = \frac{\pi}{4}$.

Figure 1.9: Examples of local behaviour of the director in vertices with angle ϕ containing defects of strength m .

We now discuss the representation of defects in three continuum theories, as well as some important results in each theory.

1.3.1 Defects in the Oseen-Frank Model

In the Oseen-Frank theory, defects are discontinuities in the director field $\mathbf{n}$ [17]. For unequal elastic constants, point defects of degree $|N| > 1$ have been shown to be unstable [56], and will split into N defects of strength $\text{sgn}(N)$. An example solution of a +1 degree point defect located at $\mathbf{x}_0$ is the radial hedgehog defect,

$$\mathbf{n}(\mathbf{x}) = \frac{\mathbf{x} - \mathbf{x}_0}{|\mathbf{x} - \mathbf{x}_0|}. \quad (1.36)$$

This radial hedgehog defect is unstable in a ball centred at $\mathbf{x}_0$ with strong radial anchoring boundary conditions degree of +1 if the elastic constants satisfy [57],

$$8(K_2 - K_1) + K_3 < 0, \quad (1.37)$$

and is locally stable within the ball [58], if

$$8(K_2 - K_1) + K_3 \geq 0. \quad (1.38)$$

In the one-constant approximation, lower bounds on the Oseen-Frank energy can be derived based on the distance between defects [28]. These lower bounds are extended to polyhedral domains with defects located in the vertices [59, 60].

Line defects can also be modelled using the Oseen-Frank theory, however, unlike point defects, the energy of line defects is unbounded. This can be seen by considering an axial line defect of strength m confined to a cylinder of radius R with strong radial anchoring conditions in the one-constant approximation. Then the director field in the plane perpendicular to the line is $\mathbf{n} = (\cos(\theta), \sin(\theta))$, where

$$\theta = m\phi + \frac{\pi}{2}. \quad (1.39)$$

The energy in an annulus about the disclination is

$$E[\theta] = \frac{K}{2} \int_0^{2\pi} \int_\epsilon^R |\nabla\theta|^2 r \, dr \, d\phi = K\pi m^2 \log\left(\frac{R}{\epsilon}\right), \quad (1.40)$$

which diverges as the inner radius $\epsilon \rightarrow 0$. Since the energy of the line defects scales like m^2 , only line defects of strength $m = \pm\frac{1}{2}, \pm 1$ are observed experimentally [61]. For lines of strength $m = \pm 1$, the energy can be made finite by allowing the core of the defect to escape in the z -axis [62].

1.3.2 Defects in the Ericksen Model

In the Ericksen theory, defects correspond to points or lines at which the order parameter $s = 0$ [2]. Here, the energy of point defects in two-dimensions and line disclinations is no longer unbounded as the order parameter approaches zero as $\mathbf{n}$ becomes discontinuous.

1.3.3 Defects in the Landau-de Gennes Model

Using a two-dimensional Landau-de Gennes model, defects correspond to points where $\mathbf{Q} = 0$. In the one-constant approximation, the Landau-de Gennes energy is equivalent to the Ginzburg-Landau energy. Properties of the singularities of the Ginzburg-Landau energy minimizers have been studied extensively, for example see [44].

In three-dimensions, the fine structure of defects is more complex. This can be illustrated by considering a ball $\mathcal{B}$ with topological degree $+1$, with homeotropic radial anchoring on $\partial\mathcal{B}$. A possible solution is the radial hedgehog defect, with a radially aligned director field and an order parameter is zero at the origin of $\mathcal{B}$ and is positive elsewhere [63]. However, the hedgehog is unstable for large droplet radii and low temperatures [64], instead forming a solution with a $+\frac{1}{2}$ strength disclination loop about the origin. Within the disclination loop, the nematic is uniaxial with a

negative order parameter, and is surrounded by a torus-shaped region of biaxiality. Similar behaviour occurs for line defects, which feature a central core of uniaxiality, surrounded by a ring of biaxiality in which the $\mathbf{Q}$ -tensor changes to match the bulk orientation [65]. We therefore see that there is no single definition of a defect in the Landau-de Gennes theory which accounts for all identified defects.

1.4 Thesis Overview

This thesis considers four problems: the first three address the effect of confinement on nematic equilibria in simple geometries, with the aim of exploring multistability in these geometries; the fourth problem concerns the fine structure of point defects, essential for future modelling of nematic equilibria in more complex geometries.

We are fortunate to have a collaboration with the Aarts Group in the Physical and Theoretical Chemistry Laboratory of the University of Oxford. This has allowed us to compare our work to experimental images and data on nematic phases of the *fd*-virus confined to rectangular and annulus wells, and has directly informed our work in Chapters 2, 3 and 4. We provide a brief overview of the *fd*-virus and experimental methodology in §2.1.3.

In Chapter 2 we study nematic liquid crystals confined to two-dimensional rectangular wells using the Oseen-Frank theory. Using shallow square wells, two distinct nematic equilibria have been identified experimentally and theoretically [41], making this domain a simple bistable device. By considering a rectangular well, we show we can have three stable equilibria. Working within the one-constant approximation, we derive expressions for the director fields and Oseen-Frank energies for all three equilibria. We then extend these expressions to include states with internal defects. Finally, we take advantage of the low rectangular aspect ratio limit to evaluate the energy difference between two equilibria without using the one-constant approxima-

tion. We discuss our finding in light of results on nematic phases of the *fd*-virus confined to shallow rectangular chambers.

In Chapter 3 we study equilibria within a semi-infinite rectangular domain with weak tangential anchoring on the surfaces. This is motivated by the experimental observation of a state with uniform alignment within a rectangle. We derive instability conditions for the uniform state in the Oseen-Frank model and explore the bifurcation behaviour. We use our results to derive an upper bound of the extrapolation length of the experimental system.

In Chapter 4 we study nematic equilibria within two-dimensional annuli. This is motivated by experiments on the confinement of nematic phases of *fd*-virus within shallow annular wells. These experiments show a number of distinct equilibria, including equilibria with boundary defects and a radially invariant defect-free state. The existence of equilibria with boundary defects is surprising, as there are no geometric constraints that require defects. In the Oseen-Frank theory, we derive conditions on the instability of the defect-free state in terms of the elastic constants, anchoring strength and ratio of the inner and outer radii of the annulus. We derive two results on the defect-free state in the Landau-de Gennes theory. The equilibria with boundary defects share structural similarities with the equilibria identified within rectangular wells, and we apply our approach from Chapter 2 to derive expressions for the director field and energy of states within an annular sector. Finally, we discuss the effects of elastic anisotropy and weak anchoring on these sector solutions.

In Chapter 5, we study the radial hedgehog defect in the Landau-de Gennes theory with a sixth order bulk potential. The radial hedgehog defect is an example of a three-dimensional point defect, which shares many structural similarities with the defect-free state in an annulus discussed in Chapter 4. The radial hedgehog has been studied extensively using a fourth order bulk potential: we show that many of these results can be extended to this more complex theory. We address the technical

complications from the use of the sixth order potential and identify some conditions on the loss of stability of the radial hedgehog defect.

We summarize our results in Chapter 6, and discuss some open problems and possible directions for future research based on our work.

Chapter 2

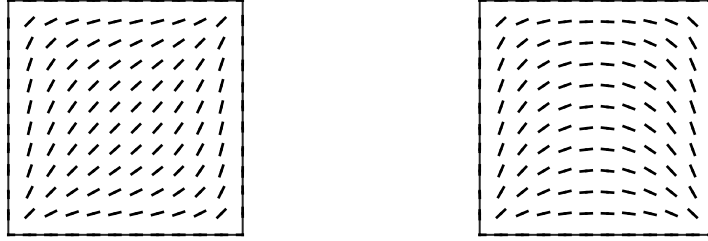
Nematic Equilibria in Shallow Rectangular Wells

2.1 Introduction

2.1.1 Literature Review

As discussed in §1.1, interest in bistable liquid crystal devices has led to a considerable amount of work on complex geometries and patterns of anchoring conditions which support multiple stable nematic equilibria. Shallow square wells are an example of a simple geometry which supports two topologically distinct stable equilibria.

In [41], the authors study an array of shallow square wells filled with nematic liquid crystal. The well surfaces are treated so as to induce degenerate planar anchoring. By studying the optical textures generated by viewing the cells through crossed polarizing filters, two distinct stable equilibria are identified. The authors also model this system numerically using a Landau-de Gennes framework. Using these numerical simulations they describe the director field of the two observed equilibria. These states, shown in Figure 2.1, are the diagonal state (D), in which the liquid crystal molecules align along the square diagonal and the rotated (or bend) state (U), in which the molecules



(a) The diagonal (D) state.

(b) The rotated (U) state.

Figure 2.1: The director fields for the diagonal and rotated states in a two-dimensional square well.

rotate by π radians across the square. States with similar structure to the diagonal state have been observed experimentally in other systems using both thermotropic liquid crystals [66] and lyotropic liquid crystals [67].

The promise of bistability in a comparatively simple geometry has inspired a number of further theoretical studies on nematic equilibria within shallow or two-dimensional square wells using both continuum and statistical approaches. In [68], the authors use conformal mapping techniques in the one-constant two-dimensional Oseen-Frank theory to describe a mechanism for switching between the U and D equilibria, by moving a defect along a wall. This idea is further extended in [69, 70], in which the authors use the Landau-de Gennes model to show that these defects should instead move through the interior of the well. A second mechanism for switching between the equilibrium states is considered in [40]. Here, the authors model the effects of electric fields and variable surface anchoring strengths to show switching between the U and D states. The structure D and U of the states is preserved when extending the geometry to a shallow three-dimensional well [71], with a more complex order reconstruction phenomenon observed for cells with dimensions below some critical value.

The diagonal and rotated states have also been studied using statistical models based on systems of hard rods or rectangles within a square well [72, 73, 74]. These

simulations capture concentration driven phase transitions, as well as the effects of confinement for small wells.

2.1.2 Chapter Outline

Motivated by this interest, as well as experimental work discussed in §2.1.3, we consider nematic equilibria confined within two-dimensional rectangular wells with strong tangential anchoring conditions.

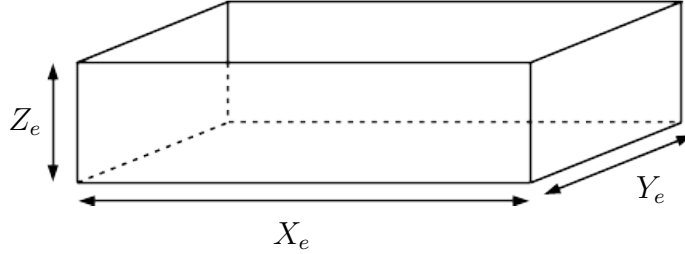


Figure 2.2: Shallow rectangular well.

The experimental systems reported in [41] are confined to shallow square wells, with depth less than half the length of the square sides. We consider a rectangular well shown in Figure 2.2, with length X_e , width Y_e and depth Z_e . If $Z_e \ll \min \{X_e, Y_e\}$, we expect any variation to the director in the z -axis to be energetically unfavourable to purely planar behaviour. We therefore consider the two-dimensional domain

$$\Omega = \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq 1, 0 \leq y \leq \lambda\}, \quad (2.1)$$

where $\lambda := \frac{Y_e}{X_e}$, the ratio of the width (Y_e) against the length (X_e). In two-dimensions, the director can be expressed in terms of the unit vector

$$\mathbf{n} = (\cos(\theta(x, y)), \sin(\theta(x, y))). \quad (2.2)$$

In terms of the function θ , the Oseen-Frank energy is

$$E[\theta] = \frac{K_3}{2} \iint_{\Omega} |\nabla \theta|^2 - \delta (\theta_y \cos(\theta) - \theta_x \sin(\theta))^2 \, d\Omega, \quad (2.3)$$

where we define our measure of elastic anisotropy $\delta := 1 - \frac{K_1}{K_3}$. Minimizers of the functional (2.3) are solutions of the Euler-Lagrange equation

$$\begin{aligned} \nabla^2 \theta + \delta \left(\frac{1}{2} \sin(2\theta) (\theta_y^2 + 2\theta_{xy} - \theta_x^2) + \theta_x \theta_y \cos(2\theta) \right. \\ \left. - \theta_{xx} \sin^2(\theta) - \theta_{yy} \cos^2(\theta) \right) = 0, \end{aligned} \quad (2.4)$$

subject to suitable boundary conditions on $\partial\Omega$.

Working within the one-constant approximation, we derive analytic expressions for the director fields and Oseen-Frank energies of generalizations of the D and U states found in a square well. We then study the properties of the director and energy in the asymptotic limit $\lambda \rightarrow 0$.

Our analytic one-constant expressions for the director and the energy can be extended to include states with internal defects. We use these expressions to discuss the properties of the states. We also use our expressions to identify the energy minimizing pathway for an internal defect to move across Ω from one corner to another and evaluate energy barriers between different stable equilibria.

Finally, we study equilibria with unequal elastic constants. Here, the non-linearity of the Euler-Lagrange equations makes it difficult to derive analytic expressions for the director field and Oseen-Frank energies. We consider the asymptotic limit $\lambda \rightarrow 0$ and derive a relation for the energy differences between two equilibrium states.

2.1.3 Experimental Work

We compare our theoretical results with experiments on the confinement of aqueous suspensions of the *fd*-virus in rectangular microchambers. Suspensions of *fd*-virus exhibit liquid crystal behaviour, including a cholesteric phase at low concentrations [16]. The constituent virus particles of these nematic systems are larger than thermotropic liquid crystal molecules, and hence can be visualized using confocal microscopy techniques.

These experiments were carried out by graduate students Oliver Dammone (Physical and Theoretical Chemistry Laboratory, University of Oxford), supervised by Dr. Pavlik Lettinga (Institut für Festkörperforschung) and Prof. Dirk Aarts (Physical and Theoretical Chemistry Laboratory, University of Oxford) and José Alvarado (FOM Institute, AMOLF), supervised by Prof. Gijsje Koenderink (FOM Institute, AMOLF). We provide a brief summary of the experimental set-up here; a more detailed explanation of the methodology can be found in [12, 75, 76].

2.1.3.1 Methodology

The *fd*-virus consists of a single strand of DNA, wrapped in a helical coating of approximately 2700 copies of the major coat protein pVIII [77], and has a contour length of $0.88\text{ }\mu\text{m}$ and a diameter of 6.6 nm . In aqueous suspension, the *fd*-virus displays behaviour in agreement with theoretical models of rod-like colloidal fluids [77]. At low virus concentration, the system exists in an isotropic phase. With increasing concentration, the system displays a cholesteric nematic phase, then smectic and columnar phases [16]. Two related viruses were considered: the first one was the semi-flexible wild-type (WT) *fd*-virus and the second one was a variant virus referred to as Y21M, which has a single mutation of the major coat protein that causes a three-fold increase of the stiffness [78]. The WT *fd*-virus has approximately equal elastic constants, [79], while for the Y21M *fd*-virus, the elastic constant ratio is

$\frac{K_3}{K_1} \approx 20$ [75]. A small volume fraction of the rods (between 2 - 4%) were fluorescently labelled with Alexa488 succinimidyl ester. These labelled rods were viewed using a confocal microscope, acting as tracers to reveal the director field.

Chips of several hundred separate rectangular microchambers were constructed using soft lithography techniques [67, 80]. The short edge had length Y_e ranging from 2 to 50 μm . The rectangular aspect ratio $\lambda = Y_e/X_e$ ranged from 0.0545 to 1, and the chamber depth was between 0.7 and 3 μm . The cholesteric pitch of the *fd*-virus was almost 2 orders of magnitude larger than the chamber depth, [81], leading to quasi-2D confinement. The chambers were filled by pipetting a droplet of the virus in aqueous suspension onto the chip, then the chambers were sealed with a microscope slide.

2.1.3.2 Experimental Results

The *fd*-virus particles spontaneously aligned into various distinct ordered steady-state patterns, as summarized in Figure 2.3. Confocal scans at different heights showed no z -dependence on the director fields and no cholesteric twist. On the top and bottom walls, the rods showed a planar alignment. There was no evidence of a preferred orientation of the rods in the plane, indicating degenerate planar anchoring conditions on the top and bottom walls of the well, and that the system is effectively two-dimensional.

The director fields were observed over a 24 hour period, during which no switching between states was observed. In total, 290 chambers containing Y21M rods and 57 chambers containing WT *fd*-rods were studied. In Figure 2.4, we show the relative frequency of each observed state in terms of the chamber dimensions, λ and Y .

Experimentally, five distinct states were observed. The diagonal (D) and rotated states (U_1) are generalizations of the states found in shallow square wells. These two states are the most common, with the D state occurring most frequently. As λ

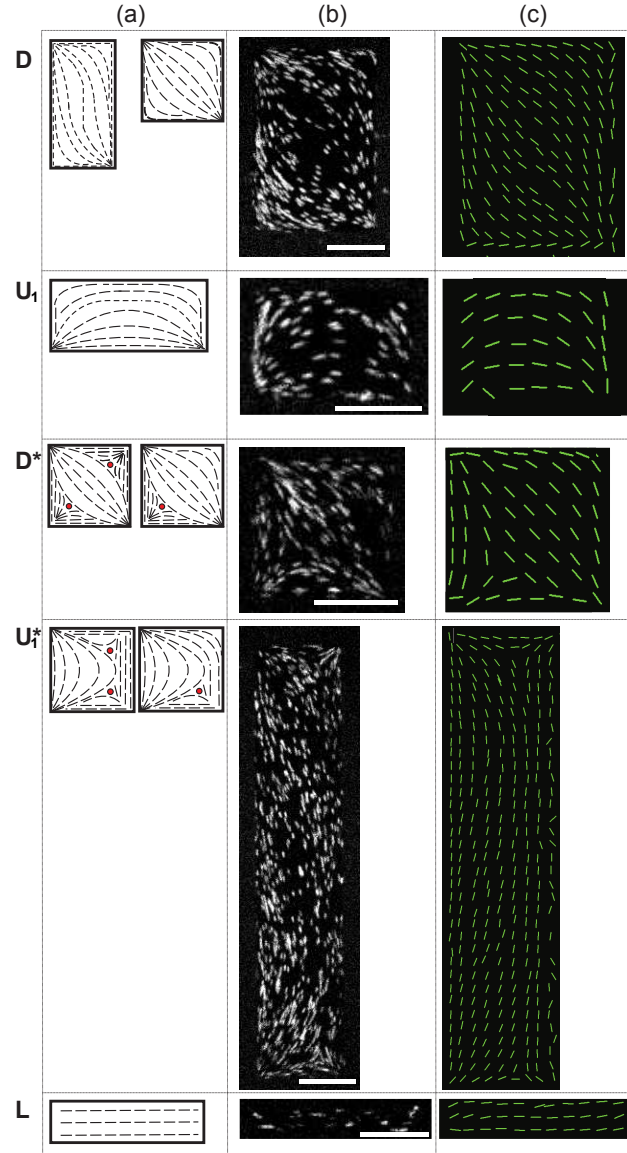


Figure 2.3: Sample director fields observed in shallow rectangular wells for WT *fd* and Y21M. (a) Sketch of the director field, with internal defects indicated by red circles. (b) Four overlaid confocal images and scale bar = 10 μm . (c) Final experimental director field, calculated from a series of 1000 confocal images. The *D* and *L* states are wild-type *fd* and U_1 , U_1^* and D^* states are the Y21M strain. *Reproduced from Ref. [12] with permission from the Royal Society of Chemistry.*

decreases from 1, the relative frequency of the U_1 state increases until the states occur at approximately the same frequency. Here, we denote the rotated state by U_1 instead of U to differentiate between the two possible directions which the director can rotate. All rotated states observed experimentally feature a rotation in the director along the long axis of the rectangle.

In addition, three further states are identified. The D^* and U_1^* feature a similar structure to the diagonal and rotated states respectively, with a corner defect of strength $-\frac{1}{4}$ replaced by a corner defect of strength $+\frac{1}{4}$ and an internal defect of strength $-\frac{1}{2}$. Additionally, we occasionally find states with two $-\frac{1}{2}$ strength defects. These states have not been observed experimentally before. Theoretical work in the Landau-de Gennes theory [70] suggests that these states are saddle points, and are therefore unstable equilibria, although these equilibria have been identified using statistical models of hard rods [72, 73, 74]. These states occur infrequently compared to the D and U_1 states, and the U_1^* state is only found for the Y21M virus. Also unreported in the literature before is the L state, in which the molecules lie tangent everywhere to the longest wall of the well. This state only occurs for very narrow channels and indicates that the assumption of strong anchoring ceases to hold for the smallest of chambers. We discuss the L state in detail in Chapter 3.

2.2 The Diagonal and Rotated Equilibria using the One-Constant Approximation

We begin by considering the generalizations of the diagonal and rotated states identified in square domains, shown in Figure 2.1, in the one-constant Oseen-Frank theory. We assume for the moment that there are no internal defects within Ω . In the one-

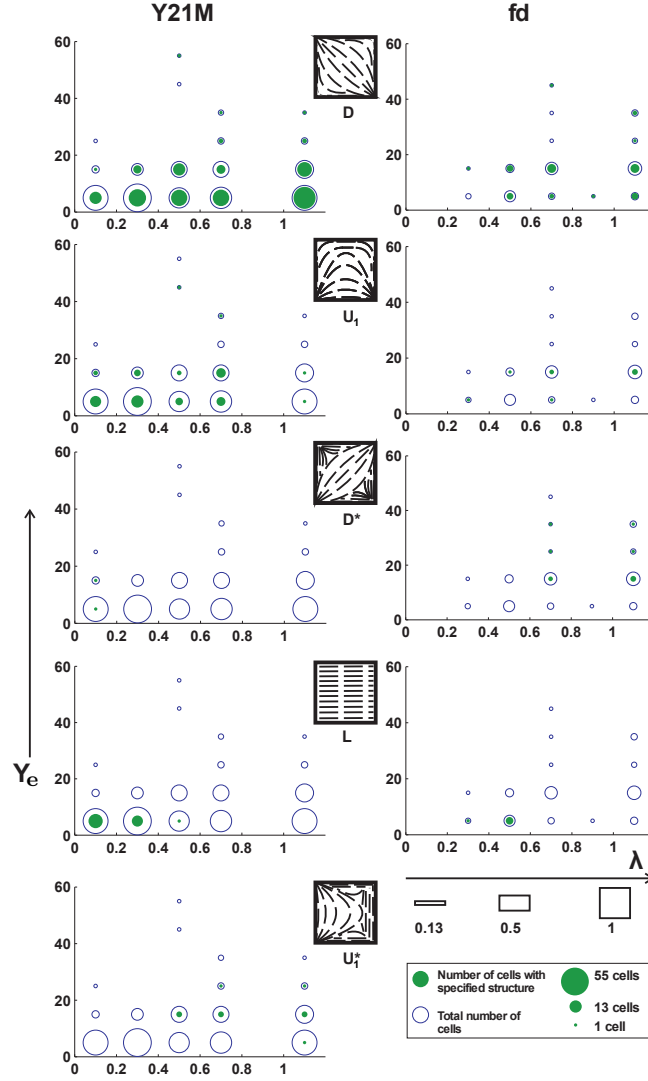


Figure 2.4: Phase space for states within rectangular cells. We plot the length of the shortest side, Y_e , versus the rectangular aspect ratio, λ , for the director fields shown in Figure 2.3. The grey circle area is proportional to the number of cells observed containing each state. The left-hand column contains results for Y21M and the right-hand column for WT *fd*-virus. *Reproduced from Ref. [12] with permission from the Royal Society of Chemistry.*

constant approximation, stable equilibria are minimizers of the energy functional

$$E[\theta] = \frac{K}{2} \iint_{\Omega} |\nabla \theta|^2 d\Omega, \quad (2.5)$$

or equivalently, solutions of

$$\nabla^2 \theta = 0, \quad (2.6)$$

subject to Dirichlet boundary conditions on $\partial\Omega$.

2.2.1 Director Fields

We now derive analytic expressions for the director fields by using linearity of the Laplace equation. We consider the solution of (2.6) subject to the boundary conditions shown in Figure 2.5.

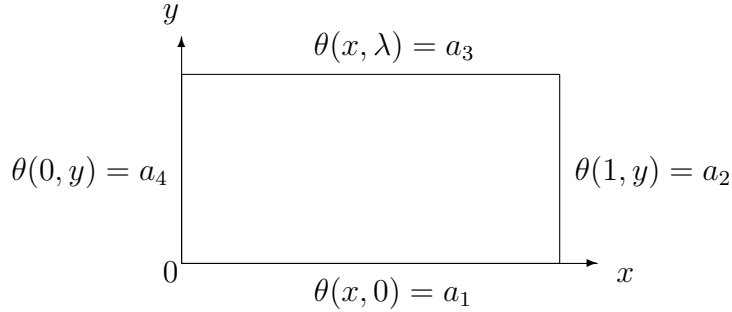


Figure 2.5: The general boundary conditions for θ .

We define the function f_1 to be the solution to $\nabla^2 f_1 = 0$, subject to the boundary conditions $f_1(x, 0; \lambda) = 1$ and $f_1(0, y; \lambda) = f_1(1, y; \lambda) = f_1(x, \lambda; \lambda) = 0$. Using the method of separation of variables, we compute f_1 to be

$$f_1(x, y; \lambda) = \sum_{n=0}^{\infty} \frac{4 \sin((2n+1)\pi x)}{(2n+1)\pi} \{ \cosh((2n+1)\pi y) - \coth((2n+1)\pi \lambda) \sinh((2n+1)\pi y) \}. \quad (2.7)$$

By rescaling and rotating the function f_1 , we define three further functions,

$$f_2(x, y; \lambda) := f_1\left(\frac{y}{\lambda}, \frac{1-x}{\lambda}; \frac{1}{\lambda}\right), \quad (2.8)$$

$$f_3(x, y; \lambda) := f_1(x, \lambda - y; \lambda), \quad (2.9)$$

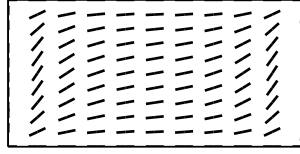
$$f_4(x, y; \lambda) := f_1\left(\frac{y}{\lambda}, \frac{x}{\lambda}; \frac{1}{\lambda}\right), \quad (2.10)$$

so each function is equal to 1 on one side of the rectangle and zero on the remaining three sides. Therefore, the director field satisfying the boundary conditions in Figure 2.5 can be expressed as the linear combination

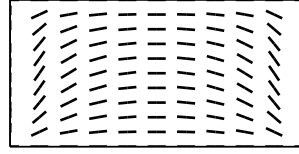
$$\theta(x, y; \lambda) = a_1 f_1(x, y; \lambda) + a_2 f_2(x, y; \lambda) + a_3 f_3(x, y; \lambda) + a_4 f_4(x, y; \lambda). \quad (2.11)$$

We now enforce some conditions on the coefficients a_i such that θ is tangent to $\partial\Omega$. Therefore, a_1 and a_3 should be equal to some integer multiples of π , and a_2 and a_4 should be equal to some integer multiples of $\frac{\pi}{2}$. These integers need not be the same for a_1 and a_3 , or for a_2 and a_4 . We only consider states with corner defects of strength $\pm\frac{1}{4}$, which requires a_i to differ from $a_{i\pm 1}$ by $\frac{\pi}{2}$ or $-\frac{\pi}{2}$.

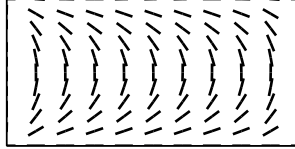
We then find that all admissible equilibria are equivalent, up to rotations or reflections, to one of the three states shown in Figure 2.6, with coefficients a_i given in Table 2.1. The D state is the generalization of the diagonal state found in a square well, with the director aligning along one of the diagonals of the rectangle. The rotated state in a square splits into two subcases, denoted U_1 and U_2 . The director of the U_1 state rotates by π radians in the x -direction. The director of the U_2 state rotates by π radians along the y -direction, and hence is considerably more distorted than the U_1 state for a narrow well with small aspect ratio λ .



(a) The D state.



(b) The U_1 state.



(c) The U_2 state.

Figure 2.6: The director fields for the three equilibrium states within a rectangle with rectangular aspect ratio $\lambda = 0.5$.

State	a_1	a_2	a_3	a_4
D	0	$\frac{\pi}{2}$	0	$\frac{\pi}{2}$
U_1	0	$-\frac{\pi}{2}$	0	$\frac{\pi}{2}$
U_2	0	$\frac{\pi}{2}$	π	$\frac{\pi}{2}$

Table 2.1: Values of the coefficients a_i for three equilibria shown in Figure 2.6.

2.2.2 The Oseen-Frank Energy

Given our analytic expression (2.11) for the director field, we now compute the Oseen-Frank energies of the D , U_1 and U_2 states. Due to the use of Dirichlet boundary conditions, θ is discontinuous at the corners of Ω . These discontinuities create point defects with infinite energy in a two-dimensional model [1, 17]. To allow for energetic comparison between the states, we regularize the energy by removing a quarter disc of radius $0 < \epsilon \ll \lambda$ centred at each of the corners and derive an asymptotic approximation to the energy in the limit as $\epsilon \rightarrow 0$. The regularized domain, shown in Figure 2.7, is denoted by Ω_ϵ . Physically, the radius ϵ represents the ‘defect core radius’, and we expect ϵ to be on the order of the nematic correlation length [64, 43]. Since all three states have equal numbers of $+\frac{1}{4}$ and $-\frac{1}{4}$ defects at the corners, we ex-

pect the corresponding contributions to the energy to be the same for all three states, and the energy difference to occur due to distortion in the bulk orientation. Despite removing the corner regions, we expect our expressions will be a good approximation to the two-dimensional Landau-de Gennes energy. Away from the corner defects, the order parameter is almost constant [40] and the energy will reduce to the Oseen-Frank energy.

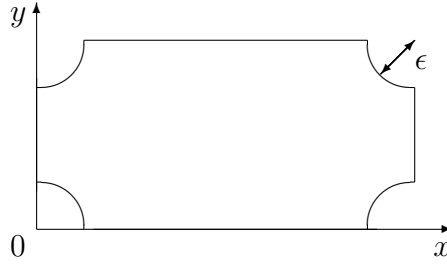


Figure 2.7: The regularized domain Ω_ϵ .

By an application of Green's First Identity [82], the regularized energy on Ω_ϵ can be reduced to a line integral about $\partial\Omega_\epsilon$,

$$E[\theta] = \frac{K}{2} \iint_{\Omega_\epsilon} |\nabla\theta|^2 dx dy = \frac{K}{2} \oint_{\partial\Omega_\epsilon} \theta \frac{\partial\theta}{\partial v} ds, \quad (2.12)$$

where $\frac{\partial\theta}{\partial v} \equiv \nabla\theta \cdot \mathbf{v}$ and $\mathbf{v}$ is the outward pointing normal to $\partial\Omega$. The boundary $\partial\Omega_\epsilon$ can be expressed as the union of the four straight edges, denoted C_i , and four curved edges, denoted γ_i , as shown in Figure 2.8. Therefore, the regularized energy is

$$E[\theta] = \frac{K}{2} \sum_{i=1}^4 \left[\int_{C_i} \theta \frac{\partial\theta}{\partial v} ds + \int_{\gamma_i} \theta \frac{\partial\theta}{\partial v} ds \right]. \quad (2.13)$$

We now consider each of these line integrals separately.

The line integrals about the arcs γ_i can be approximated by considering the local solutions θ_c in each corner. Using the arc denoted by γ_4 in Figure 2.8 as an example,

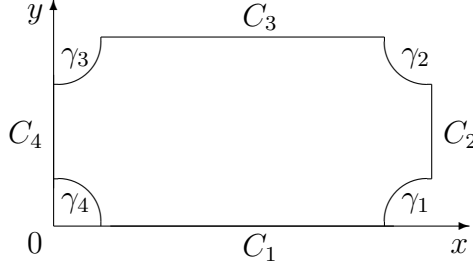


Figure 2.8: The boundary $\partial\Omega_\epsilon$ expressed terms of straight edges C_i and arcs γ_i .

this corresponds to solving

$$\nabla^2 \theta_c = 0, \quad (2.14)$$

in a polar coordinate system centred at $(x, y) = (0, 0)$, subject to boundary conditions $\theta_c(r, 0) = a_1$ and $\theta_c(r, \frac{\pi}{2}) = a_4$ and a tangential boundary condition $\theta_c(r, \phi) = \theta(x, y)$ on the line $r = \sqrt{x^2 + y^2} = \epsilon$. Solving, we find that the local solution in the corner is

$$\theta_c = a_1 + \frac{2}{\pi}(a_4 - a_1)\phi + \sum_{n=1}^{\infty} b_n r^{2n} \sin(2n\phi), \quad (2.15)$$

where the coefficients b_n can, in principle, be determined by matching with the outer solution for θ .

Thus, the contribution to the Oseen-Frank energy from the arc γ_4 is given by

$$-\int_0^{\frac{\pi}{2}} \theta_c \frac{\partial \theta_c}{\partial r} \Big|_{r=\epsilon} d\phi = \int_0^{\pi/2} \left(a_1 + \frac{2}{\pi}(a_4 - a_1)\phi + \sum_{n=1}^{\infty} b_n \epsilon^{2n} \sin(2n\phi) \right) \times \\ \left(-\sum_{n=1}^{\infty} 2nb_n \epsilon^{2n-1} \sin(2n\phi) \right) \epsilon d\phi \quad (2.16)$$

$$\sim -(a_1 + a_4)b_1 \epsilon^2 + O(\epsilon^4). \quad (2.17)$$

Similarly, it follows that all the contributions to the energy from the integrals about the arcs γ_i are order ϵ^2 .

From our definitions (2.7)–(2.10) of the functions f_i , we have $f_i = \delta_{ij}$ on wall C_j .

Therefore, the sum of the integrals about the edges C_i is

$$\sum_{i=1}^4 \int_{C_i} \theta \frac{\partial \theta}{\partial v} ds = \sum_{i,j=1}^4 a_i a_j \int_{C_i} \frac{\partial f_j}{\partial v} ds. \quad (2.18)$$

Using symmetries of the functions f_i , we reduce the 16 line integrals to six integrals,

$$I_1 := \int_{C_1} \frac{\partial f_1}{\partial v} ds = \int_{C_3} \frac{\partial f_3}{\partial v} ds, \quad (2.19)$$

$$I_2 := \int_{C_1} \frac{\partial f_3}{\partial v} ds = \int_{C_3} \frac{\partial f_1}{\partial v} ds, \quad (2.20)$$

$$I_3 := \int_{C_2} \frac{\partial f_1}{\partial v} ds = \int_{C_4} \frac{\partial f_1}{\partial v} ds = \int_{C_2} \frac{\partial f_3}{\partial v} ds = \int_{C_4} \frac{\partial f_3}{\partial v} ds, \quad (2.21)$$

$$I_4 := \int_{C_2} \frac{\partial f_2}{\partial v} ds = \int_{C_4} \frac{\partial f_4}{\partial v} ds, \quad (2.22)$$

$$I_5 := \int_{C_2} \frac{\partial f_4}{\partial v} ds = \int_{C_4} \frac{\partial f_2}{\partial v} ds, \quad (2.23)$$

$$I_6 := \int_{C_1} \frac{\partial f_2}{\partial v} ds = \int_{C_3} \frac{\partial f_2}{\partial v} ds = \int_{C_1} \frac{\partial f_4}{\partial v} ds = \int_{C_3} \frac{\partial f_4}{\partial v} ds. \quad (2.24)$$

By an application of Green's First Identity to the functions f_i and noting that $\nabla^2 f_i = 0$, we have

$$\oint_{\partial \Omega_\epsilon} \frac{\partial f_i}{\partial v} ds = 0 \quad \text{for } i = 1, \dots, 4. \quad (2.25)$$

Therefore, it must hold that

$$I_1 + I_2 + 2I_3 \sim O(\epsilon^2), \quad I_4 + I_5 + 2I_6 \sim O(\epsilon^2). \quad (2.26)$$

Using the relations in (2.26), we eliminate I_3 and I_6 and express the regularized Oseen-Frank energy in terms of four integrals and four coefficients a_i ;

$$E[\theta] \sim \frac{K}{2} \left((a_1^2 + a_3^2) I_1 + 2a_1 a_3 I_2 + (a_2^2 + a_4^2) I_4 + 2a_2 a_4 I_5 - \frac{(a_1 + a_3)(a_2 + a_4)}{2} (I_1 + I_2 + I_4 + I_5) \right) + O(\epsilon^2). \quad (2.27)$$

Using our expressions (2.7)–(2.10) for f_i , we evaluate the integrals I_1 , I_2 , I_4 and I_5 in the limit as $\epsilon \rightarrow 0$. We first consider the integral I_1 ;

$$I_1 = - \int_{\epsilon}^{1-\epsilon} \frac{\partial f_1}{\partial y} \Big|_{y=0} dx = \sum_{n=0}^{\infty} \frac{8 \cos((2n+1)\pi\epsilon) \coth((2n+1)\pi\lambda)}{(2n+1)\pi}. \quad (2.28)$$

We split this sum as follows;

$$I_1 = \underbrace{\sum_{n=0}^{\infty} \frac{8 \cos((2n+1)\pi\epsilon) (\coth((2n+1)\pi\lambda) - 1)}{(2n+1)\pi}}_{(1)} + \underbrace{\sum_{n=0}^{\infty} \frac{8 \cos((2n+1)\pi\epsilon)}{(2n+1)\pi}}_{(2)}. \quad (2.29)$$

Term (1) in (2.29) is a converging series, and therefore

$$(1) \sim \frac{8}{\pi} \sum_{n=0}^{\infty} \frac{(\coth((2n+1)\pi\lambda) - 1)}{(2n+1)} + O(\epsilon^2) \quad (2.30)$$

$$\sim \frac{4}{\pi} s_1(\lambda) + O(\epsilon^2), \quad (2.31)$$

where we define the function s_1 to be

$$s_1(\lambda) := 2 \sum_{n=0}^{\infty} \frac{\coth((2n+1)\pi\lambda) - 1}{(2n+1)}. \quad (2.32)$$

The sum denoted (2) in (2.29) is a Fourier series given in [83],

$$\sum_{n=0}^{\infty} \frac{8 \cos((2n+1)\pi\epsilon)}{(2n+1)\pi} = \frac{4}{\pi} \ln \left(\cot \left(\frac{\pi\epsilon}{2} \right) \right) \sim \frac{4}{\pi} \ln \left(\frac{2}{\pi\epsilon} \right) + O(\epsilon^2). \quad (2.33)$$

Hence, we have

$$I_1 \sim \frac{4}{\pi} \ln \left(\frac{2}{\pi\epsilon} \right) + \frac{4}{\pi} s_1(\lambda) + O(\epsilon^2). \quad (2.34)$$

Likewise, it follows that

$$I_2 \sim -\frac{4}{\pi}s_2(\lambda) + O(\epsilon^2), \quad (2.35)$$

$$I_4 \sim \frac{4}{\pi} \ln \left(\frac{2\lambda}{\pi\epsilon} \right) + \frac{4}{\pi}s_1 \left(\frac{1}{\lambda} \right) + O(\epsilon^2), \quad (2.36)$$

$$I_5 \sim -\frac{4}{\pi}s_2 \left(\frac{1}{\lambda} \right) + O(\epsilon^2), \quad (2.37)$$

where we define

$$s_2(\lambda) := 2 \sum_{n=0}^{\infty} \frac{\text{csch}((2n+1)\pi\lambda)}{(2n+1)}. \quad (2.38)$$

Using the expressions (2.34)–(2.37), the energies of all three states can be expressed in the form

$$E[\theta] \sim K\pi \left(\ln \left(\frac{1}{\epsilon} \right) + \tilde{E}[\theta] + O(\epsilon^2) \right). \quad (2.39)$$

The logarithmic contribution arises from the corner defects. This contribution is the same for all three states, as all three states contains the same number of $+\frac{1}{4}$ and $-\frac{1}{4}$ strength defects. The normalized energy $\tilde{E}[\theta]$ represents the energy due to the internal structure of the director. The expressions for $\tilde{E}[\theta]$ for each of the equilibrium states are

$$\tilde{E}_D = \ln \left(\frac{2\lambda}{\pi} \right) + s_1 \left(\frac{1}{\lambda} \right) - s_2 \left(\frac{1}{\lambda} \right), \quad (2.40)$$

$$\tilde{E}_{U_1} = \ln \left(\frac{2\lambda}{\pi} \right) + s_1 \left(\frac{1}{\lambda} \right) + s_2 \left(\frac{1}{\lambda} \right), \quad (2.41)$$

$$\tilde{E}_{U_2} = \ln \left(\frac{2}{\pi} \right) + s_1(\lambda) + s_2(\lambda). \quad (2.42)$$

From Equations (2.40)–(2.42), it follows that $\tilde{E}_D < \tilde{E}_{U_1} < \tilde{E}_{U_2}$ for $\lambda < 1$. In Figure 2.9, we plot the three normalized energies versus λ . We see that the energy of the U_2 state diverges as $\lambda \rightarrow 0$, while the normalized energies of the D and U_1

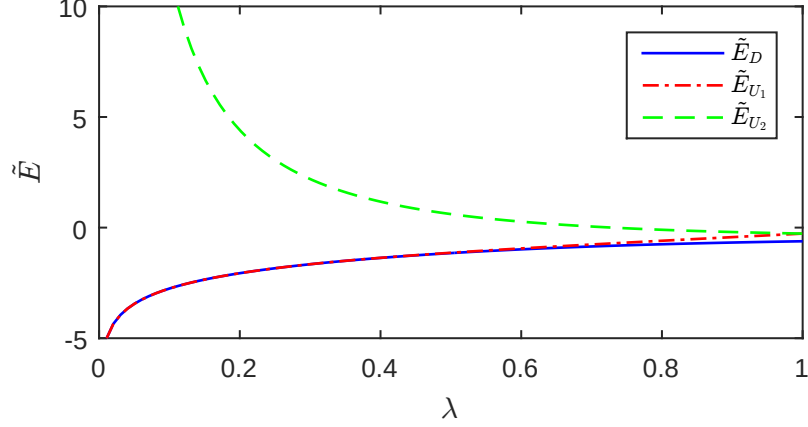


Figure 2.9: The normalized energies of the three equilibrium states plotted against the rectangular aspect ratio λ .

states converge. We explore these energetic trends in the following section. These expressions for the energies (2.40)–(2.42) may explain why the low energy diagonal state is more frequently observed experimentally using the *fd*-virus. The U_2 state is never observed experimentally, consistent with the high energy cost induced by the distortion to the director.

2.2.3 Small Rectangular Aspect Ratio

We now explore the behaviour of the director and the energy in the limit as $\lambda \rightarrow 0$. We derive alternative expressions for the functions f_i as $\lambda \rightarrow 0$ and evaluate the integrals I_1 , I_2 , I_4 and I_5 . This also gives us information on how the director behaves for small λ . We assume throughout that the defect core size $\epsilon \ll \lambda$.

We consider the function $f_3(x, y; \lambda)$; the remaining three functions follow similarly by rescaling and rotating the coordinate system. We introduce the variable $Y := \frac{y}{\lambda}$, and let $F_3(Y, x; \lambda) = f_3(y, x; \lambda)$. The function F_3 satisfies

$$\lambda^2 F_{3xx} + F_{3YY} = 0, \quad (2.43)$$

subject to $F_3(0, Y; \lambda) = F_3(1, Y; \lambda) = F_3(x, 0; \lambda) = 0$ and $F_3(x, 1; \lambda) = 1$. We let

$F_3(x, Y; \lambda) = Y - \phi(x, Y)$, where ϕ satisfies

$$\lambda^2 \phi_{xx} + \phi_{YY} = 0, \quad (2.44)$$

subject to $\phi(0, Y) = \phi(1, Y) = Y$ and $\phi(x, 0) = \phi(x, 1) = 0$. From the solution

$$\phi(x, Y) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1} \sin(n\pi Y) \cosh\left(\frac{n\pi}{\lambda} \left(x - \frac{1}{2}\right)\right)}{n\pi \cosh\left(\frac{n\pi}{2\lambda}\right)}, \quad (2.45)$$

we see that $\phi(x, Y)$ is exponentially small away from the boundaries at $x = 0$ and $x = 1$ as $\lambda \rightarrow 0$. Using the resulting solution for F_3 , we evaluate the integral I_1 ,

$$I_1 = \frac{1}{\lambda} \int_{\epsilon}^{1-\epsilon} \frac{\partial F_3}{\partial Y} \Big|_{Y=1} dx = \frac{1-2\epsilon}{\lambda} - \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sinh\left(\frac{n\pi}{2\lambda} (2\epsilon - 1)\right)}{n \cosh\left(\frac{n\pi}{2\lambda}\right)} \quad (2.46)$$

$$= \frac{1-2\epsilon}{\lambda} + \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left(\cosh\left(\frac{\pi n \epsilon}{\lambda}\right) \tanh\left(\frac{\pi n}{2\lambda}\right) - \sinh\left(\frac{\epsilon \pi n}{\lambda}\right) \right). \quad (2.47)$$

We use a series expansion for $\tanh\left(\frac{1}{x}\right)$ in the limit as $x \rightarrow 0$, namely

$$\tanh\left(\frac{1}{x}\right) \sim 1 + 2 \sum_{k=1}^{\infty} (-1)^k e^{-\frac{2k}{x}}. \quad (2.48)$$

Using this series in (2.47), we have

$$\begin{aligned} I_1 &\sim \frac{1-2\epsilon}{\lambda} + \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left(\cosh\left(\frac{n\pi\epsilon}{\lambda}\right) - \sinh\left(\frac{n\pi\epsilon}{\lambda}\right) \right) \\ &\quad + \frac{8}{\pi} \sum_{n,k=1}^{\infty} \frac{(-1)^k}{n} \cosh\left(\frac{n\pi\epsilon}{\lambda}\right) e^{-\frac{kn\pi}{\lambda}}. \end{aligned} \quad (2.49)$$

The first series in (2.49) may be simplified using

$$\sum_{n=1}^{\infty} \frac{1}{n} \left(\cosh\left(\frac{n\pi\epsilon}{\lambda}\right) - \sinh\left(\frac{n\pi\epsilon}{\lambda}\right) \right) = \sum_{n=1}^{\infty} \frac{e^{-\frac{n\pi\epsilon}{\lambda}}}{n} = -\ln(1 - e^{-\frac{\pi\epsilon}{\lambda}}) \quad (2.50)$$

$$\sim \ln\left(\frac{4}{\pi\epsilon}\right) + \frac{\pi\epsilon}{2\lambda} + O(\epsilon^2). \quad (2.51)$$

We note that

$$\frac{8}{\pi} \sum_{n,k=1}^{\infty} \frac{(-1)^k}{n} \cosh\left(\frac{n\pi\epsilon}{\lambda}\right) e^{-\frac{kn\pi}{\lambda}} = \frac{4}{\pi} \sum_{n,k=1}^{\infty} \frac{(-1)^k}{n} \left(e^{\frac{\pi n}{\lambda}(\epsilon-k)} + e^{-\frac{\pi n}{\lambda}(\epsilon+k)} \right) \quad (2.52)$$

$$\sim \frac{8}{\pi} \sum_{k=1}^{\infty} (-1)^k \ln\left(1 - e^{-\frac{k}{\lambda}\pi}\right) + O(\epsilon^2) \quad (2.53)$$

$$\sim -\frac{8}{\pi} e^{-\frac{\pi}{\lambda}} + O\left(\epsilon^2, e^{-\frac{2\pi}{\lambda}}\right). \quad (2.54)$$

In total, we therefore have

$$I_1 \sim \frac{1}{\lambda} + \frac{4}{\pi} \ln\left(\frac{\lambda}{\pi\epsilon}\right) - \frac{8}{\pi} e^{-\frac{\pi}{\lambda}} + O\left(\epsilon^2, e^{-\frac{2\pi}{\lambda}}\right). \quad (2.55)$$

By comparing terms with Equation (2.34), then as $\lambda \rightarrow 0$ it holds that

$$s_1(\lambda) \sim \frac{\pi}{4\lambda} + \ln\left(\frac{\lambda}{2}\right) - 2e^{-\frac{\pi}{\lambda}} + O\left(e^{-\frac{2\pi}{\lambda}}\right). \quad (2.56)$$

Similarly, we find that

$$s_2(\lambda) \sim \frac{\pi}{4\lambda} - \ln(2) + 2e^{-\frac{\pi}{\lambda}} + O\left(e^{-\frac{2\pi}{\lambda}}\right), \quad (2.57)$$

$$s_1\left(\frac{1}{\lambda}\right) \sim 4e^{-\frac{2\pi}{\lambda}} + O\left(e^{-\frac{3\pi}{\lambda}}\right), \quad (2.58)$$

$$s_2\left(\frac{1}{\lambda}\right) \sim 4e^{-\frac{\pi}{\lambda}} + O\left(e^{-\frac{2\pi}{\lambda}}\right). \quad (2.59)$$

From the expressions (2.40)–(2.42) and (2.56)–(2.59), we conclude that as $\lambda \rightarrow 0$,

$$\tilde{E}_D \sim \ln\left(\frac{2\lambda}{\pi}\right) - 4e^{-\frac{\pi}{\lambda}} + O\left(e^{-\frac{2\pi}{\lambda}}\right), \quad (2.60)$$

$$\tilde{E}_{U_1} \sim \ln\left(\frac{2\lambda}{\pi}\right) + 4e^{-\frac{\pi}{\lambda}} + O\left(e^{-\frac{2\pi}{\lambda}}\right), \quad (2.61)$$

$$\tilde{E}_{U_2} \sim \frac{\pi}{2\lambda} + \ln\left(\frac{\lambda}{2\pi}\right) + O\left(e^{-\frac{2\pi}{\lambda}}\right). \quad (2.62)$$

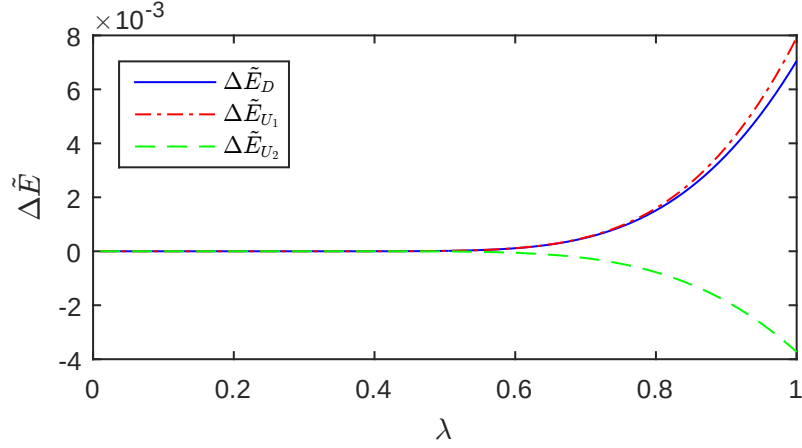


Figure 2.10: Comparison of the normalised energies given in (2.40)–(2.42), and the small λ asymptotic expressions given in (2.60)–(2.62).

Here, we see that difference $\tilde{E}_{U_1} - \tilde{E}_D \sim 8e^{-\frac{\pi}{\lambda}} + O\left(e^{-\frac{2\pi}{\lambda}}\right)$, confirming the behaviour shown in Figure 2.9. The errors are exponentially small, so the estimates (2.60)–(2.62) are accurate even for moderate values of λ . In this limit, the energies $\tilde{E}_D$ and $\tilde{E}_{U_1}$ are dominated by distortion in boundary layers near $x = 0$ and 1 , where θ rotates by $\pi/2$ radians from the edge to the bulk orientation, which is approximately uniform. The normalized energy of the U_2 state diverges as $\lambda \rightarrow 0$ as the director is constrained to rotate by π radians across a distance λ .

In Figure 2.10, we plot the difference between the normalized energies and the asymptotic approximations ($\Delta\tilde{E}$). Due to the exponentially small errors, we find that these asymptotic expressions provide a good approximation for $\tilde{E}$ even for large values of λ close to 1.

2.3 Internal Defects

We now consider states with internal defects, such as the D^* and U_1^* states identified in Figure 2.3. We show that by taking advantage of the linearity of the Laplace equation we can construct a solution that features a single internal defect of strength m located at position $(x_1, y_1) \in \Omega$. We use this solution to derive an expression for

the one-constant Oseen-Frank energy with an internal defect which can be evaluated numerically.

2.3.1 Director Fields

We need a function that induces a rotation in θ of $2\pi m$ radians at (x_1, y_1) . In polar coordinates, the director behaves like

$$\theta \approx m\phi + \text{const} \quad (2.63)$$

at (x_1, y_1) . Guided by this behaviour, we introduce a function

$$h(x, y; x_1, y_1, \lambda) := m \operatorname{atan2}(a, b) \quad (2.64)$$

where $\operatorname{atan2}(y, x)$ is the four quadrant inverse tangent [84], defined to be

$$\operatorname{atan2}(y, x) := \begin{cases} \arctan\left(\frac{y}{x}\right) & \text{if } x > 0, \\ \arctan\left(\frac{y}{x}\right) + \pi & \text{if } x < 0 \text{ and } y \geq 0, \\ \arctan\left(\frac{y}{x}\right) - \pi & \text{if } x < 0 \text{ and } y < 0, \end{cases} \quad (2.65)$$

and

$$a := y \cos(\phi') - x \sin(\phi') - y_1 \cos(\phi') + x_1 \sin(\phi'), \quad (2.66)$$

$$b := x \cos(\phi') + y \sin(\phi') - x_1 \cos(\phi') - y_1 \sin(\phi'), \quad (2.67)$$

$$\phi' := -\arctan\left(\frac{\lambda - y_1}{x_1}\right). \quad (2.68)$$

Here, h is undefined at the point $(x, y) = (x_1, y_1)$ and is discontinuous on the line from (x_1, y_1) to $(0, \lambda)$. We use the $\operatorname{atan2}$ function for the purposes of calculations instead of $\arctan$ so that the expression for the director has a single discontinuous

line. This function creates a director field with a defect of strength m , as shown in Figure 2.11a.

Next, we introduce functions to cancel out the effect of h on the boundary $\partial\Omega$. We introduce four functions g_i , which satisfy $\nabla^2 g_i = 0$ and $g_i = -\delta_{ij}h$ on the edges C_j ($j = 1, \dots, 4$) as defined in Figure 2.13. The functions g_i are

$$g_1(x, y; x_1, y_1, \lambda) := \sum_{n=1}^{\infty} A_n \sin(n\pi x) (\cosh(n\pi y) - \coth(n\pi\lambda) \sinh(n\pi y)), \quad (2.69)$$

$$g_2(x, y; x_1, y_1, \lambda) := \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi y}{\lambda}\right) \operatorname{csch}\left(\frac{n\pi}{\lambda}\right) \sinh\left(\frac{n\pi x}{\lambda}\right), \quad (2.70)$$

$$g_3(x, y; x_1, y_1, \lambda) := \sum_{n=1}^{\infty} C_n \sin(n\pi x) \operatorname{csch}(n\pi\lambda) \sinh(n\pi y), \quad (2.71)$$

$$g_4(x, y; x_1, y_1, \lambda) := \sum_{n=1}^{\infty} D_n \sin\left(\frac{n\pi y}{\lambda}\right) \left(\cosh\left(\frac{n\pi x}{\lambda}\right) - \coth\left(\frac{n\pi}{\lambda}\right) \sinh\left(\frac{n\pi x}{\lambda}\right) \right), \quad (2.72)$$

where the coefficients A_n , B_n , C_n and D_n are

$$A_n := -2 \int_0^1 h(x, 0; x_1, y_1, \lambda) \sin(n\pi x) \, dx, \quad (2.73)$$

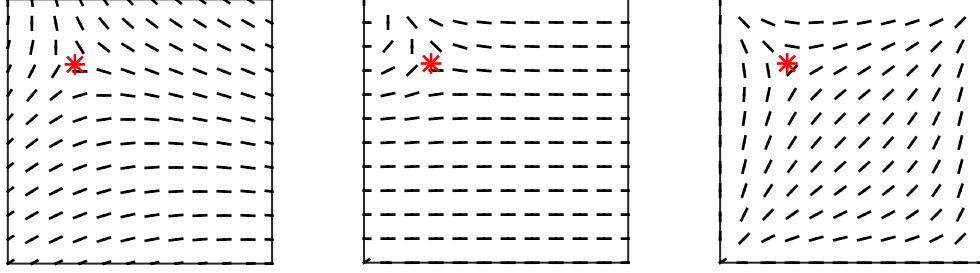
$$B_n := -\frac{2}{\lambda} \int_0^\lambda h(1, y; x_1, y_1, \lambda) \sin\left(\frac{n\pi y}{\lambda}\right) \, dy, \quad (2.74)$$

$$C_n := -2 \int_0^1 h(x, \lambda; x_1, y_1, \lambda) \sin(n\pi x) \, dx, \quad (2.75)$$

$$D_n := -\frac{2}{\lambda} \int_0^\lambda h(0, y; x_1, y_1, \lambda) \sin\left(\frac{n\pi y}{\lambda}\right) \, dy. \quad (2.76)$$

In general, these integrals cannot be evaluated in closed form, so these coefficients are evaluated numerically for given x_1 , y_1 and λ . The sum of the functions h and g_i generates a director field with a single interior defect, and $\mathbf{n}$ constant on the boundary, as shown in Figure 2.11b.

Finally, we introduce functions which enforce tangent Dirichlet boundary conditions. We use the functions defined in §2.2.1, and therefore the angle of the director



(a) $\theta = h$. (b) $\theta = h + \sum_{i=1}^4 g_i$. (c) $\theta = h + \sum_{i=1}^4 (g_i + a_i f_i)$.

Figure 2.11: Stages showing the construction of the director field. Internal defect location is indicated by red star. Here, we use the coefficients $\lambda = 1$, $m = -\frac{1}{2}$, $(x_1, y_1) = (0.2, 0.8)$, $a_1 = a_3 = 0$ and $a_2 = a_4 = \frac{\pi}{2}$.

field is given by the linear superposition

$$\theta(x, y; x_1, y_1, \lambda) = h(x, y; x_1, y_1, \lambda) + \sum_{i=1}^4 (a_i f_i(x, y; \lambda) + g_i(x, y; x_1, y_1, \lambda)). \quad (2.77)$$

Equation (2.77) generates a director field with a defect at (x_1, y_1) with tangential Dirichlet boundary conditions, for example see Figure 2.11c. Our expression for θ is discontinuous on the line running from the internal defect to the top left-hand corner. However, the director $\mathbf{n}$ is continuous everywhere except the four corners and the internal defect itself. Therefore our solution (2.77) satisfies the Euler-Lagrange equations for $\mathbf{n}$ with tangent boundary conditions and a singularity at the point (x_1, y_1) .

To satisfy Equation (1.35), the introduction of an internal defect of strengths m must alter the strength of the corner defects. In Figure 2.12, we show the effects of introducing $+\frac{1}{2}$ and $-\frac{1}{2}$ strength internal defects. The new states maintain the overall structural behaviour of the D , U_1 and U_2 states, with a single corner defect changed sign from $+\frac{1}{4}$ to $-\frac{1}{4}$ for internal defects of strength $+\frac{1}{2}$, and from $-\frac{1}{4}$ to $+\frac{1}{4}$ for internal defects of strength $-\frac{1}{2}$. The experimentally observed states, denoted D^* and U_1^* in Figure 2.3, correspond to the states shown in Figures 2.12d and 2.12e

respectively.

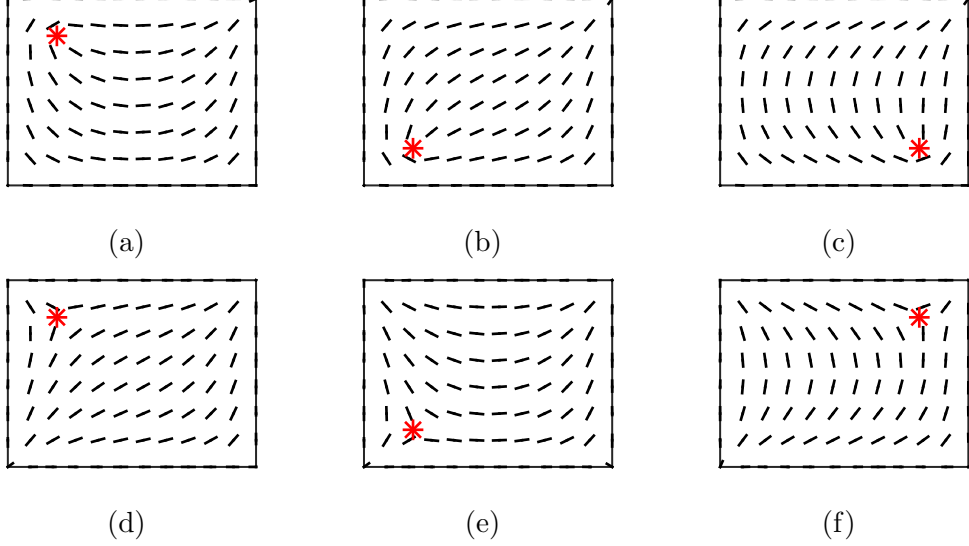


Figure 2.12: Director fields of states with internal defects of strength $m = \pm\frac{1}{2}$ in a rectangle with $\lambda = 0.75$.

2.3.2 The Oseen-Frank Energy

Using our expression (2.77) for the director, we evaluate the Oseen-Frank energy for a given (x_1, y_1) and strength m . We regularize our domain by removing discs of radius ϵ centred at each the four corners and the point (x_1, y_1) , and introduce a branch cut from $(0, \lambda)$ to (x_1, y_1) . The boundary of our regularized domain is expressed as a union of the edges shown in Figure 2.13. The Oseen-Frank energy is found using Green's First Identity:

$$E[\theta] = \frac{K}{2} \sum_{i=1}^6 \left[\int_{C_i} \theta \frac{\partial \theta}{\partial v} ds + \int_{\gamma_i} \theta \frac{\partial \theta}{\partial v} ds \right]. \quad (2.78)$$

Each of the terms in (2.78) can be evaluated individually. From the local behaviour about the arcs γ_i , we have

$$\sum_{i=1}^6 \int_{\gamma_i} \theta \frac{\partial \theta}{\partial v} ds = O(\epsilon^2), \quad (2.79)$$

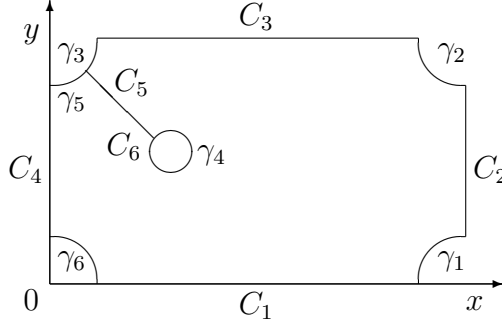


Figure 2.13: The regularized domain Ω_ϵ , with the boundary $\partial\Omega_\epsilon$ in terms of the union of straight edges C_i and arcs γ_i .

as in (2.15)–(2.17). The integrals on the edges C_i can be reduced by using the definitions of f_j , g_j and h . On the edges C_i (for $i = 1, \dots, 4$), the integral reduces to

$$\sum_{i=1}^4 \int_{C_i} \theta \frac{\partial \theta}{\partial v} ds = \underbrace{\sum_{i,j=1}^4 a_i a_j \int_{C_i} \frac{\partial f_j}{\partial v} ds}_{(1)} + \underbrace{\sum_{i,j=1}^4 a_i \int_{C_i} \frac{\partial g_j}{\partial v} ds}_{(2)} + \underbrace{\sum_{i=1}^4 a_i \int_{C_i} \frac{\partial h}{\partial v} ds}_{(3)}. \quad (2.80)$$

The first term in (2.80), (1), has been evaluated in §2.2.2 and is independent of the internal defect position. The remaining terms (2) and (3) are listed in Appendix A, and must be evaluated numerically.

On the edges C_5 and C_6 , f_i , g_i and ∇h are continuous. Therefore, the line integrals on C_5 and C_6 reduce to

$$\begin{aligned} \int_{C_5} \theta \frac{\partial \theta}{\partial v} ds + \int_{C_6} \theta \frac{\partial \theta}{\partial v} ds &= \underbrace{\int_{C_5} h \frac{\partial}{\partial v} \sum_{i=1}^4 (a_i f_i + g_i) ds + \int_{C_6} h \frac{\partial}{\partial v} \sum_{i=1}^4 (a_i f_i + g_i) ds}_{(4)} \\ &\quad + \underbrace{\int_{C_5} h \frac{\partial h}{\partial v} ds + \int_{C_6} h \frac{\partial h}{\partial v} ds}_{(5)}. \end{aligned} \quad (2.81)$$

On C_5 , $h = 2\pi m$ and on C_6 , $h = -2\pi m$. Therefore, the integrals in term (4) can be evaluated numerically by using the expressions (2.7)–(2.10) and (2.69)–(2.72) for f_i and g_i respectively, and changing to a coordinate system on C_5 . Using the function

f_1 as an example, we have:

$$\int_{C_5} h \frac{\partial f_1}{\partial v} ds + \int_{C_6} h \frac{\partial f_1}{\partial v} ds = 2\pi m \int_{C_5} \frac{\partial f_1}{\partial v} ds \quad (2.82)$$

$$= -2\pi m \int_{\epsilon}^{\sqrt{x_1^2 + (\lambda - y_1)^2} - \epsilon} \left(\cos(\phi') \frac{\partial f_1}{\partial y} - \sin(\phi') \frac{\partial f_1}{\partial x} \right) \bigg|_{\substack{x=s \cos(\phi') \\ y=\lambda + s \sin(\phi')}} ds. \quad (2.83)$$

The integrand of (2.83) can be expressed analytically in terms of an sum of an infinite series using symbolic mathematical software. By truncating this sum at some suitably large of n , we can numerically evaluate the contribution from the edges C_5 and C_6 , or, by carefully considering the infinite series, we can express the energy in terms of logarithmically terms and converging infinite summations (see Appendix A). The integrals for f_3 , f_4 , g_3 and g_4 must be evaluated with some care, as they contain a term of order $\ln(\frac{1}{\epsilon})$ due to their discontinuous behaviour at the point $(0, \lambda)$. Finally, the integrals in term (5) can be calculated exactly,

$$\int_{C_5} h \frac{\partial h}{\partial v} ds + \int_{C_6} h \frac{\partial h}{\partial v} ds = 2m^2 \pi \ln \left(\frac{\sqrt{(\lambda - y_1)^2 + x_1^2}}{\epsilon} \right) + O(\epsilon). \quad (2.84)$$

2.3.3 Results

Following the procedure outlined above, we can numerically evaluate the energy of a director field with an internal defect for given position and strength. Here, we consider the properties of states with internal defects of strength $\pm \frac{1}{2}$, as states with higher strength defects will necessarily have higher energy due to the logarithmic contribution from the defects. Due to the nature of the Fourier coefficients of the functions g_i , analytic expressions of E are difficult to work with. However, evaluating E using a mesh on the domain $A := \{(x_1, y_1) \in \mathbb{R}^2 : 4\epsilon \leq x_1 \leq 1 - 4\epsilon, 4\epsilon \leq y_1 \leq \lambda - 4\epsilon\}$ for a range of λ , we are able to visualize the energy landscape and identify some common features. Here, we use the domain A instead of the whole rectangle Ω so as

to avoid defects overlapping in the corners. We show an example contour plot of E for $\lambda = 0.6$ in Figure 2.14, derived using a regularly spaced 100×100 mesh on A .

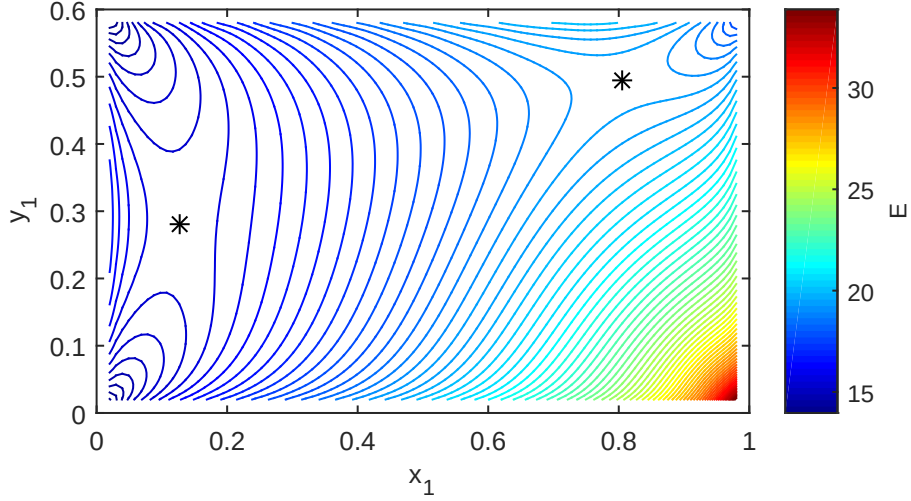


Figure 2.14: Contour plot of E in terms of x_1 and y_1 , with $\lambda = 0.6$, $m = -\frac{1}{2}$, $\epsilon = 0.005$ and $a_1 = a_3 = 0$, $a_2 = a_4 = \frac{\pi}{2}$.

We first observe that there is no energetic difference between states with $+\frac{1}{2}$ and $-\frac{1}{2}$ strength defects in equivalent locations, for example each of the pairs of states shown in Figures 2.12a and 2.12d, 2.12b and 2.12e, and 2.12c and 2.12f have identical energies up to terms of order ϵ . This is consistent with numerical studies on a similar problem using the Landau-de Gennes framework [70]. It is therefore surprising that only states with $-\frac{1}{2}$ strength internal defects are found experimentally. One possible explanation is the low number of cells filled with the *fd*-virus, a larger sample size might produce a greater range of states with internal defects. For the Y21M virus, with elastic constant ratio $\frac{K_1}{K_3} \approx 20$, the energetic contribution from $+\frac{1}{2}$ and $-\frac{1}{2}$ strength defects is no longer the same. This difference may cause states with $+\frac{1}{2}$ strength internal defects to be energetically unfavourable, providing a second possible explanation as to why these states are never experimentally observed.

For all values of λ , we find two critical points of E in A . These are shown by the (*) points in Figure 2.14. Inspection of these critical points shows that they both

are saddle-splay points. The energy achieves the global minimum in a corner of A , specifically the corner which would cause the internal defect to annihilate with the corner defect and form the diagonal state. In Figure 2.14, this corresponds to the corner at $(0, \lambda)$. The energy also features local minimizers at two further corners, where annihilation of the corner defect and internal defect will form the rotated states. The final corner contains a defect of the same strength as the internal defect, and therefore the energy achieves its maximum in this corner (the corner $(x_1, y_1) = (1, 0)$ in Figure 2.14). The energy increases close to the edges of A , which is consistent with calculations in [1] for the energy of a point defect approaching a wall. We conclude that states with internal defects can never be stable equilibria, as the energy can always be decreased by moving the internal defect towards one of the corners containing an opposing sign strength defect. This is consistent with other continuum modelling in [69, 70]. The saddle-splay points occur due to the competing attractive and repulsive forces acting on the internal defect from the four corner defects. It is therefore somewhat surprising that the D^* and U_1^* states are ever observed experimentally. We note that the energy about the saddle-splay points is approximately constant (see the gradient plot in Figure 2.16a), and it is possible that a combination of this low energy gradient coupled with some finite size effects allows the internal defects to persist using the fd -virus.

Using our evaluated energies in terms of x_1 and y_1 , we explore the optimal energy minimizing pathways for an internal defect to move through the rectangle, allowing for switching between equilibria, and calculate energy barriers between stable equilibria. The idea of using an internal defect to allow for switching between equilibria in a square well was originally discussed in [68]. Starting with a rotated state, a corner defect of strength $-\frac{1}{4}$ is split into a corner defect of $+\frac{1}{4}$ and a defect on the wall of strength $-\frac{1}{2}$. The defect on the wall along the edge to a corner containing a $+\frac{1}{4}$ defect, creating the diagonal state. Using the full expression for the energy

given in Equation (A.26), we normalize the energy by removing the constant term corresponding to the energy of the diagonal state and the energy contribution from the internal defect ($\frac{\pi}{4} \log(\frac{1}{\epsilon})$), giving us a normalized energy $\tilde{E}(x_1, y_1)$ independent of ϵ . Comparing Figures 2.14 and 2.15, we see that the normalized energy behaves similarly to the full expression for the energy, although, like the normalized energies of the diagonal and rotated states, it can be negative for some parameters.

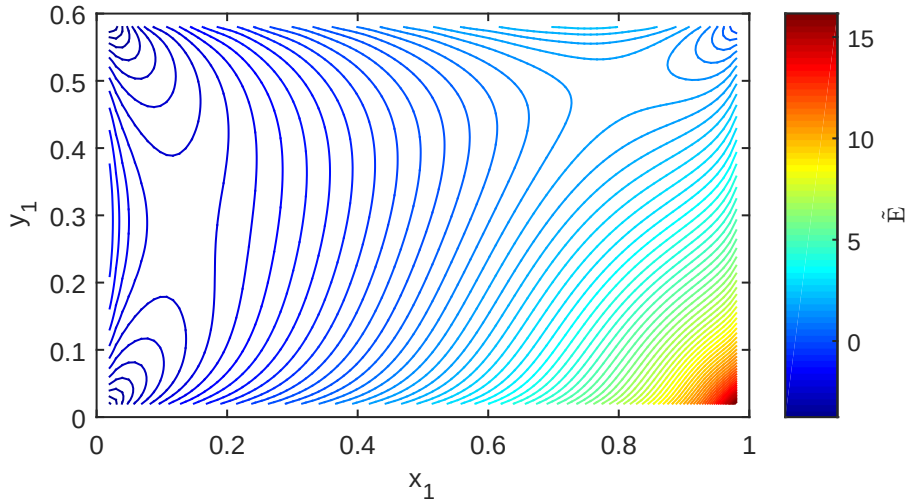


Figure 2.15: Contour plot of $\tilde{E}$, with $\lambda = 0.6$, $m = -\frac{1}{2}$ and $a_1 = a_3 = 0$, $a_2 = a_4 = \frac{\pi}{2}$.

We define our energy minimizing pathways as follows: for each value $x_1 \in (4\epsilon, 1 - 4\epsilon)$ in our mesh, we evaluate the $\min_{y_1} \tilde{E}(x_1, y_1)$ and identify the corresponding value of y_1 . This defines a line, denoted (1), in the domain A , which is the minimizing pathway for the internal defect to travel in the x -direction. Similarly, we calculate a second line (2) by fixing y_1 and minimizing $\tilde{E}(x_1, y_1)$ over x_1 . We show both of these pathways in Figure 2.16a, as well as the numerically computed gradient $-\nabla \tilde{E}$. This gradient shows the preferred direction that an internal defect will move in order to minimize the energy. Pathway (1) corresponds to a optimal pathway from the U_2 to D state, while pathway (2) corresponds to the optimal line for a defect to move from the U_1 to the D state. It is interesting to note that there is no obvious pathway for a defect to move from the U_1 to U_2 states (or vice versa) directly, instead it is always

energetically preferable to move toward the D state from one of the rotated states.

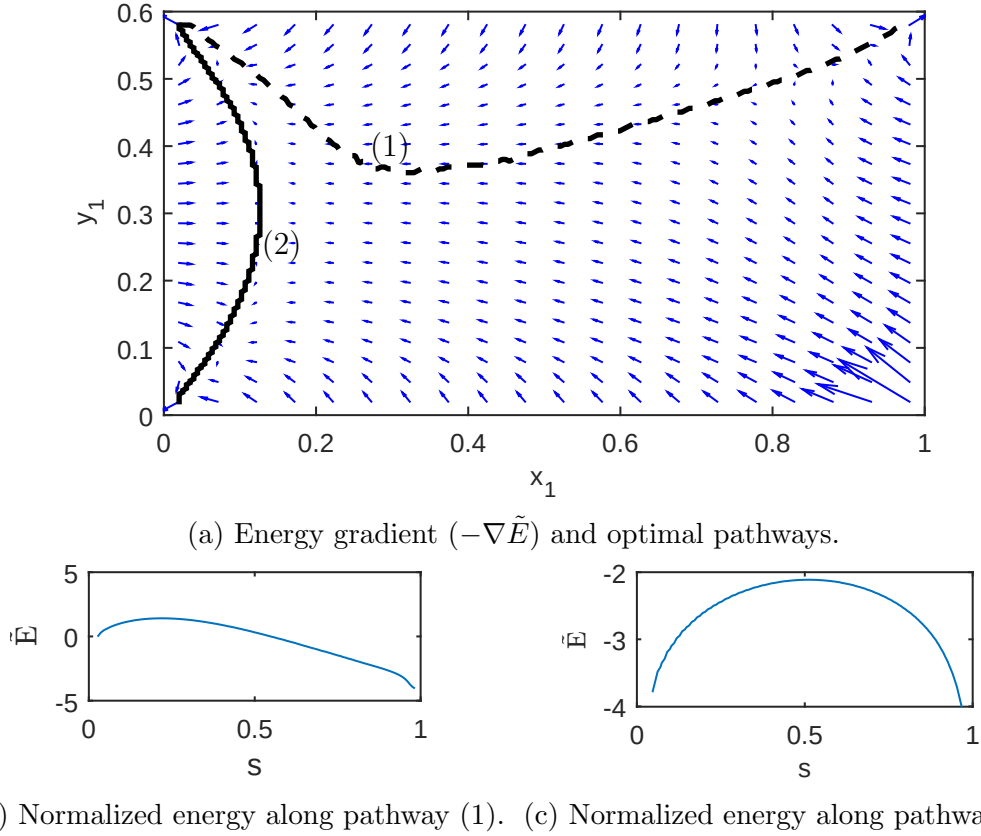


Figure 2.16: Energy minimizing pathways and the normalized energies along normalized path length s , calculated for $\lambda = 0.6$, $a_1 = a_3 = 0$, $a_2 = a_4 = \frac{\pi}{2}$ and $m = -\frac{1}{2}$.

In Figures 2.16b and 2.16c, we show the normalized energy along the pathways (1) and (2) as a function of normalized path length starting in a corner corresponding to a rotated state. We see that the pathways pass through a different saddle-splay point, which is the maximum value of $\tilde{E}$ on the pathway. We define these values of $\tilde{E}$ to be the normalized energy barrier, denoted by $\tilde{E}_{(i)}$ ($i = 1, 2$). These values can be evaluated numerically for some fixed λ , for example, see Figure 2.17. We denote the total energy barrier to be overcome to go from state i to state j to be E_{i-j} (where i ,

$j \in \{D, U_1, U_2\}$). These barriers can be expressed analytically as

$$E_{D-U_1} := \tilde{E}_{(1)} + \frac{\pi}{4} \ln \left(\frac{1}{\epsilon} \right), \quad (2.85)$$

$$E_{U_1-D} := \tilde{E}_{(1)} + \frac{\pi}{4} \ln \left(\frac{1}{\epsilon} \right) - (\tilde{E}_{U_1} - \tilde{E}_D), \quad (2.86)$$

$$E_{D-U_2} := \tilde{E}_{(2)} + \frac{\pi}{4} \ln \left(\frac{1}{\epsilon} \right), \quad (2.87)$$

$$E_{U_2-D} := \tilde{E}_{(2)} + \frac{\pi}{4} \ln \left(\frac{1}{\epsilon} \right) - (\tilde{E}_{U_2} - \tilde{E}_D). \quad (2.88)$$

It follows immediately that going from the diagonal state to either of the rotated states imposes a greater energy barrier than travelling from either rotated state to the diagonal state. The barrier to be overcome travelling from the D to U_1 states (pathway (2)) will be considerably lower than the barrier on pathway (1).

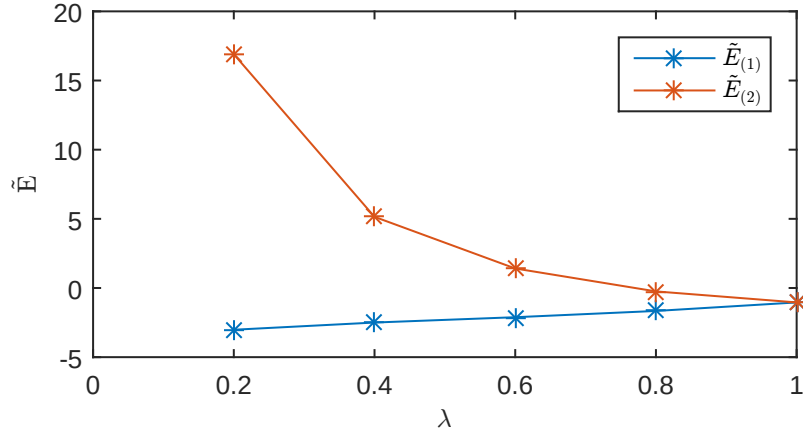


Figure 2.17: Value of normalized energy at the saddle splay points in terms of λ .

Finally, we compare these energy barriers with the energy associated with thermal fluctuations, $k_B T$. For comparison, we consider the liquid crystal material MBBA confined to geometries similar to those discussed in [41], with square wells of length $X_e = Y_e = 80 \mu\text{m}$ and depth $Z_e = 12 \mu\text{m}$. Here, the elastic constant is approximately $1 \times 10^{-11} \text{N}$ and we estimate the nematic correlation length is

$$\xi = \sqrt{\frac{27CL}{B^2}} \approx 1.79 \times 10^{-8} \text{m}. \quad (2.89)$$

Dividing ξ by the chamber length to account for the rescaling of the defect core, we estimate

$$\epsilon = 2.24 \times 10^{-4}. \quad (2.90)$$

We multiply our energy barrier by the chamber depth Z_e and the elastic constant K to find

$$KZE_{D-U_1} = 6.67 \times 10^{-16} J, \quad (2.91)$$

$$KZE_{U_1-D} = 5.36 \times 10^{-16} J, \quad (2.92)$$

which compare favourably with similar estimates in [70]. We note that this barrier is much greater than $k_B T$, which is approximately $4 \times 10^{-21} J$ for temperatures close to the nematic-isotropic transition temperature. In order to bring the energy barrier down to values close to $k_B T$ would require reducing the chamber depth Z_e to the nanometer scale.

By removing the constraint that the defect must be confined to the wall used in [68], we find that the energetically favourable pathway for an internal defect to move is through the bulk of the well. This has the effect of lowering the predicted energy barrier between the different equilibria in [68]. Our work serves as a more analytic version of the numerical work carried out in [69, 70], in which the authors use a Landau-de Gennes model to study a similar problem. One limitation of our work here is that our model cannot capture the behaviour as internal defect approaches a corner, as our method for evaluating the Oseen-Frank energy requires that the removed defect cores cannot overlap.

2.4 Equilibria with Unequal Elastic Constants

In this section, we consider the effect of elastic anisotropy on stable equilibria. Equilibria must be solutions of the Euler-Lagrange equation (2.4) subject to suitable boundary conditions. Equation (2.4) is highly nonlinear, making it difficult to derive analytic expressions for the director and the energy.

We solve Equation (2.4) numerically using COMSOL (see Appendix B for some details on COMSOL). Using suitable boundary conditions, we find the D , U_1 and U_2 states for any $\delta < 1$. Structurally, these states are similar to the one-constant solutions, with increased regions of splay distortion (for $\delta > 0$) or increased regions of bend distortion (for $\delta < 0$).

We observe that for small λ , the director field of both the D and U_1 states is almost everywhere parallel to the long walls of the rectangle, except around the edges at $x = 0$ and $x = 1$ where the director field rotates by $\frac{\pi}{2}$ radians to match the boundary conditions, as shown in Figure 2.18. From the frame invariance of the Oseen-Frank energy we obtain symmetry relations on the director fields of the D and U_1 states, both of which are observable in Figure 2.18. The director field of the D state has rotational symmetry of order 2 about the point $(\frac{1}{2}, \frac{\lambda}{2})$, or equivalently θ satisfies $\theta(x, y) = \theta(1 - x, \lambda - y)$. The director field of the U_1 state has reflective symmetry in the line $x = \frac{1}{2}$, which is equivalent to $\theta(x, y) = -\theta(1 - x, y)$.

We use these conditions to demonstrate that the D state has a lower energy than the U_1 state for all values of $\delta < 1$ in the limit $\lambda \rightarrow 0$. We first consider the D state and show that as $\lambda \rightarrow 0$, the angle of the director θ has an outer solution and two boundary layers. We calculate the leading-order contributions to the outer solution and derive an expression for the energy. We then consider the U_1 state and show how the inner and outer solutions for θ differ from the equivalent solutions for the D state in order to quantify the difference in energy between the states.

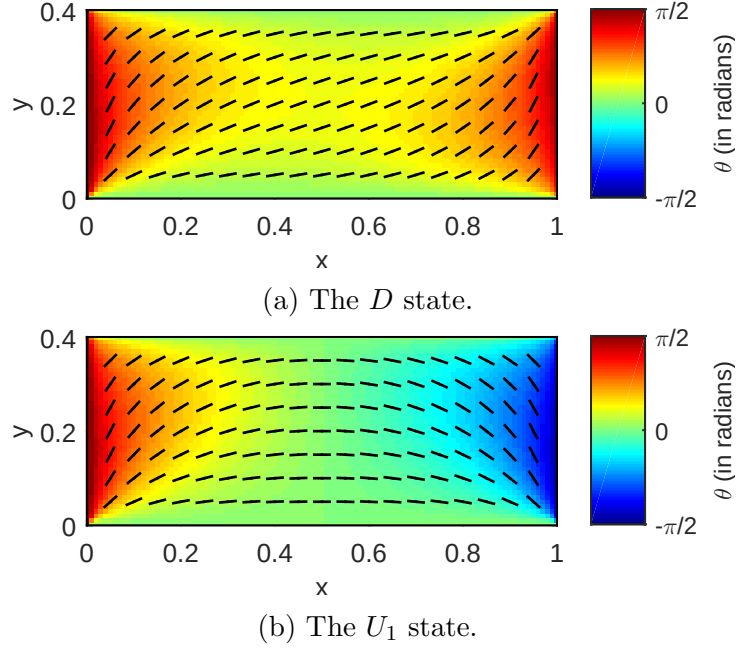


Figure 2.18: Numerically calculated director fields for the D and U_1 states for $\delta = 0.5$ and $\lambda = 0.4$.

2.4.1 The Diagonal State

The diagonal state is described by the solution to Equation (2.4) with the boundary conditions as shown in Figure 2.19.

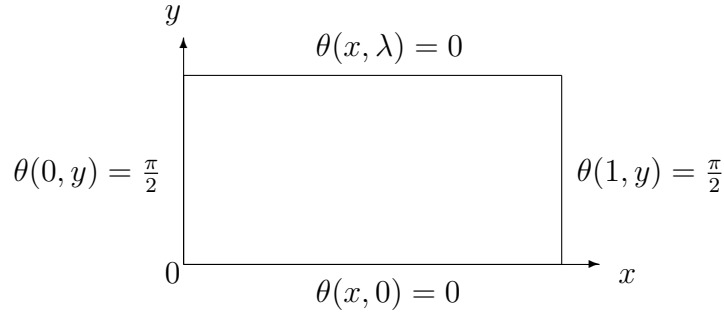


Figure 2.19: Boundary conditions for the D state.

We introduce the rescaled variable $Y := \frac{y}{\lambda}$ and let $\Theta(x, Y) = \theta(x, \lambda Y)$. The

Euler-Lagrange equation for Θ is

$$(1 - \delta \cos^2 \Theta) \Theta_{YY} + \frac{\delta}{2} \sin(2\Theta) \Theta_Y^2 + \lambda \delta (\sin(2\Theta) \Theta_{xY} + \cos(2\Theta) \Theta_x \Theta_Y) + \lambda^2 \left(\Theta_{xx} (1 - \delta \sin^2 \Theta) - \frac{\delta}{2} \sin(2\Theta) \Theta_x^2 \right) = 0, \quad (2.93)$$

subject to $\Theta(x, 0) = \Theta(x, 1) = 0$ and $\Theta(0, Y) = \Theta(1, Y) = \frac{\pi}{2}$.

2.4.1.1 The Outer Problem

Using the fact that the director field is approximately uniform, we linearize Equation (2.93) about $\Theta = 0$ to find

$$(1 - \delta) \Theta_{YY} + \lambda^2 \Theta_{xx} = 0, \quad (2.94)$$

subject to $\Theta(x, 0) = \Theta(x, 1) = 0$, $\Theta(x, Y) = \Theta(1 - x, 1 - Y)$. Solving by separation of variables, we find that

$$\Theta = \sum_{n=1}^{\infty} A_n \sin(n\pi Y) X_n(x), \quad (2.95)$$

where X_n is the solution to

$$\lambda^2 X_n'' - (1 - \delta) n^2 \pi^2 X_n = 0. \quad (2.96)$$

By solving Equation (2.96), we find that as $\lambda \rightarrow 0$

$$\Theta \sim A_1 \sin(\pi Y) \cosh \left(\frac{\pi}{\lambda} \sqrt{1 - \delta} \left(x - \frac{1}{2} \right) \right) e^{-\frac{\pi}{2\lambda} \sqrt{1 - \delta}} + O \left(e^{-\frac{\pi}{\lambda} \sqrt{1 - \delta}} \right). \quad (2.97)$$

We see that we must have an outer solution which is exponentially small, and boundary layers about $x = 0$ and $x = 1$. We note that this exponential behaviour is consistent with one-constant approximation solution derived in §2.2.3.

Motivated by the linearized behaviour of θ in (2.97), we define an exponentially small parameter

$$\mu := \exp\left(-\frac{\pi}{2\lambda}\sqrt{1-\delta}\right), \quad (2.98)$$

and expand the outer solution as a series in μ ,

$$\Theta_{\text{Outer}} \sim \mu\Theta_1(x, Y) + \mu^2\Theta_2(x, Y) + \dots \quad (2.99)$$

Substituting into Equation (2.93), we find that Θ_1 satisfies

$$(1-\delta)\Theta_{1YY} + \lambda^2\Theta_{1xx} = 0, \quad (2.100)$$

and Θ_2 satisfies

$$(1-\delta)\Theta_{2YY} + \lambda^2\Theta_{2xx} = -\lambda\delta(2\Theta_1\Theta_{1xY} + \Theta_{1x}\Theta_{1Y}), \quad (2.101)$$

subject to $\Theta_i(x, 0) = \Theta_i(x, 1) = 0$ and $\Theta_i(x, Y) = \Theta_i(1-x, 1-Y)$. Solving, we find that

$$\Theta_1(x, Y) = A_1 \sin(\pi Y) \cosh\left(\frac{\pi}{\lambda}\sqrt{1-\delta}\left(x - \frac{1}{2}\right)\right), \quad (2.102)$$

in agreement with Equation (2.97), and

$$\begin{aligned} \Theta_2(x, Y) = & A_2 \sin(2\pi Y) \sinh\left(\frac{2\pi}{\lambda}\sqrt{1-\delta}\left(x - \frac{1}{2}\right)\right) \\ & + \frac{3A_1^2\delta\pi}{16\lambda} \sin(2\pi Y) \left(\frac{1}{2} - x\right) \cosh\left(\frac{2\pi}{\lambda}\sqrt{1-\delta}\left(x - \frac{1}{2}\right)\right), \end{aligned} \quad (2.103)$$

where A_1 and A_2 are coefficients that can be determined by matching with the inner solution.

2.4.1.2 The Inner Problem

We now consider the solution in the inner region at $x = 0$. Analysis of the second inner region at $x = 1$ follows identically. We introduce $X := \frac{x}{\lambda}$ and $f(X, Y) = \Theta(x, Y)$. Then the inner director field satisfies

$$f_{XX} + f_{YY} = \delta \left[f_{XX} \sin^2(f) + f_{YY} \cos^2(f) - \cos(2f) f_X f_Y + \frac{1}{2} \sin(2f) (f_X^2 - 2f_{XY} - f_Y^2) \right], \quad (2.104)$$

on the semi-infinite rectangular domain, subject to the boundary conditions shown in Figure 2.20. We are unable to solve Equation (2.104) analytically; however, we can take advantage of the far field behaviour in order to estimate the coefficients of the outer solution.

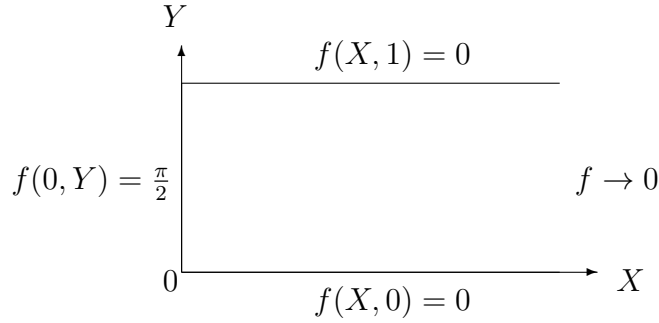


Figure 2.20: Boundary conditions for the inner problem at $x = 0$.

By expressing the outer solution (2.99) in terms of the variables X and Y ,

$$\begin{aligned} \Theta_{\text{Outer}} \sim & \frac{A_1}{2} \sin(\pi Y) \left[e^{-\pi\sqrt{1-\delta}X} + \mu^2 e^{\pi\sqrt{1-\delta}X} \right] \\ & + \sin(2\pi Y) \left[\frac{A_2}{2} \left(e^{-2\pi\sqrt{1-\delta}X} - \mu^4 e^{2\pi\sqrt{1-\delta}X} \right) \right. \\ & \left. + \frac{3A_1^2\delta\pi}{64\lambda} (1 - 2\lambda X) \left(\mu^4 e^{2\pi\sqrt{1-\delta}X} + e^{-2\pi\sqrt{1-\delta}X} \right) \right] + \dots, \quad (2.105) \end{aligned}$$

we see that as $\mu \rightarrow 0$, f must have the form

$$f \sim f_0 + \mu^2 f_2 + O(\mu^4). \quad (2.106)$$

The leading order term f_0 satisfies

$$\begin{aligned} f_{0XX} + f_{0YY} = & \delta \left[f_{0XX} \sin^2(f_0) + f_{0YY} \cos^2(f_0) \right. \\ & \left. + \frac{1}{2} \sin(2f_0)(f_{0X}^2 - 2f_{0XY} - f_{0Y}^2) - \cos(2f_0)f_{0X}f_{0Y} \right], \end{aligned} \quad (2.107)$$

with boundary conditions $f_0(X, 0) = f_0(X, 1) = 0$, $f_0(0, Y) = \frac{\pi}{2}$ and $f_0 \rightarrow 0$ as $X \rightarrow \infty$.

The next term in the expansion, f_2 , is the solution to

$$\begin{aligned} f_{2XX} + f_{2YY} = & \delta \left[\sin^2(f_0)f_{2XX} + \cos^2(f_0)f_{2YY} \right. \\ & + \sin(2f_0)(f_2(f_{0XX} + 2f_{0X}f_{0Y} - f_{0YY}) + f_{0X}f_{2X} - f_{0Y}f_{2Y} - f_{2XY}) \\ & \left. + \cos(2f_0)(f_2(f_{0X}^2 - 2f_{0XY} - f_{0Y}^2) - f_{0Y}f_{2X} - f_{0X}f_{2Y}) \right], \end{aligned} \quad (2.108)$$

with boundary conditions $f_2(X, 0) = f_2(X, 1) = f_2(0, Y) = 0$. By matching with the outer solution, we see that as $X \rightarrow \infty$

$$f_2 \sim \frac{A_1}{2} \sin(\pi Y) e^{\pi\sqrt{1-\delta}X}. \quad (2.109)$$

As $X \rightarrow \infty$, we expand f_0 as a series in terms of $e^{-\pi\sqrt{1-\delta}X}$ and calculate that

$$\begin{aligned} f_0 \sim & B_1 \sin(\pi Y) e^{-\pi\sqrt{1-\delta}X} + \left(B_2 - \frac{3B_1^2\delta\pi X}{8} \right) \sin(2\pi Y) e^{-2\pi\sqrt{1-\delta}X} \\ & + O(e^{-3\pi\sqrt{1-\delta}X}). \end{aligned} \quad (2.110)$$

By comparing Equations (2.105) and (2.110), the coefficients of the outer series

A_1 and A_2 , can be expressed in terms of the coefficients B_1 and B_2 , as

$$A_1 = 2B_1, \quad A_2 = 2B_2 - \frac{3B_1^2\delta}{8\lambda}. \quad (2.111)$$

The coefficient B_1 depends solely on δ and is given by

$$B_1(\delta) := \lim_{X \rightarrow \infty} 2 \exp(\pi\sqrt{1-\delta}X) \int_0^1 f_0(X, Y) \sin(\pi Y) dY. \quad (2.112)$$

Using COMSOL, we can calculate B_1 by solving Equation (2.107) and the boundary conditions in a long, but finite, rectangle and then evaluating the Equation (2.112) at some large value of X . In the one constant approximation, we can solve the inner problem exactly, giving us $B_1 = 2$. This is in agreement with our numerical estimate shown in Figure 2.21.

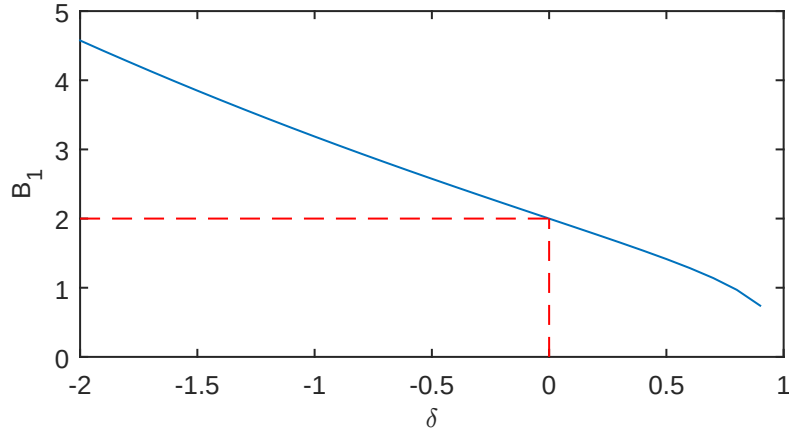


Figure 2.21: Numerical solution for $B_1(\delta)$, by solving Equation (2.107) on a rectangle of length 10, and evaluating Equation (2.112) at $X = 8$.

2.4.1.3 The Oseen-Frank Energy

We now estimate the Oseen-Frank energy. In terms of the inner and outer solutions, the energy is

$$E[\theta] = 2E_{\text{Inner}} + E_{\text{Outer}}, \quad (2.113)$$

where the inner energy is

$$E_{\text{Inner}} := \frac{1}{2} \int_0^1 \int_0^{\frac{\alpha}{\lambda}} f_X^2 + f_Y^2 - \delta (f_Y \cos(f) - f_X \sin(f))^2 dX dY, \quad (2.114)$$

and the outer energy is

$$E_{\text{Outer}} := \frac{\lambda}{2} \int_0^1 \int_\alpha^{1-\alpha} \Theta_x^2 + \frac{\Theta_Y^2}{\lambda^2} - \delta \left(\frac{\Theta_Y}{\lambda} \cos(\Theta) - \Theta_x \sin(\Theta) \right)^2 dx dY, \quad (2.115)$$

where α is a matching parameter, chosen such that $\lambda \ll \alpha \ll 1$.

Using the expression for the outer solution (2.99), the energy of the outer region is found to be

$$E_{\text{Outer}} \sim \frac{B_1^2 \pi \sqrt{1-\delta}}{2} e^{-\frac{2\pi\alpha}{\lambda} \sqrt{1-\delta}} + O(\mu^3). \quad (2.116)$$

Using the expansion (2.106) for the inner solution, we expand the integrand of (2.114) in terms of μ to get

$$\frac{1}{2} (f_X^2 + f_Y^2) - \frac{\delta}{2} (f_Y \cos(f) - f_X \sin(f))^2 \sim F_0 + \mu^2 F_2 + O(\mu^4), \quad (2.117)$$

where

$$F_0 := \frac{1}{2} (f_{0X}^2 + f_{0Y}^2) - \frac{\delta}{2} (f_{0Y} \cos(f_0) - f_{0X} \sin(f_0))^2, \quad (2.118)$$

$$F_2 := \delta (f_{0Y} \cos(f_0) - f_{0X} \sin(f_0)) \left[\sin(f_0) f_{2X} - \cos(f_0) f_{2Y} \right. \\ \left. + (f_{0X} \cos(f_0) + f_{0Y} \sin(f_0)) f_2 \right] + f_{0X} f_{2X} + f_{0Y} f_{2Y}. \quad (2.119)$$

By rearranging and applying Equation (2.107), we see that F_2 simplifies to

$$F_2 = \left[((1 - \delta \sin^2(f_0))f_{0X} + \delta \sin(f_0) \cos(f_0)f_{0Y}) f_2 \right]_X + \left[(\delta \sin(f_0) \cos(f_0)f_{0X} + (1 - \delta \cos^2(f_0))f_{0Y}) f_2 \right]_Y. \quad (2.120)$$

The energy in the inner region at $x = 0$ is therefore

$$E_{\text{Inner}} \sim \int_0^1 \int_0^{\frac{\alpha}{\lambda}} F_0 \, dX \, dY + \mu^2 \int_0^1 \int_0^{\frac{\alpha}{\lambda}} F_2 \, dX \, dY + O(\mu^4). \quad (2.121)$$

We exploit the far-field behaviour (2.110) by writing

$$\int_0^1 \int_0^{\frac{\alpha}{\lambda}} F_0 \, dX \, dY = \int_0^1 \int_0^\infty F_0 \, dX \, dY - \int_0^1 \int_{\frac{\alpha}{\lambda}}^\infty F_0 \, dX \, dY \quad (2.122)$$

$$\sim \int_0^1 \int_0^\infty F_0 \, dX \, dY - \frac{\pi \sqrt{1 - \delta} B_1^2}{4} e^{-\frac{2\pi\alpha}{\lambda} \sqrt{1 - \delta}} + O\left(e^{-\frac{3\alpha\pi}{\lambda} \sqrt{1 - \delta}}\right). \quad (2.123)$$

Here, the integral $\int_0^1 \int_0^\infty F_0 \, dX \, dY$ can be evaluated numerically by regularizing the domain to remove singularities at the corners. More importantly, we observe that this integral over the semi-infinite domain is completely independent of the outer solution and will only depend on the elastic anisotropy δ and defect core size ϵ .

The order μ^2 contribution to the inner energy is

$$\int_0^1 \int_0^{\frac{\alpha}{\lambda}} F_2 \, dX \, dY \sim \int_0^1 \left((1 - \delta \sin^2(f_0))f_{0X} + \delta \sin(f_0) \cos(f_0)f_{0Y} \right) f_2 \Big|_{X=\frac{\alpha}{\lambda}} dY \quad (2.124)$$

$$\sim -\frac{\pi B_1^2 \sqrt{1 - \delta}}{2} + O\left(e^{-\frac{\pi \sqrt{1 - \delta} \alpha}{\lambda}}\right). \quad (2.125)$$

The contribution from the second inner region at $x = 1$ is the same as the inner region

at $x = 0$. Therefore, the total energy of the diagonal state in the limit as $\lambda \rightarrow 0$ is

$$E_D \sim 2 \int_0^1 \int_0^\infty F_0 dX dY - \pi \mu^2 B_1^2 \sqrt{1-\delta} + O(\mu^3). \quad (2.126)$$

2.4.2 The Rotated (U_1) State

For the U_1 state, we follow the same procedure as for the D state. The rescaled angle Θ satisfies Equation (2.93) subject to $\Theta(x, 0) = \Theta(x, 1) = 0$ and $\Theta(0, Y) = -\Theta(1-x, Y)$ in the outer region. We again expand the outer solution in terms of μ ,

$$\Theta_{\text{Outer}} = \mu \Theta_1 + \mu^2 \Theta_2 + \dots, \quad (2.127)$$

with boundary conditions $\Theta_i(x, 0) = \Theta_i(x, 1) = 0$ and $\Theta_i(0, Y) = -\Theta_i(1-x, Y)$.

Here, the symmetry condition gives us a different outer solution, namely

$$\Theta_1(x, Y) = C_1 \sin(\pi Y) \sinh\left(\frac{\pi}{\lambda} \sqrt{1-\delta} \left(\frac{1}{2} - x\right)\right), \quad (2.128)$$

$$\begin{aligned} \Theta_2(x, Y) = C_2 \sin(2\pi Y) \sinh\left(\frac{2\pi}{\lambda} \sqrt{1-\delta} \left(x - \frac{1}{2}\right)\right) \\ + \frac{3C_1^2 \delta \pi}{16\lambda} \sin(2\pi Y) \left(\frac{1}{2} - x\right) \cosh\left(\frac{2\pi}{\lambda} \sqrt{1-\delta} \left(x - \frac{1}{2}\right)\right). \end{aligned} \quad (2.129)$$

Expressing the outer solution in terms of the inner variables, we have

$$\begin{aligned} \Theta_{\text{Outer}}(\lambda X, Y) \sim \frac{C_1}{2} \sin(\pi Y) \left[e^{-\pi \sqrt{1-\delta} X} - \mu^2 e^{\pi \sqrt{1-\delta} X} \right] \\ + \sin(2\pi Y) \left[\frac{C_2}{2} \left(e^{-2\pi \sqrt{1-\delta} X} - \mu^4 e^{2\pi \sqrt{1-\delta} X} \right) \right. \\ \left. + \frac{3C_1^2 \delta \pi}{64\lambda} (1 - 2\lambda X) \left(\mu^4 e^{2\pi \sqrt{1-\delta} X} + e^{-2\pi \sqrt{1-\delta} X} \right) \right] + \dots, \end{aligned} \quad (2.130)$$

and therefore that the inner solution f must have the form

$$f \sim f_0 - \mu^2 f_2 + O(\mu^4) \quad (2.131)$$

as $\mu \rightarrow 0$. The differential equations governing f_0 and f_2 are the same as for the diagonal case. It therefore follows that $C_1 = A_1$ and $C_2 = A_2$.

The leading order contribution to the outer energy is

$$E_{\text{Outer}} \sim \frac{B_1^2 \pi \sqrt{1-\delta}}{2} e^{-\frac{2\pi\alpha}{\lambda} \sqrt{1-\delta}} + O(\mu^3), \quad (2.132)$$

Expanding the inner energy in terms of μ , then, due to Equation (2.131), the inner energy differs from the diagonal inner energy in the order μ^2 contribution,

$$E_{\text{Inner}} \sim \int_0^1 \int_0^\infty F_0 \, dX \, dY - \frac{\pi \sqrt{1-\delta} B_1^2}{4} e^{-\frac{2\pi\alpha}{\lambda} \sqrt{1-\delta}} + \frac{\pi \mu^2 B_1^2 \sqrt{1-\delta}}{2} + O(\mu^3). \quad (2.133)$$

Therefore, the energy of the U_1 state is

$$E_{U_1} \sim 2 \int_0^1 \int_0^\infty F_0 \, dX \, dY + \pi \mu^2 B_1^2 \sqrt{1-\delta} + O(\mu^3). \quad (2.134)$$

2.4.3 Results

In the limit as $\lambda \rightarrow 0$, the energies of the D and U_1 states are dominated by the energy due to the distortion induced by the corner defects. This energy is the same for both the D and U_1 states up to an exponentially small difference, namely

$$E_{U_1} - E_D \sim 2\pi B_1^2 \sqrt{1-\delta} e^{-\frac{\pi}{\lambda} \sqrt{1-\delta}} + O\left(e^{-\frac{3\pi}{2\lambda} \sqrt{1-\delta}}\right). \quad (2.135)$$

The diagonal state is therefore the lower energy state for all δ in the limit as $\lambda \rightarrow 0$. When $\delta = 0$, we recover the difference in normalized energies identified in §2.2.3.

Using COMSOL, we evaluate the energies of the D and U_1 states for a selection of small values of λ and variable δ . We compare the differences in the numerically computed energies, along with our asymptotic result (2.135), in Figure 2.22. We see a good agreement between the numerics and our asymptotics, even for values of λ

up to 0.5. This suggests that COMSOL is successfully capturing the small effects of elastic anisotropy. Physically, this limiting behaviour is caused by the difference in the distance between pairs of opposing strength defects becoming equal as $\lambda \rightarrow 0$. We note that for small λ and $\delta < 0$, the asymptotic result and the computed energy differences from COMSOL begin to diverge. In this parameter regime, the exponentially small quantity (Equation (2.135)) is the same order of magnitude as errors arising from the regularization of the energy, which are $O(\epsilon^2)$.

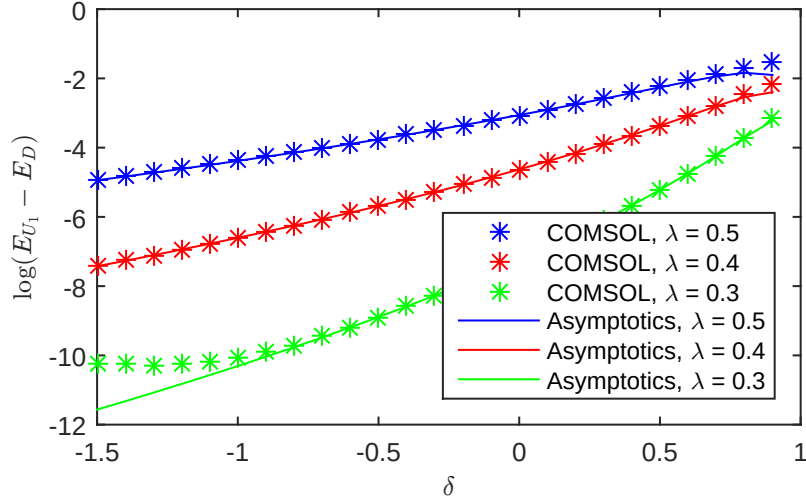


Figure 2.22: Difference in energies of the D and U_1 states with unequal elastic constants. Numerical results from COMSOL using a defect-core size of $\epsilon = 0.005$ and asymptotic results (2.135).

2.5 Summary

In this chapter, we have investigated nematic equilibria confined to two-dimensional rectangular wells with strong tangent anchoring. We identify three distinct stable equilibria: the diagonal state and two rotated states. Using the one-constant approximation, we obtain analytic expressions for the director fields and Oseen-Frank energies of the three equilibria. These expressions allow us to separate the contribution to the energy from defects from the contribution due to the bulk distortion.

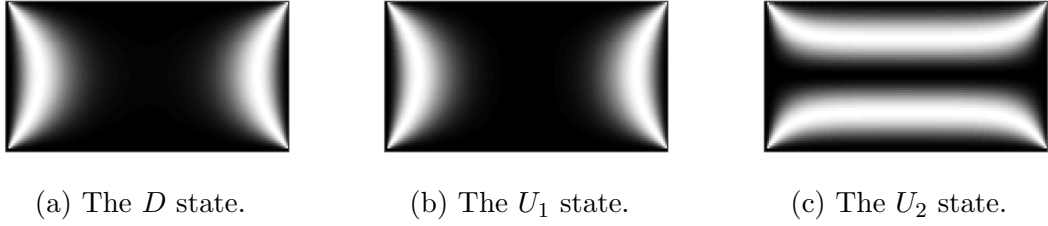


Figure 2.23: Optical textures for the D , U_1 and U_2 states between horizontal and vertical polarising filters for $\lambda = 0.4$, with white corresponding to the maximum transmitted light and black corresponding to zero transmitted light.

Our analysis shows that the diagonal state always has the minimum energy. For low rectangular aspect ratios, we show that the energies of the D and U_1 states converge. This behaviour occurs due to the distortion to the director being concentrated in boundary layers at the ends of the well. For small rectangular aspect ratios, λ , the energy of the U_2 state scales like $\frac{1}{\lambda}$ due to the high distortion caused the director rotating by π radians over a distance λ . This significantly higher energy may explain why this state is never observed experimentally using the fd -virus.

The U_2 state could have potential industrial applications for a bistable device. When viewed under crossed polarizers, the D and U_1 states are effectively indistinguishable, as shown in Figure 2.23. Here, the optical intensity between crossed polarising filters is given by

$$I = \frac{I_0}{2} \sin^2(2\theta) \sin^2\left(\frac{\pi d \Delta n}{\lambda}\right). \quad (2.136)$$

where I_0 on the intensity of incoming light, d is the thickness of the liquid crystal, λ is the wavelength of light, and Δn is the difference between the extraordinary and ordinary refractive indices [85, 86]. In contrast, the U_2 state has a very different optical texture. Unfortunately, reliably switching between the D or U_1 states and U_2 state may be difficult due to their large difference in energies, as well as the difficulty in creating a field which suitably reorientates the liquid crystal molecules.

By constructing a solution containing a singularity in the director, we derive an

expression for the director with an internal defect. We use this expression to evaluate the Oseen-Frank energy in terms of rectangular aspect ratio and defect location. We then discuss the properties of states with internal defects and conclude that these are never local minimizers of the energy: it will always be energetically preferable to move the internal defect towards one of the corners containing a defect of opposing sign strength. We also consider energy minimizing paths for an internal defect to take between states and calculate energy barriers between the stable equilibria. The increased energy cost from an internal defect may explain why these states are rarely seen experimentally using the *fd*-virus. However, our results indicate that these states will always be unstable, and it is therefore surprising that these states persist.

Lastly, we work with unequal elastic constants and take advantage of the properties of the low rectangular aspect to show that the diagonal state always has the lowest energy in the limit as $\lambda \rightarrow 0$ for any ratio of the elastic constants K_1 and K_3 . We find that our asymptotic results compare very favourably with numerical results from COMSOL, even for relatively large values of λ .

Chapter 3

Stability Analysis of the Uniform State in a Rectangular Well

3.1 Introduction

3.1.1 The Uniform State

In the previous chapter, we discussed the equilibrium states of nematic liquid crystals confined to rectangular wells with strong tangential anchoring. This was motivated in part by the experimental results presented in Figure 2.3 and Figure 2.4 on the confinement of a suspension of the *fd*-virus in shallow rectangular wells. There is one final state which we did not consider in Chapter 2, the uniform state denoted by L . This uniform state, shown in Figure 3.1, is characterized by an approximately constant director field, aligned parallel to the longest wall of the rectangle. This state occurs for small wells with low rectangular aspect ratios ($\lambda < 0.5$) and with small heights ($Y_e < 8\mu\text{m}$) [75]. The presence of this state indicates a breakdown of the strong anchoring assumption for cells of these dimensions, although interestingly, both the diagonal and rotated states are still found for similar dimension chambers.

In [12], this coexistence is used to derive an estimate for the extrapolation length

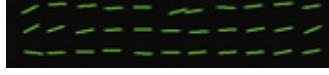


Figure 3.1: Experimental image of uniform state. *Adapted from [12] with permission from the Royal Society of Chemistry.*

$\xi := \frac{K}{W}$, by assuming that if the relative frequencies of two states are equal, then the energies are equal. The authors introduce a Rapini-Papoular surface energy to describe the energy of the L state, and calculate that

$$\xi = \frac{K}{W} \approx \frac{Y_e}{\pi \ln \left(\frac{2Y_e}{\pi \hat{\epsilon}} \right)}, \quad (3.1)$$

The defect core size $\hat{\epsilon}$ is assumed to be the length of the virus, $0.88 \mu\text{m}$, which is inferred from the experimental images in Figure 2.3. The value of Y_e used in (3.1) is determined from the experimental frequencies of each state.

State	Y (μm)	λ	ξ (μm)
D	6.8	0.4	1.4
U_1	7.4	0.5	1.4

Table 3.1: Interpolated values of Y_e and λ when the frequencies of the D and U_1 states coincide with the frequencies of the L state for the WT fd -virus and the associated estimate of the extrapolation length. *Adapted from Ref. [12] with permission from the Royal Society of Chemistry.*

The resulting estimate of the extrapolation length ξ , given in Table 3.1, is on the order of the particle length and compares favourably with the previously reported theoretical estimate of ξ for the fd -virus [87].

However, this estimate is dependent on a number of assumptions, the most significant of which is that both the D , U_1 and L states are local minimizers of the Oseen-Frank energy. In this chapter, we discuss the relative stability of these equilibria using a semi-infinite rectangular well. This precise problem has not been considered before using a continuum theory, although there are a number of related problems. We shall see that the stability of the uniform state is similar to the classical Fréedericksz tran-

sition between two parallel plates [88, 17], with the electric or magnetic field replaced by a localized anchoring energy. In the strong anchoring limit, different equilibria within semi-infinite rectangular wells are described using a conformal mapping approach in [68]. Using a mean-field model, the authors in [12] study possible equilibria within a rectangle and find the L state for small anchoring strengths. In [89], a computational model based on a system of hard rods finds smectic phases which break the surface anchoring conditions. However, this model does not capture the behaviour identified experimentally in Figure 2.3, as the smectic phase is generated by increasing the concentration, while the experimental rod concentration remains constant for all wells.

3.1.2 Chapter Outline

In this chapter, we are interested in studying the transition from the L state to the U_1 or D states found experimentally. Our analysis of the equilibria within shallow rectangular wells in Chapter 2 shows that for small rectangular aspect ratios the important characteristics of the director and energies can be captured (up to some exponentially small terms) by working in the semi-infinite domain

$$\Omega = \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq \infty, 0 \leq y \leq 1\}. \quad (3.2)$$

In the Oseen-Frank theory, we express the two-dimensional director field in terms of the unit vector

$$\mathbf{n} = (\cos(\theta(x, y)), \sin(\theta(x, y))), \quad (3.3)$$

and we work with the rescaled Oseen-Frank energy with a Rapini-Papoular surface energy,

$$E[\theta]/K_3 = \frac{1}{2} \iint_{\Omega} |\nabla \theta|^2 - \delta (\theta_y \cos(\theta) - \theta_x \sin(\theta))^2 \, d\Omega + \frac{\alpha}{2} \oint_{\partial\Omega} \sin^2(\theta - \phi_0) \, ds, \quad (3.4)$$

where our measure of elastic anisotropy is $\delta := 1 - \frac{K_1}{K_3}$ and the rescaled anchoring coefficient $\alpha := \frac{WY_e}{K_3}$, where W is the Rapini-Papoular anchoring strength and Y_e is the chamber width defined in Figure 2.2. The preferred direction of alignment on $\partial\Omega$ is given by ϕ_0 , shown in Figure 3.2.

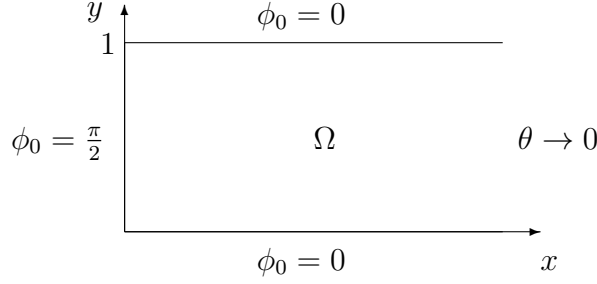


Figure 3.2: Preferred direction of alignment ϕ_0 on the boundary of Ω .

Critical points of (3.4) are solutions of the Euler-Lagrange equation

$$\begin{aligned} \nabla^2 \theta + \delta \left(\frac{1}{2} \sin(2\theta) (\theta_y^2 + 2\theta_{xy} - \theta_x^2) + \theta_x \theta_y \cos(2\theta) \right. \\ \left. - \theta_{xx} \sin^2(\theta) - \theta_{yy} \cos^2(\theta) \right) = 0, \end{aligned} \quad (3.5)$$

subject to the boundary conditions

$$- \left(\frac{\delta}{2} \sin(2\theta) \theta_x + \theta_y (1 - \delta \cos(\theta)^2) \right) + \frac{\alpha}{2} \sin(2\theta) = 0 \quad \text{on } y = 0, \quad (3.6)$$

$$\left(\frac{\delta}{2} \sin(2\theta) \theta_x + \theta_y (1 - \delta \cos(\theta)^2) \right) + \frac{\alpha}{2} \sin(2\theta) = 0 \quad \text{on } y = 1, \quad (3.7)$$

$$\left(\frac{\delta}{2} \sin(2\theta) \theta_y + \theta_x (1 - \delta \sin(\theta)^2) \right) + \frac{\alpha}{2} \sin(2\theta) = 0 \quad \text{on } x = 0, \quad (3.8)$$

$$\theta \rightarrow 0 \quad \text{as } x \rightarrow \infty. \quad (3.9)$$

We apply the final condition (3.9) so that any critical points are uniform across the bulk of the well, as found experimentally for the D , U_1 and L states.

We define the L state to be the state with the constant director field with angle $\theta_L = 0$, so that the director is parallel to the x -axis everywhere in Ω . The L state

θ_L satisfies Equation (3.5) and the boundary conditions (3.6)–(3.9) for all values of α and δ , and has Oseen-Frank energy

$$E_L = \frac{\alpha}{2}. \quad (3.10)$$

We begin by working in the one-constant Oseen-Frank theory with $\delta = 0$. In §3.2.1, we study the stability of the L state by identifying conditions for the loss of stability and performing a weakly nonlinear analysis to determine the bifurcation behaviour. In §3.2.2, we consider the large anchoring strength limit and identify possible equilibria. Finally, we minimize the Oseen-Frank energy numerically using COMSOL in order to study equilibria between the bifurcation point and the large anchoring strength limit. In §3.3, we perform a similar analysis for the Oseen-Frank energy with unequal elastic constants. We summarize our results and discuss their implications in terms of the experimental work on the *fd*-virus in §3.4.

3.2 The One-Constant Oseen-Frank Theory

3.2.1 Stability Analysis of the Uniform State

We consider the stability of the L state in the one-constant approximation. The second variation about the L state is given by

$$\begin{aligned} \delta^2 E := \frac{\partial^2 E[\theta_L + \epsilon\eta]}{\partial \epsilon^2} \Big|_{\epsilon=0} &= \iint_{\Omega} |\nabla \eta|^2 \, d\Omega - \int_0^1 \alpha \eta^2 \Big|_{x=0} \, dy \\ &\quad + \int_0^\infty \alpha \eta^2 \Big|_{y=0} \, dx + \int_0^\infty \alpha \eta^2 \Big|_{y=1} \, dx. \end{aligned} \quad (3.11)$$

For L to be locally stable, $\delta^2 E$ must be positive for any continuous perturbation η . We see immediately from Equation (3.11) that any instability must be driven by the anchoring on the wall at $x = 0$.

Minimizers of $\delta^2 E$ are solutions of the Euler-Lagrange equation

$$\nabla^2 \eta = 0, \quad (3.12)$$

with boundary conditions

$$\begin{aligned} \frac{\partial \eta}{\partial y} - \alpha \eta &= 0 & \text{on } y = 0, & \quad \frac{\partial \eta}{\partial y} + \alpha \eta = 0 & \text{on } y = 1, \\ \frac{\partial \eta}{\partial x} + \alpha \eta &= 0 & \text{on } x = 0, & \quad \eta \rightarrow 0 & \text{as } x \rightarrow \infty. \end{aligned} \quad (3.13)$$

We solve by separation of variables and find the following non-trivial solutions

$$\eta_n = A_n \left(\cos \left(\frac{(2n+1)\pi y}{2} \right) + \sin \left(\frac{(2n+1)\pi y}{2} \right) \right) e^{-\frac{(2n+1)\pi x}{2}}, \quad (3.14)$$

which are the orthogonal eigenfunctions with associated eigenvalues $\alpha_n = \frac{(2n+1)\pi}{2}$, where $n \in \mathbb{N}$. Expressing a general perturbation as a linear combination of these eigenfunctions,

$$\eta = \sum_{n=0}^{\infty} A_n \eta_n, \quad (3.15)$$

we calculate that

$$\iint_{\Omega} |\nabla \eta|^2 d\Omega = \sum_{n=0}^{\infty} \frac{\pi}{2} (2n+1) A_n^2, \quad (3.16)$$

and

$$-\int_0^1 \alpha \eta^2 \Big|_{x=0} dy + \int_0^{\infty} \alpha \eta^2 \Big|_{y=0} dx + \int_0^{\infty} \alpha \eta^2 \Big|_{y=1} dx = -\alpha \sum_{n=0}^{\infty} A_n^2, \quad (3.17)$$

and conclude that the linear state is unstable for $\alpha > \alpha_0 \equiv \frac{\pi}{2}$.

We next demonstrate that the linear state undergoes a supercritical pitchfork bifurcation by carrying out a weakly nonlinear analysis about α_0 . We express θ in

terms of the series expansion

$$\theta = \theta_L + \epsilon \eta_1 + \epsilon^2 \eta_2 + \epsilon^3 \eta_3 + \dots \quad (3.18)$$

and let $\alpha = \alpha_0 + \epsilon^2 \alpha_2$, where $0 < \epsilon \ll 1$ and the functions η_i are continuous functions. We substitute these series into the Euler-Lagrange equation (3.5) for θ and the associated boundary conditions (3.6)–(3.9), and compare terms of different order in ϵ .

Solving for terms of order ϵ , we see that

$$\eta_1 = A \left(\cos \left(\frac{\pi y}{2} \right) + \sin \left(\frac{\pi y}{2} \right) \right) e^{-\frac{\pi x}{2}}, \quad (3.19)$$

with unknown amplitude A . Comparing terms of order ϵ^2 , we see that η_2 is proportional to η_1 , and can be absorbed into terms of order ϵ .

By comparing terms of order ϵ^3 , we see that η_3 is a solution to

$$\nabla^2 \eta_3 = 0, \quad (3.20)$$

subject to the boundary conditions

$$\begin{aligned} \frac{\partial \eta_3}{\partial y} - \alpha_0 \eta_3 &= -\frac{2\alpha_0}{3} \eta_1^3 + \alpha_2 \eta_1 & \text{on } y = 0, \\ \frac{\partial \eta_3}{\partial y} + \alpha_0 \eta_3 &= \frac{2\alpha_0}{3} \eta_1^3 - \alpha_2 \eta_1 & \text{on } y = 1, \\ \frac{\partial \eta_3}{\partial x} + \alpha_0 \eta_3 &= \frac{2\alpha_0}{3} \eta_1^3 - \alpha_2 \eta_1 & \text{on } x = 0, \\ \eta_3 &\rightarrow 0 & \text{as } x \rightarrow \infty. \end{aligned} \quad (3.21)$$

The homogeneous problem η_{3h} , with the right-hand side of the boundary condi-

tions (3.21) set to zero, has the non-trivial solution

$$\eta_{3h} = \left(\cos\left(\frac{\pi y}{2}\right) + \sin\left(\frac{\pi y}{2}\right) \right) e^{-\frac{\pi x}{2}}. \quad (3.22)$$

Following from [90] we derive a compatibility condition using Green's First Identity.

We consider the integral

$$\iint_{\Omega} (\eta_{3h} \nabla^2 \eta_3 - \eta_3 \nabla^2 \eta_{3h}) \, d\Omega = \oint_{\partial\Omega} \left(\eta_{3h} \frac{\partial \eta_3}{\partial v} - \eta_3 \frac{\partial \eta_{3h}}{\partial v} \right) \, ds. \quad (3.23)$$

Since both η_3 and η_{3h} are solutions of the Laplace equation, the left-hand side of (3.23) is identically zero. Using the boundary conditions for the inhomogeneous problem, we rearrange the right-hand side of (3.23) to get the compatibility condition:

$$\begin{aligned} 0 = & - \int_0^1 \eta_{3h} \left(\frac{2\alpha_0}{3} \eta_1^3 - \alpha_2 \eta_1 \right) \Big|_{x=0} \, dy - \int_0^\infty \eta_{3h} \left(-\frac{2\alpha_0}{3} \eta_1^3 + \alpha_2 \eta_1 \right) \Big|_{y=0} \, dx \\ & + \int_0^\infty \eta_{3h} \left(\frac{2\alpha_0}{3} \eta_1^3 - \alpha_2 \eta_1 \right) \Big|_{y=1} \, dx, \end{aligned} \quad (3.24)$$

or, equivalently,

$$A (A^2(\pi + 2) - 2\alpha_2) = 0. \quad (3.25)$$

The amplitude of the perturbation may be non-zero only for $\alpha_2 > 0$, therefore, there is a supercritical pitchfork bifurcation at $\alpha = \frac{\pi}{2}$.

For α close to $\frac{\pi}{2}$, the director field of this perturbed state behaves like

$$\theta \sim \sqrt{\frac{2(\alpha - \alpha_0)}{\pi + 2}} \left(\cos\left(\frac{\pi y}{2}\right) + \sin\left(\frac{\pi y}{2}\right) \right) e^{-\frac{\pi x}{2}}. \quad (3.26)$$

and has Oseen-Frank energy

$$E \sim \frac{\alpha}{2} + \frac{\epsilon^4 A^2}{8} (A^2(\pi + 2) - 4\alpha_2) + O(\epsilon^6) \quad (3.27)$$

$$\sim \frac{\alpha}{2} - \frac{(\pi - 2\alpha)^2}{8(\pi + 2)} + O(\epsilon^6). \quad (3.28)$$

Plotting the director field of this perturbed state for small α in Figure 3.3, we see that the L state loses stability to a perturbation which causes the director to distort in order to minimize the surface energy on the $x = 0$ line.

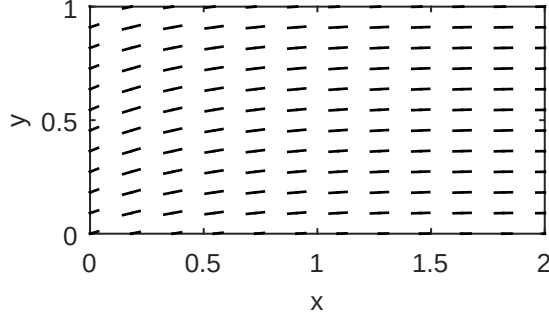


Figure 3.3: Director field of perturbation about θ_L , for $\alpha - \alpha_0 = 0.2$.

3.2.2 The Large Anchoring Strength Limit

In order to understand how the L state deforms away from the bifurcation point at $\alpha = \alpha_0$, we now consider critical points of the Oseen-Frank energy (3.4) for large anchoring strengths ($\alpha \gg \alpha_0$).

3.2.2.1 Outer Problem

We consider the limit $\alpha \rightarrow \infty$ and express θ in terms of a series expansion of the form

$$\theta \sim \theta_0 + \frac{\theta_1}{\alpha} + \frac{\theta_2}{\alpha^2} + O(\alpha^{-3}). \quad (3.29)$$

We substitute this series expansion into the Euler-Lagrange equation (3.5) and boundary conditions (3.6)–(3.9), and compare terms of each order in α .

Comparing terms of order 1, θ_0 is the solution of

$$\nabla^2 \theta_0 = 0, \quad (3.30)$$

subject to

$$\begin{aligned} \sin(2\theta_0) &= 0 && \text{on } x = 0, y = 0 \text{ and } y = 1, \\ \theta_0 &\rightarrow 0 && \text{as } x \rightarrow \infty. \end{aligned} \quad (3.31)$$

Equation (3.30) has multiple solutions, including the L state characterized by $\theta_0 = 0$. We know that L is unstable in this regime, so we consider other possible solutions. The lowest energy solution will contain defects of strength $+\frac{1}{4}$ and $-\frac{1}{4}$ at the corners $(0, 0)$ and $(0, 1)$. Without loss of generality we consider the boundary conditions $\theta_0(0, y) = \frac{\pi}{2}$ and $\theta_0(x, 0) = \theta_0(x, 1) = 0$. Solving, θ_0 has the solution

$$\theta_0(x, y) = \sum_{n=0}^{\infty} \frac{2}{2n+1} \sin((2n+1)\pi y) e^{-(2n+1)\pi x}. \quad (3.32)$$

This is the solution to the Laplace equation in a semi-infinite domain with strong anchoring, and the director field will resemble one end of the D or U_1 states found in a rectangular well in the limit as the rectangular aspect ratio $\lambda \rightarrow 0$.

The next term in the expansion (3.29) is the solution of

$$\nabla^2 \theta_1 = 0, \quad (3.33)$$

subject to

$$\begin{aligned} \frac{\partial \theta_0}{\partial y} - \theta_1 &= 0 & \text{on } y = 0, & \quad \frac{\partial \theta_0}{\partial y} + \theta_1 = 0 & \text{on } y = 1, \\ \frac{\partial \theta_0}{\partial x} - \theta_1 &= 0 & \text{on } x = 0, & \quad \theta_1 \rightarrow 0 & \text{as } x \rightarrow \infty. \end{aligned} \quad (3.34)$$

The solution θ_1 can be written explicitly in terms of θ_0 ; however, we will see that the contribution to the energy from this term can be calculated by using the definition of the boundary conditions (3.34).

When x and y are $O(\alpha^{-1})$, the leading order solution θ_0 no longer satisfies the boundary conditions. There must exist inner regions surrounding the corners at $(0, 0)$ and $(1, 0)$.

3.2.2.2 Inner Problem

We consider the inner problem in the region about $(0, 0)$ and introduce rescaled variables $X = \alpha x$, $Y = \alpha y$ and $\Theta(X, Y) = \theta(X/\alpha, Y/\alpha)$. The second inner problem in the region about $(0, 1)$ follows similarly by making the substitution $Y = 1 - \alpha y$. Then, the inner problem is

$$\nabla^2 \Theta = 0, \quad (3.35)$$

subject to

$$\begin{aligned} \frac{\partial \Theta}{\partial X} + \frac{1}{2} \sin(2\Theta) &= 0 & \text{on } X = 0, & \quad \frac{\partial \Theta}{\partial Y} - \frac{1}{2} \sin(2\Theta) = 0 & \text{on } Y = 0. \\ \Theta(X, 0) &\rightarrow 0 & \text{as } X \rightarrow \infty, & \quad \Theta(0, Y) \rightarrow \frac{\pi}{2} & \text{as } Y \rightarrow \infty. \end{aligned} \quad (3.36)$$

A similar problem has been addressed in [91] in the half-plane, where the author considers

$$\nabla^2 f = 0 \quad \text{for } x \in \mathbb{R}, y > 0, \quad (3.37)$$

$$\frac{\partial f}{\partial y} + \sin(f) = 0 \quad \text{on } y = 0. \quad (3.38)$$

The solution of this system is shown to be

$$f = \pm 2 \arctan \left(\frac{x+a}{y+1} \right) + 2\pi m, \quad (3.39)$$

where $a \in \mathbb{R}$ and $m \in \mathbb{N}$. Similar solutions have been used to study the effects of weak anchoring on the dynamics of disclination lines in nematic liquid crystals [92, 93] and boundary vortices in magnetic fields [94].

Using the solution (3.39) as a guide, we find that our boundary value problem (3.35)–(3.36) has the solution

$$\Theta = m \arctan \left(\frac{Y+1}{X+1} \right), \quad (3.40)$$

where $m = +1$. If we had chosen the first order outer solution to satisfy $\theta_0(0, y) = -\frac{\pi}{2}$, then $m = -1$. This solution creates a director field with a virtual defect, where the defect is outside of the domain Ω [95, 96], as shown in Figure 3.4. Equation (3.40) automatically satisfies the matching conditions as $X, Y \rightarrow \infty$. The virtual defect is located at the point $(x, y) = \left(-\frac{1}{\alpha}, -\frac{1}{\alpha}\right)$, and in the limit as $\alpha \rightarrow \infty$ the virtual defect will approach the boundary $\partial\Omega$, recovering the strong anchoring behaviour discussed in Chapter 2.

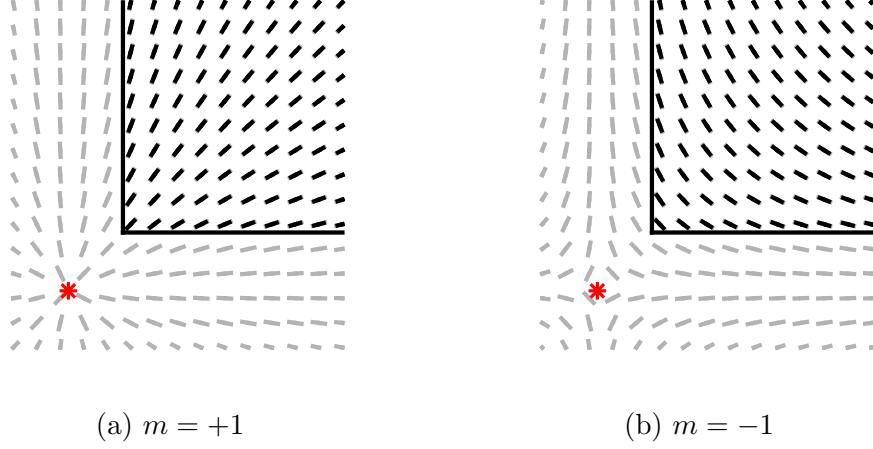


Figure 3.4: Virtual defects of strength $m = \pm 1$, in red, and the director field. Here, the physical part of the director field is shown in black, and the virtual component in grey.

3.2.2.3 The Oseen-Frank Energy

We use our outer and corner solutions to evaluate the Oseen-Frank energy for large α . We define the outer region Ω_ϵ to be the semi-infinite domain with quadrants of radius ϵ removed from the corners at $(0, 0)$ and $(1, 0)$, shown in Figure 3.5. Here, $\frac{1}{\alpha} \ll \epsilon \ll 1$ is a matching parameter.

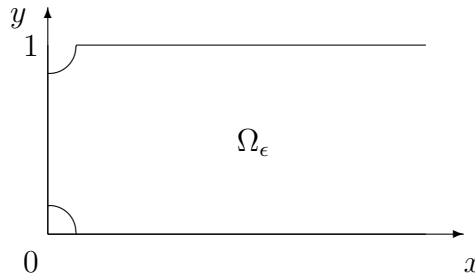


Figure 3.5: The outer domain Ω_ϵ .

The outer energy is

$$\begin{aligned}
E_O \sim & \oint_{\partial\Omega_\epsilon} \frac{\alpha}{2} \sin(\theta_0)^2 ds + \frac{1}{2} \iint_{\Omega_\epsilon} |\nabla\theta_0|^2 d\Omega + \frac{1}{2} \int_\epsilon^\infty \sin(2\theta_0)\theta_1 \Big|_{y=0} dx \\
& + \frac{1}{2} \int_\epsilon^\infty \sin(2\theta_0)\theta_1 \Big|_{y=1} dx - \frac{1}{2} \int_\epsilon^{1-\epsilon} \sin(2\theta_0)\theta_1 \Big|_{x=0} dy \\
& + \frac{1}{\alpha} \iint_{\Omega_\epsilon} \nabla\theta_0 \cdot \nabla\theta_1 d\Omega + \frac{1}{2\alpha} \oint_{\partial\Omega_\epsilon} \theta_1^2 ds + O(\alpha^{-2}). \tag{3.41}
\end{aligned}$$

Since we have chosen $\theta_0 = 0$ on $y = 0, 1$ and $\theta_0 = \frac{\pi}{2}$ on $x = 0$, the outer energy simplifies to

$$E_O \sim \frac{1}{2} \iint_{\Omega_\epsilon} |\nabla\theta_0|^2 d\Omega + \frac{1}{\alpha} \iint_{\Omega_\epsilon} \nabla\theta_0 \cdot \nabla\theta_1 d\Omega + \frac{1}{2\alpha} \oint_{\partial\Omega_\epsilon} \theta_1^2 ds + O(\alpha^{-2}). \tag{3.42}$$

The integral of order 1 is the energy evaluated in the strong anchoring limit, given in §2.2.3,

$$\frac{1}{2} \iint_{\Omega_\epsilon} |\nabla\theta_0|^2 d\Omega \sim \frac{\pi}{2} \log\left(\frac{2}{\pi\epsilon}\right) + O(\epsilon^2). \tag{3.43}$$

From an application of Green's First Identity and the definition of the boundary conditions for θ_1 in (3.34) the order α^{-1} terms simplify to

$$\iint_{\Omega_\epsilon} \nabla\theta_0 \cdot \nabla\theta_1 d\Omega + \frac{1}{2} \oint_{\partial\Omega_\epsilon} \theta_1^2 ds = -\frac{1}{2} \oint_{\partial\Omega_\epsilon} \theta_1^2 ds \tag{3.44}$$

$$\begin{aligned}
& = -\frac{1}{2} \int_\epsilon^\infty \left(\frac{\partial\theta_0}{\partial y}\right)^2 \Big|_{y=0} dx - \frac{1}{2} \int_\epsilon^\infty \left(\frac{\partial\theta_0}{\partial y}\right)^2 \Big|_{y=1} dx \\
& \quad - \frac{1}{2} \int_\epsilon^{1-\epsilon} \left(\frac{\partial\theta_0}{\partial x}\right)^2 \Big|_{x=0} dy \tag{3.45}
\end{aligned}$$

$$\sim \frac{\pi}{2} - \frac{2}{\epsilon} + O(\epsilon^2). \tag{3.46}$$

Therefore, the energy in the outer region is

$$E_O \sim \frac{\pi}{2} \log\left(\frac{2}{\pi\epsilon}\right) + \frac{\pi}{2\alpha} - \frac{2}{\alpha\epsilon} + O(\epsilon^2, \alpha^{-2}) \tag{3.47}$$

We next evaluate the contribution to the Oseen-Frank energy from the corner region at $(0,0)$. The energy from the second corner at $(1,0)$ will have identical energy, as both virtual defects have strength $|m| = 1$. The total corner energy is

$$E_C = \frac{1}{2} \int_0^{\alpha\epsilon} \int_0^{\sqrt{\epsilon^2\alpha^2 - Y^2}} |\nabla\Theta|^2 dX dY + \frac{1}{2} \int_0^{\alpha\epsilon} \sin(\Theta)^2 \Big|_{Y=0} dX + \frac{1}{2} \int_0^{\alpha\epsilon} \cos(\Theta)^2 \Big|_{X=0} dY, \quad (3.48)$$

which we evaluate in the limit as $\alpha\epsilon \rightarrow \infty$. We rewrite the Dirichlet energy using Green's First Identity,

$$\begin{aligned} \frac{1}{2} \int_0^{\alpha\epsilon} \int_0^{\sqrt{\epsilon^2\alpha^2 - Y^2}} |\nabla\Theta|^2 dX dY &= -\frac{1}{2} \int_0^{\epsilon\alpha} \Theta \frac{\partial\Theta}{\partial Y} \Big|_{Y=0} dX - \frac{1}{2} \int_0^{\epsilon\alpha} \Theta \frac{\partial\Theta}{\partial X} \Big|_{X=0} dY \\ &\quad + \frac{1}{2} \int_0^{\frac{\pi}{2}} \Theta \frac{\partial\Theta}{\partial r} r \Big|_{r=\epsilon\alpha} d\phi. \end{aligned} \quad (3.49)$$

Integrating by parts and taking the limit as $\epsilon\alpha \rightarrow \infty$,

$$-\frac{1}{2} \int_0^{\epsilon\alpha} \Theta \frac{\partial\Theta}{\partial Y} \Big|_{Y=0} dX - \frac{1}{2} \int_0^{\epsilon\alpha} \Theta \frac{\partial\Theta}{\partial X} \Big|_{X=0} dY \sim \frac{\pi}{4} \log\left(\frac{\epsilon\alpha}{2}\right) - \frac{C}{2} + \frac{4+\pi}{4\epsilon\alpha} + O\left(\frac{1}{\epsilon^2\alpha^2}\right), \quad (3.50)$$

where C is Catalan's constant [97], defined to be

$$C := \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2} \approx 0.9160. \quad (3.51)$$

Using a series expansion for Θ and $\frac{\partial\Theta}{\partial r}$ in the limit as $\epsilon\alpha \rightarrow \infty$, we find that

$$\begin{aligned} \frac{1}{2} \int_0^{\frac{\pi}{2}} \theta \frac{\partial\Theta}{\partial r} r \Big|_{r=\epsilon\alpha} d\phi &\sim \frac{1}{2} \int_0^{\frac{\pi}{2}} \frac{\phi (\sin(\phi) - \cos(\phi))}{\epsilon\alpha} d\phi + O\left(\frac{1}{\epsilon^2\alpha^2}\right) \\ &\sim \frac{4-\pi}{4\epsilon\alpha} + O\left(\frac{1}{\epsilon^2\alpha^2}\right). \end{aligned} \quad (3.52)$$

Finally, the surface energy terms are

$$\frac{1}{2} \int_0^{\epsilon\alpha} \sin^2(\Theta) \Big|_{\phi=0} dr + \frac{1}{2} \int_0^{\epsilon\alpha} \cos^2(\Theta) \Big|_{\phi=\frac{\pi}{2}} dr = -\frac{\pi}{4} + \arctan(\epsilon\alpha + 1) \quad (3.53)$$

$$\sim \frac{\pi}{4} - \frac{1}{\epsilon\alpha} + O\left(\frac{1}{\epsilon^2\alpha^2}\right). \quad (3.54)$$

The total energy from a corner region is thus given by

$$E_C \sim \frac{\pi}{4} \log\left(\frac{\epsilon\alpha}{2}\right) - \frac{C}{2} + \frac{\pi}{4} + \frac{1}{\epsilon\alpha} + O(\alpha^{-2}). \quad (3.55)$$

Thus, the net Oseen-Frank energy in Ω is given by

$$E = E_O + 2E_C \sim \frac{\pi}{2} \log\left(\frac{\alpha}{\pi}\right) - C + \frac{\pi}{2} + \frac{\pi}{\alpha} + O(\alpha^{-2}). \quad (3.56)$$

This expression tells us that for large anchoring strengths, the energy of the state with two virtual corner defects is much less than the energy of the uniform state. The finite anchoring strength provides a regularization of the strong anchoring problem, resulting in a finite Oseen-Frank energy without removing the corners of the domain Ω . In the strong anchoring limit $\alpha \rightarrow \infty$, we can derive an estimate for the effective defect core size ϵ by comparing the leading order terms in Equations (3.47) and (3.56):

$$\epsilon = \frac{2e^{\frac{2C}{\pi}-1}}{\alpha} \approx \frac{1.3132}{\alpha}. \quad (3.57)$$

3.2.3 Numerics

Our stability analysis in §3.2.1 and large anchoring strength asymptotics in §3.2.2 indicate that the L state will always lose stability for $\alpha > \frac{\pi}{2}$, and that for large anchoring strengths, the stable equilibrium approaches the rotated or diagonal solutions found in a rectangle using strong anchoring boundary conditions. We now use

COMSOL to compute the bifurcation diagram, and investigate values of α between the bifurcation point $\frac{\pi}{2}$ and the large anchoring strength limit.

We solve Equation (3.5) subject to the boundary conditions (3.6)–(3.6) on a domain

$$\Omega_H = \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq H, 0 \leq y \leq 1\}, \quad (3.58)$$

for some fixed $H \gg 1$. We use COMSOL's parametric sweep to vary the anchoring parameter α . We start the sweep by choosing some large α with initial conditions corresponding to the strong anchoring solution Equation (3.32). Using the previous solution as an initial condition, we then vary α backwards towards $\alpha = 0$. This allows us to model the effects of the moderate values of α on the large anchoring solution with two virtual defects. Here, we choose $H = 10$ and our initial value of $\alpha = 20$.

For small values of α , we find that the director adopts an intermediate state between the L state and the strong anchoring solution, which is shown in Figure 3.6b for $\alpha = 2$. Here, the director shows some slight distortion about the line $x = 0$, then reorientates to a constant as $x \rightarrow H$.

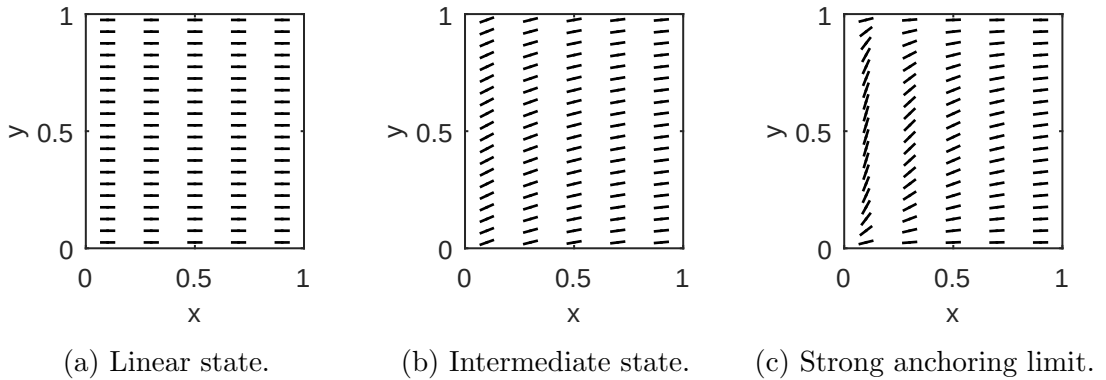
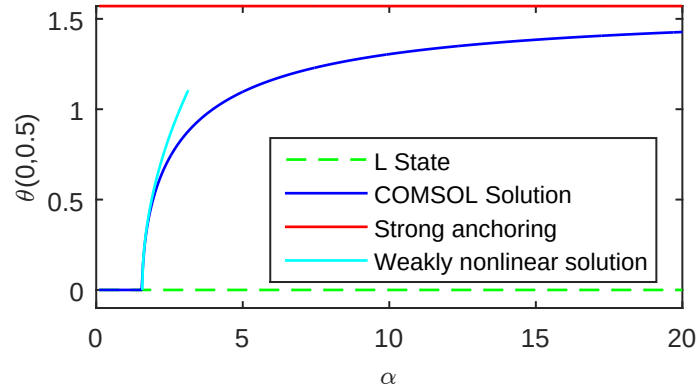


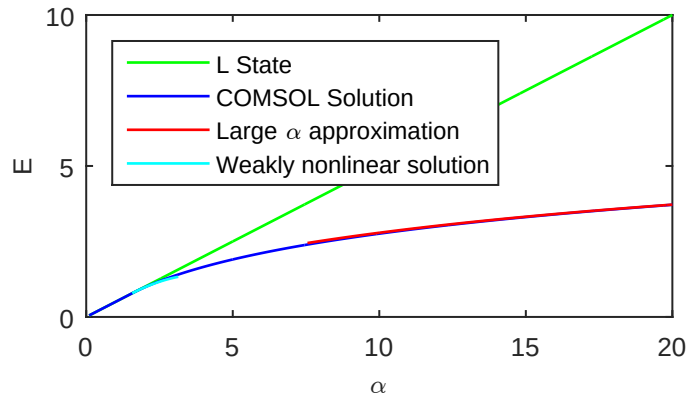
Figure 3.6: The director field of the linear state, intermediate state and strong anchoring limit.

In Figure 3.7, we plot the value of θ at a point on the $x = 0$ line and energies of the COMSOL solution, with the director and energies of the L state and asymptotics shown for comparison. The large α asymptotics successfully describe the behaviour

of the energy for moderate values of α . As α approaches $\frac{\pi}{2}$ from above, the director of the distorted state continuously deforms into the uniform state. For $\alpha < \frac{\pi}{2}$, we are unable to find a distorted solution and our numerical analysis indicates that there is no value of α for which the L state and the D or U_1 states are both stable equilibria.



(a) Value of θ at $(0, 0.5)$.



(b) Oseen-Frank energy in Ω_H .

Figure 3.7: The value of the angle θ at the point $(0, 0.5)$ and Oseen-Frank energy for the computed solutions, with the large α asymptotics and weakly nonlinear solutions shown for comparison.

3.3 The Oseen-Frank Theory with Elastic Anisotropy

Now we relax the one-constant approximation and analyse the stability of the L state when $\delta \neq 0$. As in §3.2.1, we consider the second variation of the Oseen-Frank energy about the L state, given by

$$\begin{aligned} \delta^2 E = & \iint_{\Omega} \eta_x^2 + (1 - \delta) \eta_y^2 \, d\Omega - \int_0^1 \alpha \eta^2 \Big|_{x=0} \, dy + \int_0^\infty \alpha \eta^2 \Big|_{y=0} \, dx \\ & + \int_0^\infty \alpha \eta^2 \Big|_{y=1} \, dx. \end{aligned} \quad (3.59)$$

Minimizers of (3.59) are solutions of the Euler-Lagrange equation

$$\eta_{xx} + (1 - \delta) \eta_{yy} = 0, \quad (3.60)$$

subject to the boundary conditions

$$\begin{aligned} -\frac{\partial \eta}{\partial y}(1 - \delta) + \alpha \eta &= 0 & \text{on } y = 0, & \quad \frac{\partial \eta}{\partial x} + \alpha \eta = 0 & \text{on } x = 0, \\ \frac{\partial \eta}{\partial y}(1 - \delta) + \alpha \eta &= 0 & \text{on } y = 1, & \quad \eta \rightarrow 0 & \text{as } x \rightarrow \infty. \end{aligned} \quad (3.61)$$

Solving, we find the first eigenfunction:

$$\eta_0 = A \left(\cos \left(\frac{\alpha_0 y}{\sqrt{1 - \delta}} \right) + \frac{1}{\sqrt{1 - \delta}} \sin \left(\frac{\alpha_0 y}{\sqrt{1 - \delta}} \right) \right) e^{-\alpha x} \quad (3.62)$$

with associated eigenvalue

$$\alpha_0 = \sqrt{1 - \delta} \left(\frac{\pi}{2} + \arctan \left(\frac{\delta}{2\sqrt{1 - \delta}} \right) \right), \quad (3.63)$$

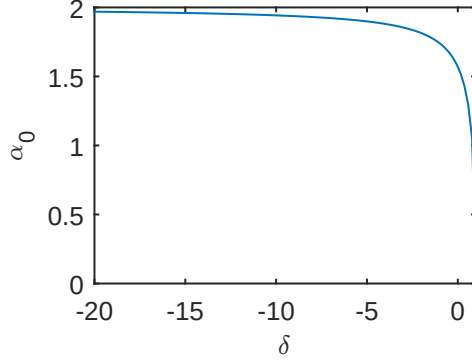


Figure 3.8: First eigenvalue α_0 in terms of δ .

or, in terms of the elastic constants, the critical anchoring strength for the loss of stability is given by

$$WY_e = \sqrt{K_1 K_3} \left(\frac{\pi}{2} - \arctan \left(\frac{K_1 - K_3}{2\sqrt{K_1 K_3}} \right) \right). \quad (3.64)$$

Plotting the first eigenvalue in Figure (3.8), we observe that as $\delta \rightarrow 1$, $\alpha_0 \rightarrow 0$ and as $\delta \rightarrow -\infty$, $\alpha_0 \rightarrow 2$. By considering Equation (3.64) in the limits as $K_1 \rightarrow \infty$ and $K_3 = O(1)$, and $K_3 \rightarrow \infty$ and $K_1 = O(1)$, we can interpret this behaviour. In the limit as $K_1 \rightarrow \infty$, splay deformations become energetically unfavourable and the critical value of W for the uniform state to become unstable is

$$WY_e \sim 2K_3 + O(K_1^{-1}). \quad (3.65)$$

In the limit as $K_3 \rightarrow \infty$, bend deformations becomes energetically unfavourable and

$$WY_e \sim \sqrt{K_1 K_3} \pi + O(1). \quad (3.66)$$

The deformation to the director induced by the perturbation η_0 on the edge $x = 0$ is primarily a bend deformation, and hence the required anchoring strength for the L state to become unstable scales with K_3 .

A weakly nonlinear analysis about bifurcation point α_0 shows that the amplitude of (3.62) satisfies

$$A = 0, \quad A = \pm 4 \sqrt{\frac{(\alpha - \alpha_0)(\delta - 1)}{f(\delta, \alpha_0)}} \quad (3.67)$$

where

$$f(\delta, \alpha_0) := \left(\frac{\alpha_0(6\delta^3 - 24\delta^2 + 32\delta - 16)}{1 - \delta} + (32\delta - 20\delta^2 - 16) \right). \quad (3.68)$$

Numerical evaluation shows that $\frac{\delta-1}{f(\delta, \alpha_0)} > 0$ for all $\delta < 1$, and hence the bifurcation at $\alpha = \alpha_0$ is unconditionally supercritical. Further simulations in COMSOL using the method described in §3.2.3 shows similar behaviour to the one-constant case, suggesting that elastic anisotropy is not sufficient to allow for the coexistence of the uniform and D or U_1 states in a narrow rectangular well.

3.4 Summary

In this chapter we have studied critical points of the Oseen-Frank energy with a Rapini-Papoular surface energy in a semi-infinite rectangular domain in order to understand the stability of the uniform state found experimentally in a rectangular well. We have identified a critical value of the anchoring coefficient $\alpha_0 = \frac{\pi}{2}$, for which the uniform state loses stability, and classified the critical value as a supercritical bifurcation. Working in the large anchoring strength limit, we recover the strong anchoring behaviour. We find a state with a distorted director field, which has the structure of an endpoint of D or U_1 state in rectangular well in the low rectangular aspect ratio limit. We derive an estimate for the energy in the large anchoring strength limit by considering a virtual defect solution. We then perform numerical simulations using COMSOL which suggest that the distorted state and uniform states cannot coexist.

Comparing our results to the experimental results on the *fd*-virus, the lack of a parameter region for which distorted and uniform states can coexist is surprising. One possible explanation for this discrepancy between the experiment and theory is that some of the L and D or U_1 states identified experimentally are the intermediate states found numerically for moderate values of α . This is supported by the experimental image in Figure 3.1, which shows some slight distortion about the two ends of the channel, similar to the behaviour in Figure 3.6b. Assuming that this state is in fact the intermediate state, then the associated parameter α must be greater than the critical value $\alpha_0 = \frac{\pi}{2}$. This allows us to put an upper bound on the extrapolation length

$$\xi < \frac{2Y_e}{\pi}. \quad (3.69)$$

For the system shown in Figure 3.6b the value of $Y_e = 5.7\mu\text{m}$, and we therefore estimate that

$$\xi < 3.6 \mu\text{m}. \quad (3.70)$$

However, we note that there are a number of other possible explanations for this experimental phenomenon. For these cell dimensions, the chamber height Y_e is only a factor of 10 greater than the particle size, and it is possible that experimentally we are observing a breakdown in the nematic ordering. A second explanation arises from a similar study in micromagnetics [98, 99, 100], where small chamber depths allow for stable equilibria resembling our diagonal state, but increasing the chamber depth leads to a more uniform alignment. It is therefore possible that variations in the experimental chamber depth Z_e could be responsible for the coexistence of equilibria, and that a two-dimensional model may not be sufficient to fully capture the behaviour observed experimentally.

Chapter 4

Nematic Equilibria in Shallow Annular Wells

4.1 Introduction

4.1.1 Motivation

In this chapter, we study nematic equilibria within two-dimensional annular wells with tangential anchoring. This work is motivated by experimental work carried out by Oliver Dammone [75] and José Alvarado [76] on the aqueous suspensions of *fd*-virus particles within confined to shallow annular and circular chambers.

The suspension of *fd*-virus and the chambers were prepared using the techniques discussed in §2.1.3. The chambers, sketched in Figure 4.1, had a depth (Z_e) of $1\text{ }\mu\text{m}$ and an outer radius (R_{outer}) between 5 and $35\text{ }\mu\text{m}$. When filled, the *fd*-virus particles lay in the plane of the annulus, and no variation in the z -axis was observed.

Six distinct states are identified in the experiments and sample director fields of each state are shown in Figure 4.2. The first state is a radially invariant defect-free state, with the director aligned tangent to the two outer walls throughout the chamber. Four of the states feature defects on the boundary, with $+\frac{1}{2}$ strength defects

on the outer wall and $-\frac{1}{2}$ strength defects on the inner wall. The last state identified is a uniform state, with an approximately constant director field.

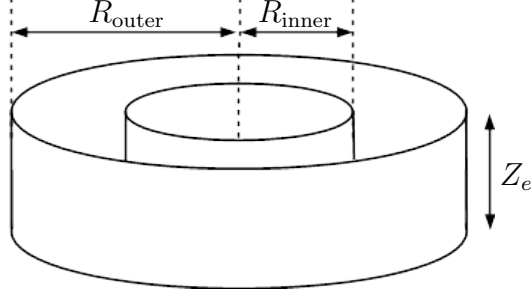


Figure 4.1: Sketch of experimental annular well.

The relative frequencies of the six experimentally observed states are shown in Figure 4.3. The preferred equilibria is set by the ratio of the inner and outer radii $b := \frac{R_{\text{inner}}}{R_{\text{outer}}}$. For narrow annuli with b close to 1, the defect-free state is the only state which occurs. As the ratio b decreases, equilibria with one and then two $+\frac{1}{2}$ strength defects on the outer boundary occur with increasing frequency. Equilibria with three $+\frac{1}{2}$ strength defects on the outer boundary occur infrequently and with no apparent dependence on the ratio of the radii. The absolute chamber size does not appear to have any discernible effect on the relative frequencies, except for the uniform state. The uniform state only occurs in the smallest chambers, with $R_{\text{outer}} = 5\mu\text{m}$.

4.1.2 Literature Review

The defect-free state within an annular well has received a considerable amount of attention in the past, particularly in the context of liquid crystals confined within concentric cylinders. In [101], the authors work with the one-constant Oseen-Frank theory and show that the director can escape out of the plane if $\frac{R_{\text{inner}}}{R_{\text{outer}}} < e^{-\pi}$. In [102], the authors identify critical values for the loss of stability of the defect-free state in the Oseen-Frank theory in terms of the elastic constants and anchoring strengths. This loss of stability is further explored in [103, 104, 105, 106, 107] in the context

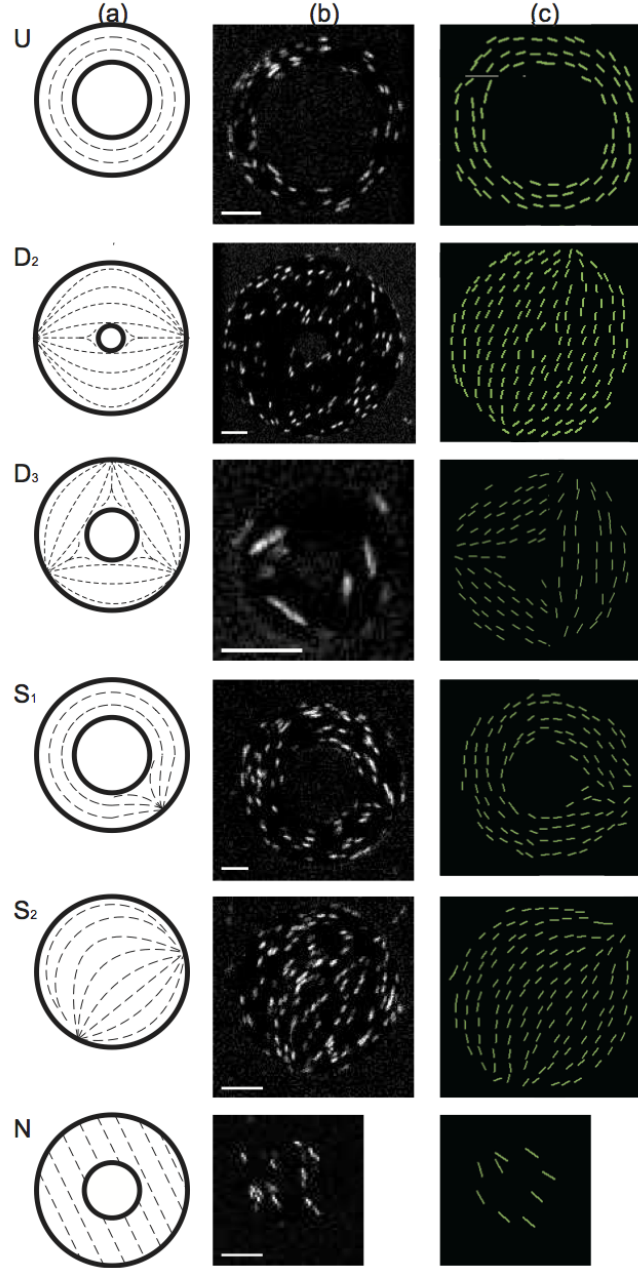


Figure 4.2: Experimentally observed states in shallow circular and annular wells for the *fd*-virus. (a) Sketch of the director field. (b) Four overlaid confocal images, with scale bar = $5 \mu\text{m}$. (c) Experimental director fields calculated from 1000 images. *Adapted from [75] with permission of the author.*

of Fréedericksz transitions with an applied electrical or magnetic field. The authors primarily consider the stability of three characteristic configurations, referred to as ‘radial’, ‘azimuthal’ and ‘uniform’ and obtain explicit estimates for the critical thresh-

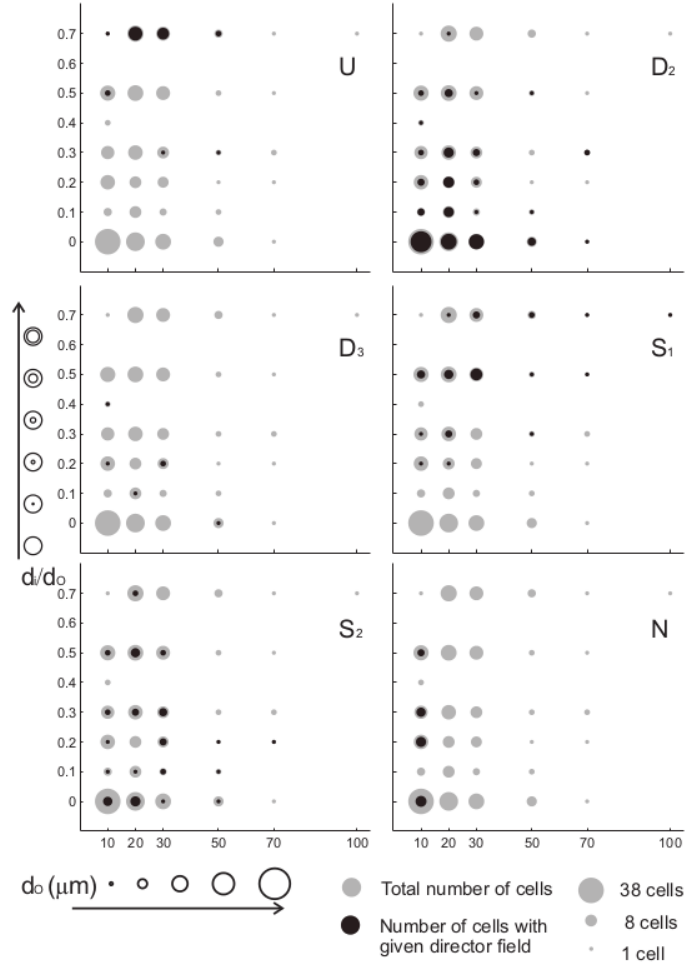


Figure 4.3: Relative frequencies for the six states found in annular wells in terms of ratio of inner diameter (d_i) to outer diameter (d_o) versus outer diameter. The grey circle is the total number of cells for given cell dimensions and the black circle is the number of cells with the director field. *Reproduced from [75] with permission of the author.*

old field in terms of the Oseen-Frank elastic constants, cylindrical aspect ratio and anchoring strength. The defect-free state in this chapter is analogous to the azimuthal state on an annulus, with tangent boundary conditions on both circular boundaries [102, 103, 104, 105]. In [108], the author considers the instability due to elastic anisotropy with strong anchoring and derives results on the bifurcation behaviour about these critical points.

Two-dimensional annular domains have also received a considerable amount of

attention in the Ginzburg-Landau theory for superconductivity. In [109], the authors show that minimizers of the Ginzburg-Landau functional are radially invariant for narrow annuli. For very thick annuli with prescribed degree on the boundaries, the global minimizer is proved to be not radially invariant by the construction of a lower energy solution with a pair of vortices approaching the boundaries [110, 111, 112].

Outside of work using the Ginzburg-Landau potential, equilibria with boundary defects have received considerably less attention than the defect-free state. Motivated by the same experiments on the *fd*-virus, the authors of [113] use an ansatz to approximate the director and derive an estimate of the distortion and surface energies. They find that for suitably small R_{outer} , the defect-free state is not the global minimizer within an annular well. Monte Carlo simulations of systems of hard rods discussed in [75, 76] suggest that boundary defects occur when the chamber size is comparable to the rod size. However, with the exception of the smallest chambers, the length of the *fd*-virus is much smaller than the experimental lengthscale of the chamber size.

4.1.3 Chapter Outline

In this chapter, we study nematic equilibria within two-dimensional annular wells using the Oseen-Frank and Landau-de Gennes theories with strong and weak tangential anchoring. In particular, we are interested in understanding the experimentally observed transition from the radially invariant defect-free state to equilibria with boundary defects as the ratio $b := \frac{R_{\text{inner}}}{R_{\text{outer}}}$ decreases.

In §4.2, we study the defect-free state. Working in the Oseen-Frank theory, we compute conditions on the local stability of the defect-free state in terms of the elastic constants, ratio of the radii and anchoring strength. Our work in the Oseen-Frank theory with strong and weak anchoring has been partially captured by results in [102, 103, 104, 105, 106, 107], although we are specifically looking for phenomena which can drive the apparent transition from the defect-free state to the states with

boundary defects found experimentally and our method of proof differs slightly. In §4.3, we study the defect-free state in the Landau-de Gennes theory with strong anchoring. We derive an explicit condition on the local stability of the defect-free state and a condition on the global minimality in terms of the ratio of inner and outer radii.

In §4.4, we consider equilibria with boundary defects. Using the arrangements of defects on the boundary, we identify a number of possible different equilibria with strong anchoring. Using similar techniques to our work on the rectangular wells in Chapter 2, we derive expressions for the director field and Oseen-Frank energy in the one-constant case. We then briefly discuss the stability of these states, as well as the effect of elastic anisotropy and weak anchoring.

We work with the rescaled two-dimensional annulus

$$\Omega = \{(r, \phi) \in \mathbb{R}^2; \quad b \leq r \leq 1, \quad 0 \leq \phi < 2\pi\}, \quad (4.1)$$

where the normalized radius $b := \frac{R_{\text{inner}}}{R_{\text{outer}}}$ is the ratio of the inner and outer radii. In polar coordinates (r, ϕ) , the Oseen-Frank energy is

$$E[\theta]/K_3 := \frac{1}{2} \iint_{\Omega} \theta_r^2 + \frac{\theta_\phi^2}{r^2} - \delta \left(\cos(\theta - \phi) \frac{\theta_\phi}{r} - \sin(\theta - \phi) \theta_r \right)^2 d\Omega, \quad (4.2)$$

where $\delta := 1 - \frac{K_1}{K_3}$ is our measure of elastic anisotropy. The corresponding Euler-Lagrange equation is:

$$\begin{aligned} \nabla^2 \theta \left(1 - \frac{\delta}{2} \right) + \delta \left(\frac{1}{2} \sin(2\theta - 2\phi) \left(\frac{2\theta_{r\phi}}{r} + \frac{\theta_\phi^2}{r^2} - \theta_r^2 - \frac{2\theta_\phi}{r^2} \right) \right. \\ \left. + \frac{1}{2} \cos(2\theta - 2\phi) \left(\theta_{rr} - \frac{\theta_{\phi\phi}}{r^2} - \frac{\theta_r}{r} + \frac{2\theta_r \theta_\phi}{r} \right) \right) = 0, \end{aligned} \quad (4.3)$$

subject to boundary conditions on $\partial\Omega$.

We work with tangent boundary conditions, which in the strong anchoring limit

requires that

$$\theta(1, \phi) = \theta(b, \phi) = \phi \pm \frac{\pi}{2}. \quad (4.4)$$

Weak anchoring conditions are included by considering Rapini-Papoular energy functional

$$E_S[\theta] = \oint_{\partial\Omega} \frac{\alpha}{2} \sin(\theta - \theta_0)^2 ds, \quad (4.5)$$

where we define the rescaled anchoring strength $\alpha := \frac{WR_{\text{outer}}}{K_3}$ and the preferred direction of alignment $\theta_0 = \phi + \frac{\pi}{2}$. Then, the boundary conditions (4.4) are replaced by:

$$\left(\frac{2-\delta}{2}\right) \theta_r + \frac{\delta}{2} \left(\frac{\theta_\phi}{r} \sin(2\theta - 2\phi) + \theta_r \cos(2\theta - 2\phi)\right) + \frac{\alpha}{2} \sin(2\theta - 2\theta_0) = 0, \quad (4.6)$$

on $r = 1$, and

$$\left(\frac{2-\delta}{2}\right) \theta_r + \frac{\delta}{2} \left(\frac{\theta_\phi}{r} \sin(2\theta - 2\phi) + \theta_r \cos(2\theta - 2\phi)\right) - \frac{\alpha}{2} \sin(2\theta - 2\theta_0) = 0, \quad (4.7)$$

on $r = b$.

The two-dimensional Landau-de Gennes energy is

$$E[\mathbf{Q}] := \iint_{\Omega} \frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{1}{4\varepsilon^2} (|\mathbf{Q}|^2 - 1)^2 d\Omega, \quad (4.8)$$

where $\varepsilon^2 := \frac{L}{|A|R_{\text{outer}}^2}$. Critical points are solutions to the Euler-Lagrange equations

$$\nabla^2 \mathbf{Q}_{ij} = \frac{1}{\varepsilon^2} (|\mathbf{Q}|^2 - 1) \mathbf{Q}_{ij}, \quad (4.9)$$

subject to suitable boundary conditions. We impose strong tangential anchoring on $\partial\Omega$, and therefore

$$\mathbf{Q}_B = \frac{1}{\sqrt{2}} (2\mathbf{n} \otimes \mathbf{n} - \mathbf{I}_2) \quad (4.10)$$

on $r = b$ and $r = 1$, where $\mathbf{n} = (\cos(\theta_0), \sin(\theta_0))$.

4.2 The Defect-Free State in the Oseen-Frank Theory with Strong and Weak Anchoring

In this section, we consider the defect-free state, with a director defined to be

$$\theta^*(r, \phi) := \phi + \frac{\pi}{2}. \quad (4.11)$$

This state is a critical point of the Oseen-Frank energy with both strong and weak anchoring for all values of δ , b and α , and has energy

$$E[\theta^*] = \pi \log \left(\frac{1}{b} \right). \quad (4.12)$$

We now investigate the stability of this state with strong and weak anchoring conditions on $\partial\Omega$ by considering the second variation of the Oseen-Frank energy.

4.2.1 Strong Anchoring

The second variation of the defect-free state with strong anchoring is

$$\delta^2 E := \left. \frac{\partial^2 E[\theta^* + \epsilon\eta]}{\partial \epsilon^2} \right|_{\epsilon=0} = \iint_{\Omega} |\nabla \eta|^2 - \delta \left(\frac{\eta}{r} + \eta_r \right)^2 d\Omega, \quad (4.13)$$

where the perturbation η satisfies $\eta(b, \phi) = \eta(1, \phi) = 0$ and is 2π -periodic in ϕ . It follows immediately that $\delta^2 E > 0$ for all $\delta \leq 0$ and any non-trivial η . Physically, the parameter regime $\delta < 0$ corresponds to splay deformations being energetically unfavourable compared to bend deformations. The defect-free state is comprised entirely of a bend deformation, therefore any perturbation to the defect-free state will induce energetically unfavourable splay deformations to the director.

In the rest of this section, we consider $\delta > 0$. In the following proposition, we show that the defect-free state becomes unstable as $\delta \rightarrow 1$.

Proposition 4.2.1. *For any admissible perturbation $\eta(r)$, there exists $\delta_\eta < 1$ such that $\delta^2 E < 0$ for $\delta_\eta < \delta \leq 1$.*

Proof. We consider the functional

$$E_2(\eta, \delta, b) := \iint_{\Omega} |\nabla \eta|^2 - \delta \left(\frac{\eta}{r} + \eta_r \right)^2 d\Omega. \quad (4.14)$$

For some η independent of ϕ , E_2 simplifies to

$$E_2(\eta(r), \delta, b) = 2\pi \int_b^1 \left\{ (\eta_r)^2 - \delta \left(\frac{\eta}{r} + \eta_r \right)^2 \right\} r dr. \quad (4.15)$$

For fixed b and $\eta(r)$, E_2 is a continuous function of δ which is bounded below by $E_2(\eta(r), 1, b)$. This lower bound is

$$E_2(\eta(r), 1, b) = -2\pi \int_b^1 \frac{\eta^2}{r} + 2\eta\eta_r dr = -2\pi \int_b^1 \frac{\eta^2}{r} dr - 2\pi\eta^2 \Big|_b^1 \quad (4.16)$$

$$= -2\pi \int_b^1 \frac{\eta^2}{r} dr < 0. \quad (4.17)$$

Since E_2 is continuous with respect to δ , we conclude that for any admissible $\eta(r)$, there exists some $0 < \delta_\eta < 1$ such that $\delta^2 E < 0$ for all $\delta_\eta < \delta < 1$. $\square$

We now improve on this condition by considering minimizers of $\delta^2 E$. The associated Euler-Lagrange equation for η is

$$\frac{\delta\eta}{r^2} + \frac{\eta_{\phi\phi}}{r^2} + (1 - \delta) \left(\eta_{rr} + \frac{\eta_r}{r} \right) = 0, \quad (4.18)$$

where $\eta(b, \phi) = \eta(1, \phi) = 0$ and η is 2π -periodic. We consider separable solutions of

the form

$$\eta = \sum_{k \in \mathbb{Z}} e^{ik\phi} f_k(r), \quad (4.19)$$

where the functions $f_k(r)$ are solutions of

$$r^2 f_k''(r) + r f_k'(r) + \frac{\delta - k^2}{1 - \delta} f_k(r) = 0, \quad (4.20)$$

subject to boundary conditions $f_k(b) = f_k(1) = 0$. Equation (4.20) is an Euler ordinary differential equation, with solutions of the form $f_k = Ar^m + Br^{-m}$, where m and k are related by

$$m^2 = \frac{k^2 - \delta}{1 - \delta}. \quad (4.21)$$

For all $k \geq 1$, the boundary conditions on f_k rule out any non-trivial solutions.

For $k = 0$, non-trivial solutions are the eigenfunctions

$$f_{0,n}(r) = \sin \left(\pi n \frac{\log(r)}{\log(b)} \right) \quad (4.22)$$

with associated eigenvalues $\delta_n = \frac{\pi^2 n^2}{\pi^2 n^2 + \log(b)^2}$. Any minimizer of the second variation, η , can therefore be expressed as linear combination of the eigenfunctions $f_{0,n}$,

$$\eta = \sum_{n=1}^{\infty} A_n f_{0,n}. \quad (4.23)$$

Substituting this series into Equation (4.13), we see that

$$\delta^2 E = \sum_{n=1}^{\infty} \frac{A_n^2 (\delta \log(b)^2 + n^2 \pi^2 (\delta - 1))}{2 \log(b)}. \quad (4.24)$$

It follows that the defect-free state is locally stable for all $\delta < \delta_1 \equiv \frac{\pi^2}{\pi^2 + \log(b)^2}$ and will lose stability for $\delta > \delta_1$. The eigenvalues, eigenfunctions and instability criterion have been previously identified using different techniques in [102, 105, 106, 108].

We now show that the defect-free state undergoes a supercritical pitchfork bifurcation at $\delta = \delta_1$ by identifying the optimal amplitude of the associated eigenfunction $f_{0,1}(r) = \sin\left(\pi \frac{\log(r)}{\log(b)}\right)$. We consider the neighbourhood about δ_1 by setting $\delta = \delta_1 + \epsilon^2 \delta_2$, where $\epsilon \ll 1$. We express θ in terms of an asymptotic expansion of the form

$$\theta = \theta^* + \epsilon \eta_1 + \epsilon^2 \eta_2 + \epsilon^3 \eta_3 + \dots, \quad (4.25)$$

where the functions satisfy $\eta_i(b, \phi) = \eta_i(1, \phi) = 0$ and are 2π -periodic in ϕ . We substitute (4.25) into the Euler-Lagrange equation (4.3) and compare terms of order ϵ . It follows that $\eta_1 = A_1 \sin\left(\pi \frac{\log(r)}{\log(b)}\right)$ and η_2 is proportional η_1 , and therefore can be included in terms of order ϵ . Comparing terms of order ϵ^3 , we find η_3 satisfies

$$\frac{\delta_1 \eta_3}{r^2} + \frac{\eta_{3\phi\phi}}{r^2} + (1 - \delta_1) \left(\eta_{3rr} + \frac{\eta_{3r}}{r} \right) = R(r), \quad (4.26)$$

where

$$\begin{aligned} R(r) := & \frac{(\log^2(b) + \pi^2) A_1 (\delta_1 A_1^2 - 2\delta_2)}{2r^2 \log^2(b)} \sin\left(\pi \frac{\log(r)}{\log(b)}\right) \\ & - \frac{\delta_1 A_1^3 (3\pi^2 + \log^2(b))}{6r^2 \log^2(b)} \sin\left(3\pi \frac{\log(r)}{\log(b)}\right). \end{aligned} \quad (4.27)$$

From the Fredholm Alternative Theorem, Equation (4.26) admits a solution if and only if the following solvability condition holds [90]:

$$\int_b^1 \sin\left(\pi \frac{\log(r)}{\log(b)}\right) R(r) r \, dr = 0, \quad (4.28)$$

Evaluating, we see that this condition reduces to

$$A_1 (A_1^2 \delta_1 - 2\delta_2) = 0. \quad (4.29)$$

and therefore the optimal amplitude, A_1 , is only defined for $\delta_2 > 0$ and we have a

supercritical pitchfork bifurcation at $\delta = \delta_1$.

Finally, we consider the behaviour of the energy minimizing defect-free state for $\delta > \delta_1$. Our analysis has shown that the optimal perturbation is independent of ϕ , and therefore we seek a solution of the form

$$\theta = \theta^* + U(r; \delta), \quad (4.30)$$

subject to $U(1; \delta) = U(b; \delta) = 0$. We make a change of variables by defining $t = -\log(r)$ and substitute (4.30) into the Equation (4.3). We find that U satisfies

$$(1 - \delta \cos^2(U)) \frac{d^2 U}{dt^2} + \frac{\delta}{2} \sin(2U) \left(\left(\frac{dU}{dt} \right)^2 + 1 \right) = 0, \quad (4.31)$$

subject to $U(0; \delta) = U(\log(1/b); \delta) = 0$. We consider functions with at most one critical point; solutions with multiple critical points exist but have a higher energy. Using MATLAB boundary-value problem solver, we solve (4.31) for $U(t)$ and thus find that the perturbed state has a spiral-like pattern, as shown in Figure 4.4a.

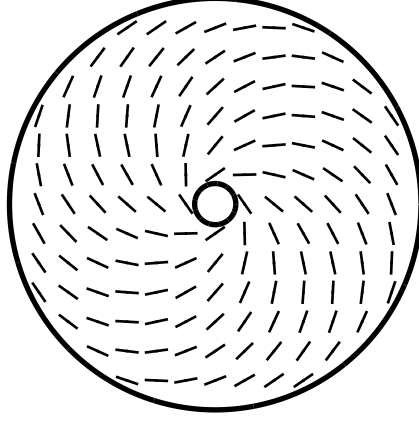
For the limiting case $\delta = 1$, we solve Equation (4.31) exactly to find

$$U(t; 1) = \arccos \left(\frac{b}{b+1} \exp(t) + \frac{1}{b+1} \exp(-t) \right), \quad (4.32)$$

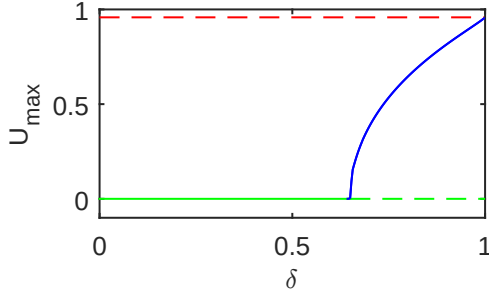
with associated energy $E = 2\pi \left(\frac{1-b}{1+b} \right)$, which acts as a lower bound on our numerically computed energy (see Figure 4.4c) We consider the second variation about the spiral state,

$$\delta^2 E := \iint_{\Omega} g^2 \eta_{\phi}^2 + (1 - g^2) \eta_t^2 + \eta^2 \left(\frac{2b - b^2 - 1}{b^2 e^{2t} + e^{-2t} - b^2 - 1} \right) d\Omega, \quad (4.33)$$

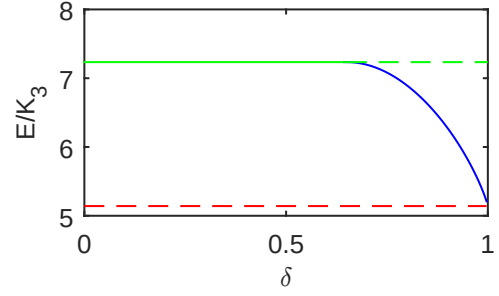
where $g(t) = \frac{b}{b+1} \exp(t) + \frac{1}{b+1} \exp(-t)$ and η is some perturbation function. For all $t \in [0, \log(1/b)]$, we have that $g \leq 1$ and $\frac{2b-b^2-1}{b^2 e^{2t} + e^{-2t} - b^2 - 1} \geq 1$. Therefore, the second variation is positive for all admissible perturbations and the spiral-like state is stable



(a) Director of the spiral state, for $b = 0.1$ and $\delta = 0.95$.



(b) Maximum value of U (blue) with the defect-free state (green) and limiting case (red) shown for comparison.



(c) Energy of defect-free state (green) and spiral state (blue).

Figure 4.4: Sample director field of the spiral state, and maximum value of U and energy in terms of δ for $b = 0.1$. The defect-free energy and maximum amplitude are shown in green, and the limiting case as $\delta \rightarrow 1$ is shown in red.

at least as $\delta \rightarrow 1$.

4.2.2 Weak Anchoring

The second variation of the Oseen-Frank energy with weak anchoring about the defect-free state is

$$\delta^2 E[\theta^*] := \iint_{\Omega} |\nabla \eta|^2 - \delta \left(\frac{\eta}{r} + \eta_r \right)^2 d\Omega + \alpha \int_{\partial\Omega} \eta^2 ds, \quad (4.34)$$

where η is a perturbation which is 2π -periodic in ϕ . As in the strong anchoring case, we consider separable solutions of the form

$$\eta(r, \phi) = \sum_{k \in \mathbb{Z}} e^{ik\phi} f_k(r), \quad (4.35)$$

where f_k is a solution of

$$r^2 f_k''(r) + r f_k'(r) + \frac{\delta - k^2}{1 - \delta} f_k(r) = 0, \quad (4.36)$$

but now with boundary conditions

$$f_k'(r) = \frac{\delta - \alpha}{1 - \delta} f_k(r) \quad \text{on } r = 1, \quad (4.37)$$

$$f_k'(r) = \frac{\alpha + \frac{\delta}{b}}{1 - \delta} f_k(r) \quad \text{on } r = b. \quad (4.38)$$

Solving, we see that for $k = 0$,

$$f_0(r) = A \sin \left(\sqrt{\frac{\delta}{1 - \delta}} \log \left(\frac{1}{r} \right) \right) + B \cos \left(\sqrt{\frac{\delta}{1 - \delta}} \log \left(\frac{1}{r} \right) \right), \quad (4.39)$$

and for $k \geq 1$,

$$f_k(r) = A \sinh \left(\sqrt{\frac{k^2 - \delta}{1 - \delta}} \log \left(\frac{1}{r} \right) \right) + B \cosh \left(\sqrt{\frac{k^2 - \delta}{1 - \delta}} \log \left(\frac{1}{r} \right) \right). \quad (4.40)$$

The boundary conditions (4.37)–(4.38) require the following compatibility conditions between the parameters α, δ, b and k :

$$\tan \left(\sqrt{\frac{\delta}{1 - \delta}} \ln \left(\frac{1}{b} \right) \right) + \frac{\alpha(1 + b)\sqrt{\delta(1 - \delta)}}{\alpha\delta - \alpha b\delta + \alpha^2 b - \delta} = 0 \quad \text{for } k = 0, \quad (4.41)$$

$$\tanh \left(\sqrt{\frac{k^2 - \delta}{1 - \delta}} \ln \left(\frac{1}{b} \right) \right) + \frac{\alpha(1 + b)\sqrt{(k^2 - \delta)(1 - \delta)}}{\delta\alpha + \alpha^2 b - \alpha b\delta - \delta + k^2(1 - \delta)} = 0 \quad \text{for } k \geq 1. \quad (4.42)$$

The compatibility condition for $k = 0$ also is identified in [102]. We consider the cases $k = 0$ and $k \geq 1$ separately.

4.2.2.1 Radial Perturbations ($\mathbf{k} = \mathbf{0}$)

The boundary-value problem (4.36)–(4.38) is a Sturm-Liouville problem with a complete set of eigenfunctions [90],

$$\begin{aligned} f_{n,0}(r) = & A_n \frac{\sqrt{\delta_{n,0}(1-\delta_{n,0})}}{\alpha - \delta_{n,0}} \cos \left(\sqrt{\frac{\delta_{n,0}}{1-\delta_{n,0}}} \log \left(\frac{1}{r} \right) \right) \\ & + A_n \sin \left(\sqrt{\frac{\delta_{n,0}}{1-\delta_{n,0}}} \log \left(\frac{1}{r} \right) \right), \end{aligned} \quad (4.43)$$

where the corresponding eigenvalues $\delta_{n,0}$ are solutions of

$$\tan \left(\sqrt{\frac{\delta}{1-\delta}} \ln \left(\frac{1}{b} \right) \right) + \frac{\alpha(1+b)\sqrt{\delta(1-\delta)}}{\alpha\delta - \alpha b\delta + \alpha^2 b - \delta} = 0. \quad (4.44)$$

Equation (4.44) has an infinite number of solutions $\delta_{n,0}$ for any fixed α and b . In Figure 4.5, we plot the first eigenvalue $\delta_{1,0}$ as a function of b , for different values of α . We see that lowering the anchoring strength reduces the value of δ for which the defect-free state becomes unstable. As $\alpha \rightarrow \infty$, the compatibility condition becomes $\tan \left(\sqrt{\frac{\delta}{1-\delta}} \ln \left(\frac{1}{b} \right) \right) \rightarrow 0$ and $\delta_{1,0} \rightarrow \frac{\pi^2}{\pi^2 + \ln(b)^2}$, and we recover the strong anchoring result.

We now investigate the loss of stability of about $\delta = \delta_{1,0}$. As in the strong anchoring case, we let

$$\theta = \theta^* + \epsilon \eta_1 + \epsilon^2 \eta_2 + \epsilon^3 \eta_3 + \dots, \quad (4.45)$$

$$\delta = \delta_{1,0} + \epsilon^2 \delta_2 + \dots \quad (4.46)$$

Then η_1 and η_2 are proportional to the first eigenfunction $f_{1,0}(r)$ in Equation (4.43)

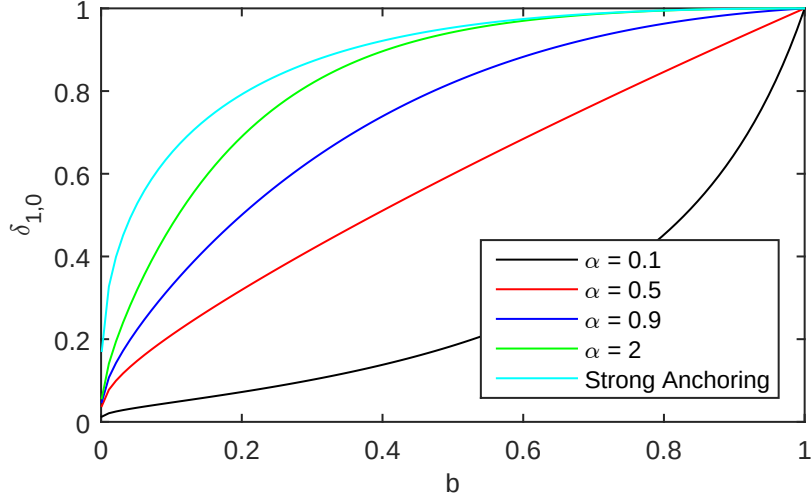


Figure 4.5: The first eigenvalue $\delta_{1,0}$ versus b for fixed α and the strong anchoring limit.

with $n = 1$. The solvability condition for η_3 is

$$\int_b^1 R\eta_{3h}r \, dr = -r\eta_{3h} \left(\delta_2 \left(\frac{\eta_1}{r} + \eta_1' \right) - \frac{2\eta_1^3}{3} \left(\alpha + \frac{\delta_{1,0}}{b} \right) - \delta_{1,0}\eta_1^2\eta_1' \right) \Big|_{r=b} + \eta_{3h} \left(\delta_2 \left(\frac{\eta_1}{r} + \eta_1' \right) + \frac{2\eta_1^3}{3} \left(\alpha - \frac{\delta_{1,0}}{r} \right) - \delta_{1,0}\eta_1^2\eta_1' \right) \Big|_{r=1}, \quad (4.47)$$

where η_{3h} is the solution of the homogeneous problem as given below:

$$\eta_{3h}(r) := \frac{\sqrt{\delta_{1,0}(1-\delta_{1,0})}}{\alpha - \delta_{1,0}} \cos \left(\sqrt{\frac{\delta_{1,0}}{1-\delta_{1,0}}} \ln \left(\frac{1}{r} \right) \right) + \sin \left(\sqrt{\frac{\delta_{1,0}}{1-\delta_{1,0}}} \ln \left(\frac{1}{r} \right) \right), \quad (4.48)$$

and

$$R := \delta_2 \left(\frac{\eta_1'}{r} + \eta_1'' - \frac{\eta_1}{r^2} \right) - \delta_{1,0} \left(\eta_1\eta_1'^2 - \frac{2\eta_1^3}{3r^2} + \eta_1^2\eta_1'' + \frac{\eta_1^2\eta_1'}{r} \right). \quad (4.49)$$

The compatibility condition yields

$$A_1^3 E_3 - \delta_2 A_1 E_1 = 0, \quad (4.50)$$

where E_3 and E_1 are functions of $\delta_{1,0}$, b and α . Numerically evaluating these functions for $\delta_{1,0}$, b and α shows that both E_1 and E_3 are positive and hence we have a supercritical pitchfork bifurcation at $\delta = \delta_{1,0}$.

4.2.2.2 Radial Symmetry Breaking Perturbations ($k \geq 1$)

For $k = 1$, the compatibility condition (4.42) simplifies to

$$-\frac{(1+b)(b^2\alpha^2 - \alpha b^2 + 2\delta\alpha b - 2\delta b + b - \alpha^2 b - \alpha + 2\delta - 1)}{(b^2 + 1)(\delta\alpha + \alpha^2 b - \delta\alpha b - 2\delta + 1)} = 0, \quad (4.51)$$

with a unique solution

$$\delta_{1,1}(\alpha, b) = \frac{1}{2} \frac{\alpha b^2 + \alpha^2 b + \alpha + 1 - b^2 \alpha^2 - b}{\alpha b - b + 1}. \quad (4.52)$$

The solution $\delta_{1,1} \in (0, 1)$ iff $0 < \alpha < 1$, and the constraint that $b \in (0, 1)$ requires that $\delta_{1,1} > \frac{1}{2}$.

For $k > 1$, the compatibility condition (4.42) has a solution if and only if

$$\frac{(1-\delta)\alpha(1+b)}{\delta\alpha + \alpha^2 b - \alpha b\delta - \delta + k^2(1-\delta)} \sqrt{\frac{k^2 - \delta}{1-\delta}} < 0. \quad (4.53)$$

In particular, this implies $\frac{k^2 + \alpha^2 b}{\alpha b - \alpha + 1 + k^2} < \delta_{1,k} < 1$, which requires that $\alpha < 1$. We conclude that the defect-free state may lose stability to perturbations with ϕ -dependence only if $\alpha < 1$. Physically, this condition corresponds to chamber sizes which are on the order of the extrapolation length of the nematic.

In Figure 4.6, we plot the instability curves in the (δ, α) -plane, for fixed values of k and b . The curves define the regions of parameter space for which the defect-free state will lose stability under different types of perturbation. We see that purely radial perturbations induce instability for a greater range of δ and α . As either α or b increases, the defect-free state is stable with respect to a larger class of perturbations.

For systems with $\alpha < 1$, purely radial perturbations induce instability for smaller values of δ than symmetry breaking perturbations. For very narrow chambers with $b \rightarrow 1$, the critical value of δ for radial perturbations is similar to radially symmetry breaking perturbations, and we might expect to see equilibria with boundary defects forming in this parameter regime.

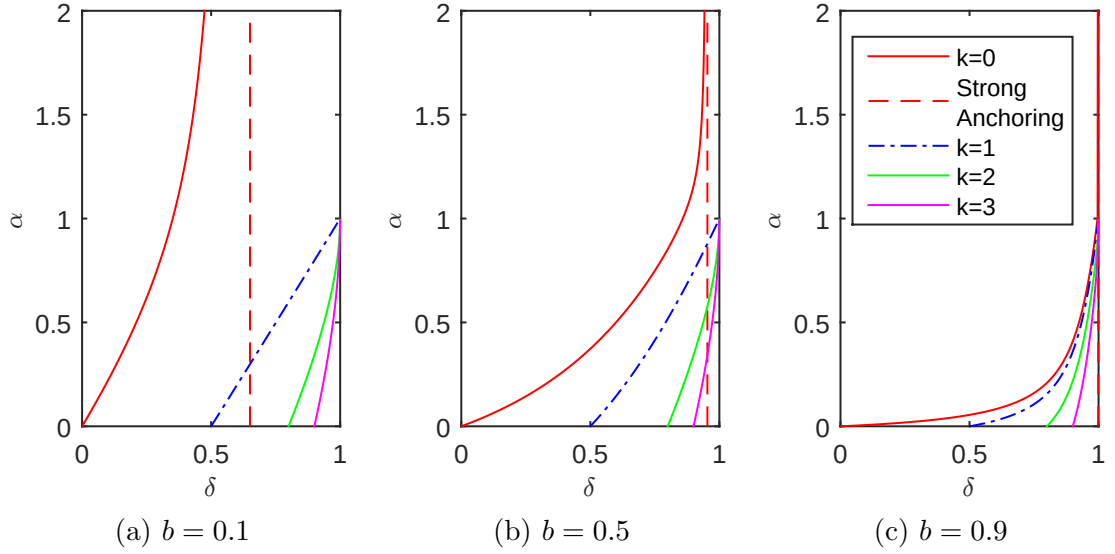


Figure 4.6: The smallest solution to the compatibility condition (4.41) and the strong anchoring limit, and the only solution to (4.42) for $k = 1, 2, 3$ in the (δ, α) -plane for fixed b .

4.3 The Defect-Free State in Landau-de Gennes Theory

In this section, we discuss the defect-free state in the Landau-de Gennes theory, and derive some results which complement our analysis in the Oseen-Frank theory.

4.3.1 Properties of the Defect-Free State

We define the defect-free state to be

$$\mathbf{Q}^* = s(r) (2\mathbf{n}^* \otimes \mathbf{n}^* - \mathbf{I}_2), \quad (4.54)$$

where $\mathbf{n}^* = (\cos(\theta^*), \sin(\theta^*))$ and the order parameter s is the admissible space.

The associated energy of the defect-free state is

$$E[\mathbf{Q}^*] = \iint_{\Omega} \frac{1}{2} \left\{ (s')^2 + \frac{4s^2}{r^2} + \frac{1}{4\varepsilon^2} (2s^2 - 1)^2 \right\} d\Omega. \quad (4.55)$$

The energy (4.55) is lower semi-continuous and satisfies the coercivity condition in [114]. Hence by direct methods in the calculus of variations [115], we are guaranteed the existence of a global minimizer which is the solution to the Euler-Lagrange equation

$$s'' + \frac{s'}{r} - \frac{4s}{r^2} = \frac{s}{\varepsilon^2} (2s^2 - 1), \quad (4.56)$$

subject to $s(b) = s(1) = \frac{1}{\sqrt{2}}$. It follows immediately that Equation (4.54) is a critical point of the Landau-de Gennes energy.

Using Equation (4.56), we can derive some elementary properties of the order parameter in the extremal state. By an application of the maximum principle, we show that s is bounded above.

Proposition 4.3.1. *The solution to Equation (4.56), $s(r)$, satisfies the following bounds for all $r \in [b, 1]$:*

$$s(r) \leq \frac{1}{\sqrt{2}}, \quad (4.57)$$

for all values of $0 < b < 1$ and $\varepsilon^2 > 0$.

Proof. If s has a maximum at $r^* \in (b, 1)$, then $s'(r^*) = 0$ and $s''(r^*) < 0$. Therefore

$$\frac{s(r^*)}{\varepsilon^2} (2s(r^*)^2 - 1) + \frac{4s(r^*)}{r_*^2} \leq 0 \quad \Rightarrow \quad (2s(r^*)^2 - 1) \leq 0. \quad (4.58)$$

If the maximum occurs at $r = b$ or 1 , then it follows immediately that the maximum value of s is $\frac{1}{\sqrt{2}}$. $\square$

The existence of a unique solution to Equation (4.56) follows from a similar proof of the uniqueness of the radial solution in a disk given in [101].

We now show that s is bounded below by using a result from [109, 116].

Proposition 4.3.2. *For all $\varepsilon^2 > 0$, the solution to Equation (4.56) is bounded below by*

$$s(r) \geq \frac{\sqrt{2}b}{b^2 + 1}. \quad (4.59)$$

Proof. We first show that the solution $s(r)$ to Equation (4.56) satisfies the relation

$$s(r) \geq \eta(r) \quad (4.60)$$

where $\eta(r)$ is the solution to

$$\eta''(r) + \frac{\eta'(r)}{r} - \frac{4\eta(r)}{r^2} = 0, \quad (4.61)$$

subject to $\eta(b) = \eta(1) = \frac{1}{\sqrt{2}}$.

We assume for a contradiction that for some $r_* \in (b, 1)$, $s(r_*) - \eta(r_*) < 0$. There-

fore, there must exist some R_1, R_2 such that $b \leq R_1 < r_* < R_2 \leq 1$ and

$$s(R_1) - \eta(R_1) = 0, \quad (4.62)$$

$$s'(R_1) - \eta'(R_1) < 0, \quad (4.63)$$

$$s(R_2) - \eta(R_2) = 0, \quad (4.64)$$

$$s'(R_2) - \eta'(R_2) > 0. \quad (4.65)$$

Multiplying (4.56) by η and (4.61) by rs , subtracting the resulting equations and integrating over (R_1, R_2) , we find that

$$\int_{R_1}^{R_2} \eta(rs')' - s(r\eta')' dr = \int_{R_1}^{R_2} \frac{\eta}{\varepsilon^2} (2s^2 - 1)r dr. \quad (4.66)$$

The right-hand side of (4.66) is always negative since $2s^2 - 1 < 0$ on $r \in (b, 1)$.

Integrating by parts, the left-hand side is

$$R_2 s(R_2)(s'(R_2) - \eta'(R_2)) - R_1 s(R_1)(s'(R_1) - \eta'(R_1)) > 0, \quad (4.67)$$

and hence we have a contradiction.

Solving Equation (4.61), we see that

$$\eta(r) = \frac{1}{\sqrt{2}} \frac{b^2 + r^4}{(b^2 + 1)r^2}. \quad (4.68)$$

The minimum of (4.68) occurs at $r = \sqrt{b}$, and $\eta(\sqrt{b}) = \frac{\sqrt{2b}}{b^2 + 1}$. $\square$

4.3.2 Local Stability of the Defect-Free State

In this section, we show that the defect-free state is locally stable in the limit as $\varepsilon^2 \rightarrow 0$ and derive an explicit condition on the local stability in terms of ε^2 and b . To

show that a state is locally stable, it suffices to show that the second variation,

$$\delta^2 E[\mathbf{Q}^*] := \iint_{\Omega} \frac{1}{2} |\nabla \mathbf{V}|^2 + \frac{|\mathbf{V}|^2}{2\varepsilon^2} (2s^2 - 1) + \frac{1}{\varepsilon^2} (\mathbf{Q}^* \cdot \mathbf{V})^2 d\Omega > 0, \quad (4.69)$$

for any admissible perturbation $\mathbf{V}$. Here, we adapt the proof of local stability from [117] for a vortex solution of the Ginzburg-Landau functional on a disk to an annulus.

We introduce a basis for the space of symmetric, traceless 2×2 matrices,

$$\mathbf{E} = \begin{pmatrix} \cos(2\phi) & \sin(2\phi) \\ \sin(2\phi) & -\cos(2\phi) \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} -\sin(2\phi) & \cos(2\phi) \\ \cos(2\phi) & \sin(2\phi) \end{pmatrix}. \quad (4.70)$$

Then, we can write any perturbation $\mathbf{V}$ in the form

$$\mathbf{V} = v(r, \phi) \mathbf{E} + w(r, \phi) \mathbf{F}, \quad (4.71)$$

where the functions v, w are 2π -periodic in ϕ and satisfy the boundary conditions $v(b, \phi) = v(1, \phi) = w(b, \phi) = w(1, \phi) = 0$.

We use a basis decomposition for the functions v and w as shown below:

$$v(r, \phi) = \sum_{n=0}^{\infty} a_n(r) \cos(n\phi) + b_n(r) \sin(n\phi), \quad (4.72)$$

$$w(r, \phi) = \sum_{n=0}^{\infty} c_n(r) \cos(n\phi) + d_n(r) \sin(n\phi), \quad (4.73)$$

where $a_n = b_n = c_n = d_n = 0$ on $r = b, 1$ for all n . In terms of these functions, the second variation is

$$\delta^2 E[\mathbf{Q}^*] = 2\pi L_0[a_0, a_0, c_0, c_0] + 2\pi \sum_{n=1}^{\infty} L_n[a_n, b_n, c_n, d_n], \quad (4.74)$$

where we define the functional L_n to be

$$L_n[a, b, c, d] := \int_b^1 \left\{ (a')^2 + (b')^2 + (c')^2 + (d')^2 + \left(\frac{n^2 + 4}{r^2} \right) (a^2 + b^2 + c^2 + d^2) \right. \\ \left. + \frac{8n}{r^2} (ad - bc) + \frac{(6s^2 - 1)}{\varepsilon^2} (a^2 + b^2) + \frac{(2s^2 - 1)}{\varepsilon^2} (c^2 + d^2) \right\} r \, dr. \quad (4.75)$$

In the following proposition, we show that to prove the local stability, it suffices to consider the functionals L_0 , L_1 and L_2 .

Proposition 4.3.3. *The second variation $\delta^2 E[\mathbf{Q}^*] > 0$ if $\min L_0 > 0$, $\min L_1 > 0$ and $\min L_2 > 0$.*

Proof. For $n \geq 1$,

$$L_{n+2}(a, b, c, d) - L_n(a, b, c, d) = \int_b^1 \left\{ \frac{4n + 4}{r} (a^2 + b^2 + c^2 + d^2) + \frac{16}{r} (ad - bc) \right\} dr. \quad (4.76)$$

Using Young's inequality, it follows that

$$(4n + 4)(a^2 + b^2 + c^2 + d^2) + 16(ad - bc) \geq (4n - 4)(a^2 + b^2 + c^2 + d^2) \geq 0. \quad (4.77)$$

and therefore if $n \geq 1$, the inequality holds. $\square$

We now show that each of the functionals L_0 , L_1 and L_2 is positive for any admissible functions a_n , b_n , c_n and d_n , although L_2 is conditional subject to some constraint on ε^2 .

For any functions a_0 and c_0 satisfying $a_0 = c_0 = 0$ on $r = b, 1$, we have that

$$L_0(a_0, a_0, c_0, c_0) \geq L_0(0, 0, 0, c_0), \quad (4.78)$$

and

$$L_0(0, 0, 0, c_0) := \int_b^1 \left\{ (c'_0)^2 + \frac{4c_0^2}{r} + \frac{1}{\varepsilon^2} (2s^2 - 1)c_0^2 \right\} r \, dr. \quad (4.79)$$

We define $c(r) := s(r)c_0(r)$ and recall the governing ordinary differential equation for s in (4.56). Then

$$L_0(0, 0, 0, c_0) = \int_b^1 \frac{d}{dr} \left(s \frac{ds}{dr} c^2 r \right) + s^2 \left(\frac{dc}{dr} \right)^2 r \, dr = \int_b^1 s^2 \left(\frac{dc}{dr} \right)^2 r \, dr > 0, \quad (4.80)$$

for any non-trivial $c : [b, 1] \rightarrow \mathbb{R}$ with $c(b) = c(1) = 0$.

For any trivial functions a_1, b_1, c_1, d_1 satisfying the required homogeneous boundary conditions, we make a change of variables $a_1 = \sqrt{a_1^2 + b_1^2} \cos \vartheta$, $b_1 = \sqrt{a_1^2 + b_1^2} \sin \vartheta$. Then, we define $a = \sqrt{a_1^2 + b_1^2}$ and $d = \sqrt{c_1^2 + d_1^2}$, and it follows that

$$L_1(a_1, b_1, c_1, d_1) \geq L_1(a, 0, d, 0). \quad (4.81)$$

We introduce a new function $u(r)$, which is a minimizer of the functional (4.55) with boundary conditions $u(b) = 0$ and $u(1) = \frac{1}{\sqrt{2}}$. This minimizer is the solution of

$$u'' + \frac{u'}{r} - \frac{4u}{r^2} = \frac{u}{\varepsilon^2} (2u^2 - 1). \quad (4.82)$$

The function u is unique and monotonically increasing. In the following proposition, we show that u acts as lower bound on s .

Proposition 4.3.4. *For all $r \in [b, 1]$ and all $b \in (0, 1)$ and $\varepsilon^2 > 0$,*

$$u(r) \leq s(r). \quad (4.83)$$

Proof. We assume for a contradiction that $s(r) < u(r)$ for some $r \in (b, 1)$. Then, there must exist r_1 and r_2 , where $b < r_1 < r_2 \leq 1$, for which $s(r_1) - u(r_1) = 0$, $s'(r_1) - u'(r_1) < 0$, $s(r_2) - u(r_2) = 0$, $s'(r_2) - u'(r_2) > 0$ and $s(r) - u(r) < 0$ for

$r \in [r_1, r_2]$. We multiply the Euler-Lagrange equations (4.56) and (4.82) for s and u by ru and rs respectively, subtract and integrate over (r_1, r_2) to find

$$\int_{r_1}^{r_2} rus'' - rsu'' + us' - su' dr = \int_{r_1}^{r_2} \frac{su}{\varepsilon^2} (2s^2 - 2u^2)r dr. \quad (4.84)$$

The right-hand side is negative since $s - u < 0$ in (r_1, r_2) . The left-hand side is

$$\begin{aligned} \text{LHS} &= \int_{r_1}^{r_2} u(rs')' - s(ru')' dr = (rus' - rsu') \Big|_{r_1}^{r_2} \\ &= r_2 s(r_2)(s'(r_2) - u'(r_2)) - r_1 s(r_1)(s'(r_1) - u'(r_1)) > 0, \end{aligned} \quad (4.85)$$

which is a contradiction. $\square$

Since $s \geq u$, we immediately have

$$\begin{aligned} L_1(a, 0, d, 0) &\geq \int_b^1 \left\{ (a')^2 + (d')^2 + \frac{5}{r^2} (a^2 + d^2) - \frac{8}{r^2} ad \right. \\ &\quad \left. + \frac{1}{\varepsilon^2} (a^2 + d^2) (2u^2 - 1) + \frac{4}{\varepsilon^2} a^2 u^2 \right\} r dr \equiv m. \end{aligned} \quad (4.86)$$

It remains to show that $\min m > 0$, which follows by analogy with [117] with some technical differences. We compute the Euler-Lagrange equations for (4.86):

$$a'' + \frac{a'}{r} - \frac{5a}{r^2} + \frac{4d}{r^2} = \frac{1}{\varepsilon^2} a(6u^2 - 1) - a \min m, \quad (4.87)$$

$$d'' + \frac{d'}{r} - \frac{5d}{r^2} + \frac{4a}{r^2} = \frac{1}{\varepsilon^2} d(2u^2 - 1) - d \min m, \quad (4.88)$$

where $\min m$ acts as a Lagrange multiplier. As in [117], this system is satisfied weakly, with $\min m = 0$ and no boundary conditions, by the functions $A = u'$ and $D = 2u/r$. Multiplying the Euler-Lagrange equations (4.87) and (4.88) by rA and rD respectively and the equations for A and D by ra and rd respectively, and integrating

over $(b, 1)$, we find that

$$-\min m \int_b^1 r(aA + dD) dr = (r(a'A + d'D)) \Big|_b^1. \quad (4.89)$$

The RHS is negative since $a, d \geq 0$, $a'(1), d'(1) < 0$, and $a'(b), d'(b) > 0$. Therefore, $\min m \geq 0$.

If $\min m = 0$, then we must have

$$a'(1)A(1) + \sqrt{2}d'(1) = ba'(b)A(b). \quad (4.90)$$

This implies $d'(1) = 0$ and $a'(b)u'(b) = a'(1)u'(1) = 0$. For $a'(1)u'(1) = 0$ to hold, we must either have $a'(1) = 0$ (and hence $a = d = 0$) or $u'(1) = 0$. If $u'(1) = 0$, then from Equation (4.82), we see that $u''(1) = 2\sqrt{2}$ which implies that $u(1)$ is a local minimum. Since u is monotonically increasing, this leads to a contradiction. We therefore conclude that $\min m > 0$ and hence $L_1 > 0$ for any non-trivial functions.

It remains to show that $L_2 > 0$ for some values of ε^2 and b . We first show that $L_2 > 0$ in the limit as $\varepsilon^2 \rightarrow 0$ by following the strategy laid out in [116], and then derive an explicit condition in terms of b and ε^2 . To show that $L_2 > 0$, it suffices to consider the functional

$$m_1 \equiv \int_b^1 \left(a_2'^2 + d_2'^2 + \frac{8(a_2 - d_2)^2}{r^2} + \frac{1}{\varepsilon^2} (a_2^2(6s^2 - 1) + d_2^2(2s^2 - 1)) \right) r dr, \quad (4.91)$$

where a_2 and d_2 are positive functions of r satisfying $a_2(b) = d_2(b) = a_2(1) = d_2(1) = 0$.

We first show that for sufficiently small ε^2 , $\min s(r)$ is controlled by ε^2 .

Proposition 4.3.5. $s \rightarrow \frac{1}{\sqrt{2}}$ uniformly as $\varepsilon^2 \rightarrow 0$.

Proof. The function s attains its minimum at some $r_* \in (b, 1)$. We define $s(r_*) = s_{\min}$.

Therefore, $s'(r_*) = 0$, $s''(r_*) \geq 0$ and

$$\frac{s_{\min}}{\varepsilon^2}(2s_{\min}^2 - 1) + \frac{4s_{\min}}{r_*^2} \geq 0. \quad (4.92)$$

Rearranging, it follows that

$$s(r) \geq s_{\min} \geq \sqrt{\frac{1}{2} - \frac{2\varepsilon^2}{r_*^2}} \rightarrow \frac{1}{\sqrt{2}} \quad \text{as } \varepsilon^2 \rightarrow 0. \quad (4.93)$$

□

We now let $a_2(r) = s(r)a(r)$, $d_2(r) = s(r)d(r)$, and use Hardy's decomposition trick (see Appendix C) to write m_1 as

$$m_1 = \int_b^1 s^2 \left\{ a'^2 + d'^2 + \frac{4(a^2 + d^2)}{r^2} - \frac{16ad}{r^2} + \frac{4s^2 a^2}{\varepsilon^2} \right\} r \, dr. \quad (4.94)$$

We consider the non-derivative terms in the integrand of (4.94), and it follows that

$$s^2 \left(\frac{4(a^2 + d^2)}{r^2} - \frac{16ad}{r^2} \right) + \frac{4s^4 a^2}{\varepsilon^2} \geq \frac{4s_{\min}^2(a^2 + d^2)}{r^2} - \frac{256a^2}{r^2} - \frac{d^2}{16r^2} + \frac{4s_{\min}^4 a^2}{\varepsilon^2}. \quad (4.95)$$

The coefficients of d^2 are positive if the order parameter $s_{\min} > \frac{1}{8}$ for all $b \in (0, 1)$. From Proposition 4.3.5, we can always find some T_1 such that $s_{\min} > \frac{1}{8}$ for all $\frac{1}{\varepsilon^2} > T_1$. The coefficients of a^2 are positive if $\frac{1}{\varepsilon^2} > T_2$, where we define $T_2 \equiv \frac{64}{s_{\min}^2 b^2}$. Therefore, $L_2 > 0$ if $\frac{1}{\varepsilon^2} > \max\{T_1, T_2\}$.

Finally, we show that L_2 is non-negative if $\frac{1}{\varepsilon^2}$ is greater than an explicit positive quantity dependent on b . We let $a(r) = \alpha(r) \cos(\vartheta(r))$ and $d(r) = \alpha(r) \sin(\vartheta(r))$, where $\alpha(b) = \alpha(1) = 0$, and then

$$m_1 \geq m_2(\alpha, \vartheta) := \int_b^1 s^2 \left(\alpha'^2 + \frac{4\alpha^2}{r^2} - \frac{8\alpha^2 \sin(2\vartheta)}{r^2} + \frac{4}{\varepsilon^2} s^2 \alpha^2 \sin^2(\vartheta) \right) r \, dr. \quad (4.96)$$

The minimum of the integrand of m_2 with respect to ϑ occurs at

$$\vartheta = \frac{1}{2} \arctan \left(\frac{4\varepsilon^2}{r^2 s(r)^2} \right) \quad (4.97)$$

and evaluating the integrand of m_2 , it follows that

$$m_2(\alpha, \vartheta) \geq \int_b^1 s^2 \left(\alpha'^2 + \frac{4\alpha^2}{r^2} - \frac{32\alpha^2}{r^4 \varepsilon^2 s^2 \sqrt{1 + \frac{16\varepsilon^4}{s^4 r^4}}} + \frac{2s^2 \alpha^2}{\varepsilon^2} \left(1 - \frac{1}{\sqrt{1 + \frac{16\varepsilon^4}{s^4 r^4}}} \right) \right) r \, dr. \quad (4.98)$$

We note that $\alpha = 0$ is always a critical point of

$$\frac{4\alpha^2}{r^2} - \frac{32\alpha^2}{r^4 \varepsilon^2 s^2 \sqrt{1 + \frac{16\varepsilon^4}{s^4 r^4}}} + \frac{2s^2 \alpha^2}{\varepsilon^2} \left(1 - \frac{1}{\sqrt{1 + \frac{16\varepsilon^4}{s^4 r^4}}} \right), \quad (4.99)$$

and is a minimum if $\frac{1}{\varepsilon^2} > \frac{3}{r^2 s^2}$. Using the lower bound on s from Proposition 4.3.2, we deduce that $L_2 > 0$, and hence $\delta^2 E[\mathbf{Q}^*] > 0$, if

$$\frac{1}{\varepsilon^2} > \frac{3(b^2 + 1)^2}{2b^4}. \quad (4.100)$$

4.3.3 Global Minimality of the Defect-Free State

We now show that the defect-free state is the global minimizer of the Landau-de Gennes energy for sufficiently large b , independent of ε^2 .

We consider the expansion about $\mathbf{Q}^*$ of the Landau-de Gennes energy,

$$\begin{aligned} E[\mathbf{Q}^* + \mathbf{V}] &= \iint_{\Omega} \frac{1}{2} |\nabla \mathbf{V}|^2 + \frac{|\mathbf{V}|^2}{2\varepsilon^2} (2s^2 - 1) + \frac{1}{4\varepsilon^2} (|\mathbf{V}|^2 + 2(\mathbf{Q}^* \cdot \mathbf{V}))^2 \, d\Omega \\ &\quad + E[\mathbf{Q}^*] + \iint_{\Omega} \nabla \mathbf{Q}^* \cdot \nabla \mathbf{V} + \frac{\mathbf{Q}^* \cdot \mathbf{V}}{\varepsilon^2} (2s^2 - 1) \, d\Omega, \end{aligned} \quad (4.101)$$

where $\mathbf{V} = 0$ on $\partial\Omega$. To show that $\mathbf{Q}^*$ is the global minimizer, it suffices to show

that

$$\iint_{\Omega} \frac{1}{2} |\nabla \mathbf{V}|^2 + \frac{|\mathbf{V}|^2}{2\varepsilon^2} (2s^2 - 1) \, d\Omega > 0, \quad (4.102)$$

for any admissible perturbation $\mathbf{V}$. The only term in Equation (4.102) which is negative is due to $2s^2 - 1 \leq 0$. We use results from §4.3.1 to derive a lower bound on this term.

Using Equation (4.92), there exists some minimizer $s(r_*) = s_{\min}$ such that

$$\frac{s_{\min}}{\varepsilon^2} (2s_{\min}^2 - 1) + \frac{4s_{\min}}{r_*^2} > 0. \quad (4.103)$$

Rearranging, it follows that

$$\frac{s_{\min}}{\varepsilon^2} (2s_{\min}^2 - 1) > -\frac{4s_{\min}}{r_*^2} > -\frac{4s_{\min}}{b^2} > -\frac{2\sqrt{2}}{b^2}. \quad (4.104)$$

We now define a function $g(s) := 2s^3 - s$. For all $r \in (b, 1)$,

$$s \geq s_{\min} \quad \Leftrightarrow \quad s(2s^2 - 1) > s_{\min}(2s_{\min}^2 - 1), \quad (4.105)$$

if g is an increasing function of s , or equivalently, if $s^2 > \frac{1}{6}$. Using our lower bound on s from Proposition 4.3.2, $g'(s) > 0$ if

$$\sqrt{3} - \sqrt{2} < b < 1. \quad (4.106)$$

Since $s_{\min}$ is a minimum, it holds that

$$\frac{s}{2\varepsilon^2} (2s^2 - 1) \leq \frac{s_{\min}}{2\varepsilon^2} (2s_{\min}^2 - 1). \quad (4.107)$$

If we assume that $\sqrt{3} - \sqrt{2} < b < 1$, then by rearranging (4.107) and applying (4.105),

we have

$$\frac{1}{2\varepsilon^2} (2s^2 - 1) \geq \frac{1}{2\varepsilon^2} \frac{s}{s_{\min}} (2s^2 - 1) > -\frac{\sqrt{2}}{b^2 s_{\min}} > -\frac{b^2 + 1}{b^3}. \quad (4.108)$$

It therefore follows that

$$\iint_{\Omega} \frac{|\mathbf{V}|^2}{2\varepsilon^2} (2s^2 - 1) \, d\Omega > \int_{\Omega} -\frac{b^2 + 1}{b^3} |\mathbf{V}|^2 \, d\Omega \quad (4.109)$$

$$\geq -\frac{(b^2 + 1)}{b^3} \int_0^{2\pi} \int_b^1 |\mathbf{V}|^2 \, dr \, d\phi. \quad (4.110)$$

We now consider the distortion term in Equation (4.102),

$$\iint_{\Omega} \frac{1}{2} |\nabla \mathbf{V}|^2 \, d\Omega \equiv \frac{1}{2} \sum_{i,j=1}^2 \int_0^{2\pi} \int_b^1 \left(\left(\frac{\partial \mathbf{V}_{ij}}{\partial r} \right)^2 + \frac{1}{r^2} \left(\frac{\partial \mathbf{V}_{ij}}{\partial \phi} \right)^2 \right) r \, dr \, d\phi \quad (4.111)$$

$$\geq \frac{b}{2} \sum_{i,j=1}^2 \int_0^{2\pi} \int_b^1 \left(\frac{\partial \mathbf{V}_{ij}}{\partial r} \right)^2 \, dr \, d\phi \quad (4.112)$$

Applying Wirtinger's inequality [118], it follows immediately that

$$\frac{b}{2} \sum_{i,j=1}^2 \int_0^{2\pi} \int_b^1 \left(\frac{\partial \mathbf{V}_{ij}}{\partial r} \right)^2 \, dr \, d\phi \geq \frac{b\pi^2}{2(b-1)^2} \int_0^{2\pi} \int_b^1 |\mathbf{V}|^2 \, dr \, d\phi. \quad (4.113)$$

Combining (4.110) and (4.113), we have

$$\iint_{\Omega} \frac{1}{2} |\nabla \mathbf{V}|^2 + \frac{|\mathbf{V}|^2}{2\varepsilon^2} (2s^2 - 1) \, d\Omega > \left(\frac{b\pi^2}{2(b-1)^2} - \frac{(b^2 + 1)}{b^3} \right) \int_0^{2\pi} \int_b^1 |\mathbf{V}|^2 \, dr \, d\phi. \quad (4.114)$$

Therefore, the right-hand side of (4.114) is always positive if

$$\frac{b\pi^2}{2(b-1)^2} - \frac{(b^2 + 1)}{b^3} > 0, \quad (4.115)$$

which is equivalent to $0.501172 < b < 1$. Comparing this condition with (4.106), we see that the defect-free state is always the global minimizer of the Landau-de Gennes

energy if $b \in (0.501172, 1)$.

We have shown the defect-free state is the global minima within a narrow annulus, and is locally stable in the limit as $\varepsilon^2 \rightarrow 0$. However, in this limit, work on the Ginzburg-Landau theory within annuli with prescribed degree on the boundary predicts the existence of vortices approaching the walls of the annulus [110, 111, 112]. In the following section, we consider such structures in the Oseen-Frank model.

4.4 Nematic Equilibria with Boundary Defects

In this section, we identify and study nematic equilibria on the annular domain Ω with defects on the boundary. Equilibria with boundary defects are identified in the experiments presented in Figure 4.2; these states feature 1, 2 or 3 defects of strength $+\frac{1}{2}$ on the outer wall and an equivalent number of $-\frac{1}{2}$ strength defects on the inner wall. This induces a director field with rotational symmetry of order 1, 2 or 3 respectively. Our analysis in §4.2 shows that if the defect-free state loses stability, the new equilibrium retains its rotational symmetry except under some very small range of values of $\alpha < 1$. Furthermore, this loss of stability requires the elastic constants $K_3 > K_1$, but the *fd*-virus used in the experiments has approximately equal elastic constants [79]. This suggests that states with boundary defects do not spontaneously arise from the instability of the defect-free state, and instead there must be a distinct class of equilibria with boundary defects. We classify these equilibria in terms of the arrangements of defects, and evaluate their director fields and energies using analytic and numerical methods.

4.4.1 Classification of Equilibria with Boundary Defects

In the strong anchoring limit, the angle of the director is constrained to take the values $\theta = \phi \pm \frac{\pi}{2}$ on $\partial\Omega$. For the director to satisfy these conditions, the director

field must rotate by a factor of $n\pi$ (with $n \in \mathbb{N}$) about any boundary defect, and so all boundary defects must be of half integer strength. Here, we consider the lowest energy equilibria with boundary defects of strength $\pm\frac{1}{2}$ and no internal defects.

The Euler characteristic of an annulus Ω is $\chi = 0$, thus the sum of defect strengths must be equal to zero (see Equation (1.35)). We consider equilibria with boundary defects which have N defects of strength $+\frac{1}{2}$ and N defects of strength $-\frac{1}{2}$, where N is some positive integer. Defects of opposing sign strength will exert an attractive force on each other and defects of the same sign will exert a repulsive force [1]. Therefore, we begin by assuming that equilibria have defects spaced at equidistant positions on $\partial\Omega$. To minimize the distortion to the director, we assume that there are N defects on each boundary and that every defect on the boundary at $r = b$ is connected to a defect on the boundary at $r = 1$ by a radial line centred at $(0, 0)$. Without loss of generality, the defects are located on the lines $\phi = 0, \phi = \frac{2\pi}{N}, \dots, \phi = \frac{2\pi(N-1)}{N}$. Thus, it suffices to consider the annular sector

$$\Omega_N = \left\{ (r, \phi) \in \mathbb{R}^2 : b \leq r \leq 1, 0 \leq \phi \leq \frac{2\pi}{N} \right\}, \quad (4.116)$$

and construct solutions for θ in Ω_N . In the strong anchoring limit, $\theta = \phi \pm \frac{\pi}{2}$ on the edges at $r = b$ and $r = 1$. On the straight edges of Ω_N , we assume that θ is tangent to the edges, so $\theta \in \{-\pi, 0, \pi\}$ on $\phi = 0$ and $\theta \in \{\frac{2\pi}{N} - \pi, \frac{2\pi}{N}, \frac{2\pi}{N} + \pi\}$ on $\phi = \frac{2\pi}{N}$. Any director field with θ non-tangent to these edges would be expected to have a higher energy than a state with θ tangent to these internal edges.

By considering the arrangement of defects in the corners of Ω_N , we identify four distinct states, shown in Figure 4.7. Three of these states correspond to generalizations of the rotated state found in square and rectangular wells, denoted U_1 , U_2 and U_3 , where the director field connects two $+\frac{1}{4}$ strength defects along an edge. The fourth state is a generalization of the diagonal state, denoted D , where the director

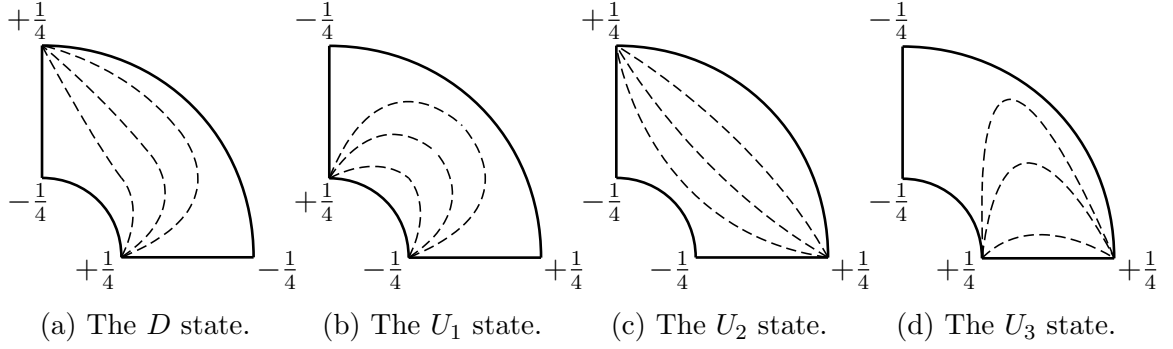


Figure 4.7: The four possible states within a sector Ω_N , with defect strength and sketches of the director field.

connects two $+\frac{1}{4}$ strength defects located on opposite corners of Ω_N .

Any equilibrium with $2N$ regularly spaced boundary defects of strength $\pm\frac{1}{2}$ can be described by dividing Ω into N equal segments, and placing one of states $\{D, U_1, U_2, U_3\}$ within each segment. The choice of state within each sector is subject to the constraint that defects of strength $+\frac{1}{4}$ and $-\frac{1}{4}$ from adjoining sectors cannot coexist at the same point. When considering the whole annulus, we restrict our attention to states composed exclusively of one sector solution, which we denote $D^{(N)}$, $U_1^{(N)}$, $U_2^{(N)}$, $U_3^{(N)}$ respectively. For odd values of N , only the $U_1^{(N)}$ and $U_2^{(N)}$ states are valid solutions. The experimentally observed states in Figure 4.2 correspond to the $U_2^{(1)}$, $U_2^{(2)}$ and $U_2^{(3)}$ states.

4.4.2 Equal Elastic Constants with Strong Anchoring

Using the one constant approximation and strong anchoring, we derive expressions for the director fields and the Oseen-Frank energy of the four sector solutions following the method discussed in §2.2. We consider the general problem

$$\nabla^2\theta = 0, \tag{4.117}$$

subject to the boundary conditions $\theta(r, 0) = 0$, $\theta(1, \phi) \in \{\phi \pm \frac{\pi}{2}\}$, $\theta(b, \phi) \in \{\phi \pm \frac{\pi}{2}\}$, and $\theta(r, 2\pi/N) \in \{\frac{2\pi}{N}, \frac{2\pi}{N} + \pi, \frac{2\pi}{N} - \pi\}$.

Any admissible θ subject to these Dirichlet boundary conditions can be expressed as a linear combination

$$\theta = a_0\phi + a_1f_1 + a_2f_2 + a_3f_3 + a_4f_4, \quad (4.118)$$

where the functions f_i are solutions of the Laplace equation with boundary conditions:

$$f_1(r, 0) = f_1(r, 2\pi/N) = 0, \quad f_1(b, \phi) = 0, \quad f_1(1, \phi) = 1, \quad (4.119)$$

$$f_2(r, 0) = f_2(r, 2\pi/N) = 0, \quad f_2(b, \phi) = 0, \quad f_2(1, \phi) = \phi, \quad (4.120)$$

$$f_3(r, 0) = f_3(r, 2\pi/N) = 0, \quad f_3(b, \phi) = 1, \quad f_3(1, \phi) = 0, \quad (4.121)$$

$$f_4(r, 0) = f_4(r, 2\pi/N) = 0, \quad f_4(b, \phi) = \phi, \quad f_4(1, \phi) = 0. \quad (4.122)$$

The coefficients a_i corresponding to the four sector solutions are given in Table 4.1.

State	a_0	a_1	a_2	a_3	a_4
D	1	$\frac{\pi}{2}$	0	$\frac{\pi}{2}$	0
U_1	$1 + \frac{N}{2}$	$\frac{\pi}{2}$	$-\frac{N}{2}$	$\frac{\pi}{2}$	$-\frac{N}{2}$
U_2	$1 - \frac{N}{2}$	$-\frac{\pi}{2}$	$\frac{N}{2}$	$-\frac{\pi}{2}$	$\frac{N}{2}$
U_3	1	$-\frac{\pi}{2}$	0	$\frac{\pi}{2}$	0

Table 4.1: Values of the coefficients a_i for the four sector solutions within Ω_N .

Using separation of variables, we compute the functions f_i to be

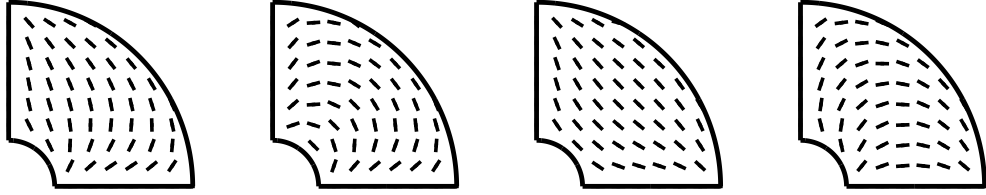
$$f_1(r, \phi) = \sum_{n=1}^{\infty} \frac{4 \sin\left(\frac{(2n-1)N\phi}{2}\right)}{(2n-1)\pi} \left(\frac{r^{-\frac{(2n-1)N}{2}} - b^{-(2n-1)N} r^{\frac{(2n-1)N}{2}}}{1 - b^{-(2n-1)N}} \right), \quad (4.123)$$

$$f_2(r, \phi) = \sum_{n=1}^{\infty} \frac{4(-1)^{n+1} \sin\left(\frac{Nn\phi}{2}\right)}{Nn} \left(\frac{r^{-\frac{nN}{2}} - b^{-nN} r^{\frac{nN}{2}}}{1 - b^{-nN}} \right), \quad (4.124)$$

$$f_3(r, \phi) = \sum_{n=1}^{\infty} \frac{4 \sin\left(\frac{(2n-1)N\phi}{2}\right)}{(2n-1)\pi} \left(\frac{r^{-\frac{(2n-1)N}{2}} - r^{\frac{(2n-1)N}{2}}}{b^{-\frac{(2n-1)N}{2}} - b^{\frac{(2n-1)N}{2}}} \right), \quad (4.125)$$

$$f_4(r, \phi) = \sum_{n=1}^{\infty} \frac{4(-1)^{n+1} \sin\left(\frac{Nn\phi}{2}\right)}{Nn} \left(\frac{r^{-\frac{nN}{2}} - r^{\frac{nN}{2}}}{b^{-\frac{nN}{2}} - b^{\frac{nN}{2}}} \right). \quad (4.126)$$

Some sample director plots using these functions are shown in Figure 4.8 for $N = 4$ and $b = 0.25$.



(a) The D state. (b) The U_1 state. (c) The U_2 state. (d) The U_3 state.

Figure 4.8: The director field of the four states within Ω_4 and $b = 0.25$ in the one-constant approximation.

We now evaluate the energy following the procedure discussed in §2.2.2. We regularize the sector Ω_N by removing quadrants of radius $0 < \epsilon \ll \min\{b, 1-b\}$ from each of the corners and denote the regularized domain as $\Omega_{N\epsilon}$. We use Green's First Identity [82] to express the energy as the sum of line integrals

$$E[\theta] = \sum_{i=1}^4 \frac{K}{2} \int_{C_i} \theta \frac{\partial \theta}{\partial v} ds + \frac{K}{2} \int_{\gamma_i} \theta \frac{\partial \theta}{\partial v} ds, \quad (4.127)$$

where the edges C_i and γ_i are defined in Figure 4.9.

The contributions from the edges γ_i are all of order ϵ . Unlike the rectangular

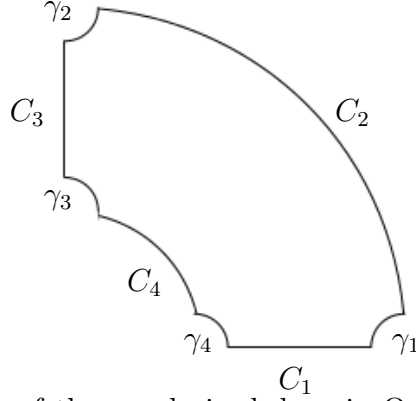


Figure 4.9: The boundary of the regularized domain $\Omega_{N\epsilon}$, expressed terms of edges C_i and γ_i .

domain, where the equivalent terms are all order ϵ^2 , the curvature of the edges C_2 and C_4 induces order ϵ terms. We list the order ϵ terms from the integrals about the arcs γ_i in Appendix D. The contributions to the energy from the edges C_i are

$$\int_{C_1} \theta \frac{\partial \theta}{\partial v} ds = 0, \quad (4.128)$$

$$\int_{C_2} \theta \frac{\partial \theta}{\partial v} ds = \sum_{i=1}^4 a_i \int_{C_2} \phi \frac{\partial f_i}{\partial v} ds + \sum_{i=1}^4 a_1 a_i \int_{C_2} \frac{\partial f_i}{\partial v} ds, \quad (4.129)$$

$$\int_{C_3} \theta \frac{\partial \theta}{\partial v} ds = \frac{2\pi}{N} a_0^2 \ln \left(\frac{1-\epsilon}{b+\epsilon} \right) + \sum_{i=1}^4 \frac{2\pi}{N} a_0 a_i \int_{C_3} \frac{\partial f_i}{\partial v} ds, \quad (4.130)$$

$$\int_{C_4} \theta \frac{\partial \theta}{\partial v} ds = \sum_{i=1}^4 a_i \int_{C_4} \phi \frac{\partial f_i}{\partial v} ds + \sum_{i=1}^4 a_2 a_i \int_{C_4} \frac{\partial f_i}{\partial v} ds. \quad (4.131)$$

We evaluate each of these line integrals and derive asymptotic approximations in the limit as $\epsilon \rightarrow 0$, listed in Appendix D. Similarly to our work on the rectangular wells in §2.2.2, the leading order terms of these integrals can be expressed as linear combination of $\ln \left(\frac{1}{\epsilon} \right)$, which arises from the discontinuities in f_i on the boundary,

and series defined as follows:

$$s_1(N, b) := 8 \sum_{n=1}^{\infty} \frac{\coth\left(\frac{N}{2}(2n-1)\ln b\right) + 1}{2n-1}, \quad (4.132)$$

$$s_2(N, b) := 8 \sum_{n=1}^{\infty} \frac{\operatorname{csch}\left(\frac{N}{2}(2n-1)\ln b\right)}{2n-1}, \quad (4.133)$$

$$s_3(N, b) := 8 \sum_{n=1}^{\infty} \frac{\coth\left(\frac{N}{2}n\ln b\right) + 1}{n}, \quad (4.134)$$

$$s_4(N, b) := 8 \sum_{n=1}^{\infty} \frac{\operatorname{csch}\left(\frac{N}{2}n\ln b\right)}{n}. \quad (4.135)$$

In the limit as $\epsilon \rightarrow 0$, the regularized energies within the sector $\Omega_{N\epsilon}$ are given by

$$E \sim K\pi \left(\ln\left(\frac{1}{\epsilon}\right) + \tilde{E} \right) + O(\epsilon), \quad (4.136)$$

where normalized energies of the four states, $\tilde{E}$, are:

$$\begin{aligned} \tilde{E}_{U_1}(N, b) &= \frac{s_1(N, b) + s_4(N, b) - s_2(N, b) - s_3(N, b)}{4} \\ &\quad + \frac{(N+2)^2}{4N} \ln\left(\frac{1}{b}\right) + \frac{1}{2} \ln\left(\frac{b}{N^2}\right), \end{aligned} \quad (4.137)$$

$$\begin{aligned} \tilde{E}_{U_2}(N, b) &= \frac{s_1(N, b) + s_4(N, b) - s_2(N, b) - s_3(N, b)}{4} \\ &\quad + \frac{(N-2)^2}{4N} \ln\left(\frac{1}{b}\right) + \frac{1}{2} \ln\left(\frac{b}{N^2}\right), \end{aligned} \quad (4.138)$$

$$\tilde{E}_{U_3}(N, b) = -\frac{s_1(N, b) + s_2(N, b)}{4} + \frac{1}{N} \ln\left(\frac{1}{b}\right) + \frac{1}{2} \ln\left(\frac{16b}{N^2}\right), \quad (4.139)$$

$$\tilde{E}_D(N, b) = \frac{s_2(N, b) - s_1(N, b)}{4} + \frac{1}{N} \ln\left(\frac{1}{b}\right) + \frac{1}{2} \ln\left(\frac{16b}{N^2}\right). \quad (4.140)$$

In Figure 4.10, we plot the normalized energies of the four states as a function of N for some fixed values of b . For small values of N , the U_2 state is the minimum energy state in the set $\{D, U_1, U_2, U_3\}$. This differs from the rectangular wells, where we found that the diagonal state is the global minimizer. By examining the director fields for small values of N , such as those shown in Figure 4.8, we see that the director

of the U_2 state features less distortion than the other three states. Furthermore, we see that for $N > 1$ and small b , the U_2 state features a large region within Ω_N for which the director is approximately constant. As N increases, there is a crossover in the energy minimizing state from the U_2 state to the D state. In the limit as $N \rightarrow \infty$, the sector Ω_N approaches the profile of a narrow rectangle, and we find that the diagonal state is the global minimizer, with the next lowest energy state being the U_3 state, recovering the behaviour identified within rectangular wells in §2.2.3.

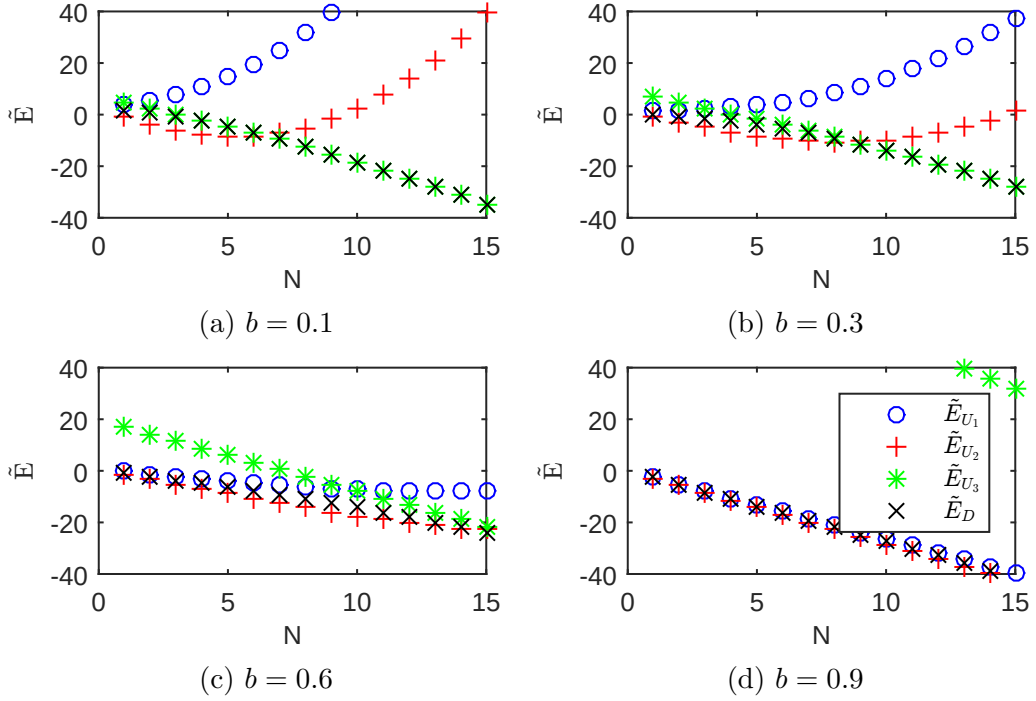


Figure 4.10: The normalized energy of the four states within Ω_N plotted against N , for fixed values of b .

The total energy within the annulus Ω will be

$$E \sim KN\pi \left(\ln \left(\frac{1}{\epsilon} \right) + \tilde{E} \right), \quad (4.141)$$

and we therefore see that states with large numbers of defects will be energetically unfavourable. Due to the contribution of the $N \log(1/\epsilon)$ term from the defects, the defect-free state will be the lowest energy state within Ω , except in the limit where

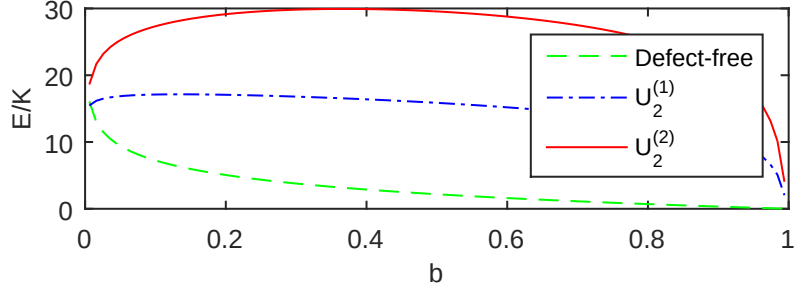
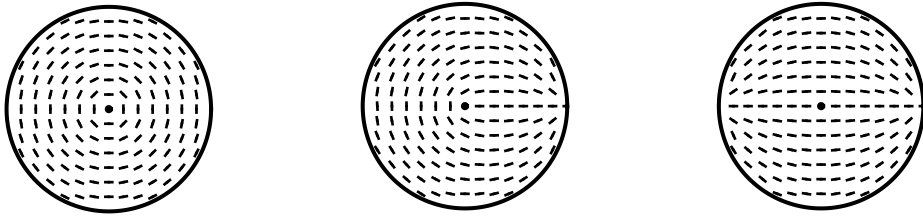


Figure 4.11: The regularized one-constant Oseen-Frank energy of the three lowest energy states; the defect-free state, the $U_2^{(1)}$ state and the $U_2^{(2)}$ state, for defect core size $\epsilon = 0.002$.

$b = O(\epsilon)$, as shown in Figure 4.11. Furthermore, we see that the $U_2^{(1)}$ state always has lower energy than the $U_2^{(2)}$ state except in the limit as where $b = O(\epsilon)$.

In the limit where $b = O(\epsilon)$, the defect-free state approaches the vortex type solution found in a disk (Figure 4.12a), the $U_2^{(1)}$ state approaches a state with a $+\frac{1}{2}$ strength defect on the boundary and a $+\frac{1}{2}$ strength defect at the origin (Figure 4.12b), and the $U_2^{(2)}$ state approaches an equilibrium with two $+\frac{1}{2}$ defects on the boundary (Figure 4.12c). In this limit, our asymptotic approximation (4.141) to the energy ceases to be valid, but from work on liquid crystal confined to disks, [113], we know that the $U_2^{(2)}$ state is the global minimizer.



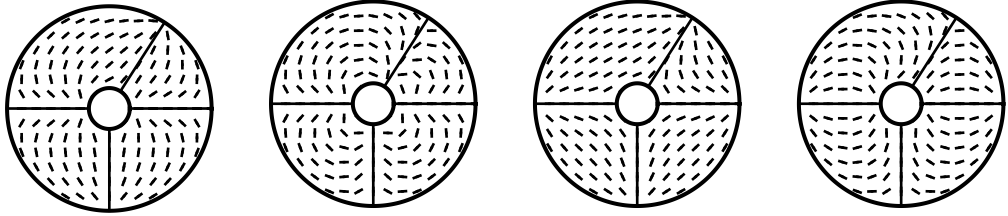
(a) The defect-free state. (b) The $U_2^{(1)}$ state. (c) The $U_2^{(2)}$ state.

Figure 4.12: Director fields of the three lowest energy states for $b = 0.02$.

Our expressions for the director and Oseen-Frank energy can be generalized to sectors with arbitrary central angle Φ ,

$$\Omega_\Phi = \{(r, \phi) \in \mathbb{R}^2 : b \leq r \leq 1, 0 \leq \phi \leq \Phi\}, \quad (4.142)$$

by making the substitution $N = \frac{2\pi}{\Phi}$. Using these modified expressions, we investigate the stability of the $D^{(N)}$, $U_1^{(N)}$, $U_2^{(N)}$ and $U_3^{(N)}$ states under perturbations which break the N -fold symmetry of the defect arrangement. We consider the $D^{(N)}$, $U_1^{(N)}$, $U_2^{(N)}$ and $U_3^{(N)}$ states, modified by moving the defects on the radial line $\phi = \frac{2\pi}{N}$ to the line $\phi = \Phi$, where $\Phi \in (0, \frac{4\pi}{N})$ and $N \geq 2$. In Figure 4.13, we show the examples of the director fields of the four states with $N = 4$, and the defects on the line $\phi = \frac{2\pi}{N}$ moved to the line $\phi = 1$.



(a) The $D^{(4)}$ state. (b) The $U_1^{(4)}$ state. (c) The $U_2^{(4)}$ state. (d) The $U_3^{(4)}$ state.

Figure 4.13: Director fields of the four modified states, with $\Phi = 1$, $b = 0.25$ and $N = 4$.

The contribution to the energy from the number of defects remains the same, so it is sufficient to consider the total normalized energy. For $j \in \{D, U_1, U_2, U_3\}$, the total normalized energy of these modified states is

$$\hat{E}_j = \tilde{E}_j\left(\frac{2\pi}{\Phi}, b\right) + \tilde{E}_j\left(\frac{2\pi}{\frac{4\pi}{N} - \Phi}, b\right) + (N - 2)\tilde{E}_j(N, b). \quad (4.143)$$

This corresponds to the normalized energy for $(N - 2)$ sectors Ω_N , and the normalized energy for sectors Ω_Φ and $\Omega_{\frac{4\pi}{N} - \Phi}$.

For all $j \in \{D, U_1, U_2, U_3\}$,

$$\left. \frac{d\hat{E}_j}{d\Phi} \right|_{\Phi = \frac{2\pi}{N}} = 0, \quad (4.144)$$

so the symmetric arrangement of defects is a critical point of the normalized energy.

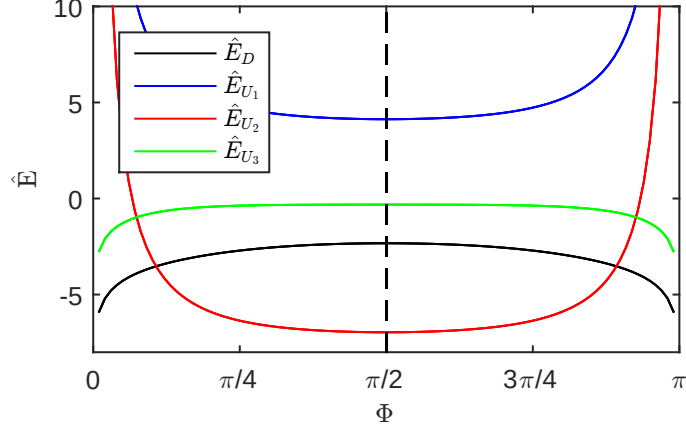


Figure 4.14: Normalized energy of the modified states in terms of Φ , with $b = 0.25$ and $N = 4$.

Numerical inspection of the normalized energy shows that this critical point is the global maximum of $\hat{E}_D$ and $\hat{E}_{U_3}$ and the global minimum of $\hat{E}_{U_1}$ and $\hat{E}_{U_2}$, for example see Figure 4.14. Therefore, the $D^{(N)}$ and $U_3^{(N)}$ states are unstable equilibria, as a perturbation which breaks the N -fold symmetry of the defect configuration will lower the total regularized energy. This behaviour arises due to the competing attractive forces between the $+\frac{1}{2}$ and $-\frac{1}{2}$ strength boundary defects on each boundary. In contrast, the $U_1^{(N)}$ and $U_2^{(N)}$ states are stable under these perturbations, as the repulsive forces from the boundary defects of the same sign strength enforces a symmetry alignment.

We note that these are not the only possible perturbations, and one obvious question concerns what would happen if the boundary defects are allowed to move into the interior on the annulus. Studying this behaviour would best be carried out using a Ginzburg-Landau model instead of the Oseen-Frank model considered here. In the following two sections, we identify two parameter regimes in the Oseen-Frank theory which can allow equilibria with boundary defects to have lower energy than the defect-free state.

4.4.3 Unequal Elastic Constants with Strong Anchoring

A sector based approach can be used to consider the effects of unequal elastic constants on the director and energies of the four states identified within a sector Ω_N . Using COMSOL, we solve Equation (4.3) on Ω_N subject to tangent Dirichlet boundary conditions and evaluate the associated regularized energies.

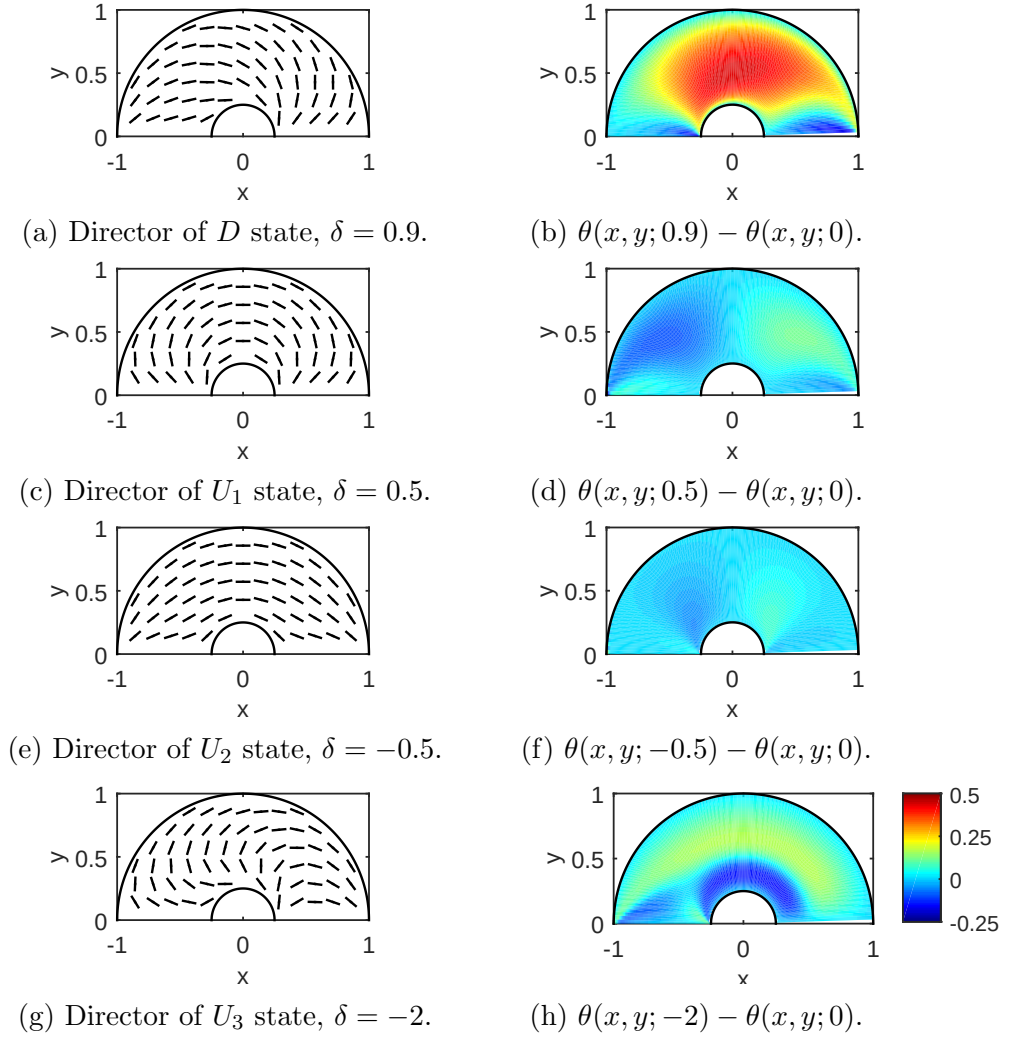


Figure 4.15: Sample sector director fields within Ω_2 with unequal elastic constants, and the difference between the computed solution for $\theta(x, y; \delta)$ and the one-constant solution $\theta(x, y; 0)$ in radians.

In Figure 4.15, we plot some of the computed director fields and the structural difference between the computed θ and the analytic one-constant solutions. As ex-

pected, the overall structure of the director of each of the sector solutions remains the same as the one-constant analytic solutions. For $\delta > 0$, we see increased regions of energetically preferable splay distortions to the director, and similarly for $\delta < 0$, we see larger regions of bend distortions.

Evaluating the Oseen-Frank energies, we find that the U_2 state remains the energy minimum in the set $\{D, U_1, U_2, U_3\}$ for small values of N . Using COMSOL to evaluate the energies of $U_2^{(1)}$ and $U_2^{(2)}$ states for a range of δ and b , we are able to build up a phase diagram showing the state with minimum energy for given δ and b . The phase diagram, shown in Figure 4.16, indicates that for small b and δ close 1, the $U_2^{(1)}$ and $U_2^{(2)}$ states can have lower energy than both the radially invariant defect-free state and the defect-free spiral state identified in §4.2.1. The precise value of δ and b for which the $U_2^{(1)}$ and $U_2^{(2)}$ states become global minimizers is dependent on the defect core size. We note that, similarly to the one-constant case, there will be an energy associated with the core of each of the defects which will also affect this transition line.

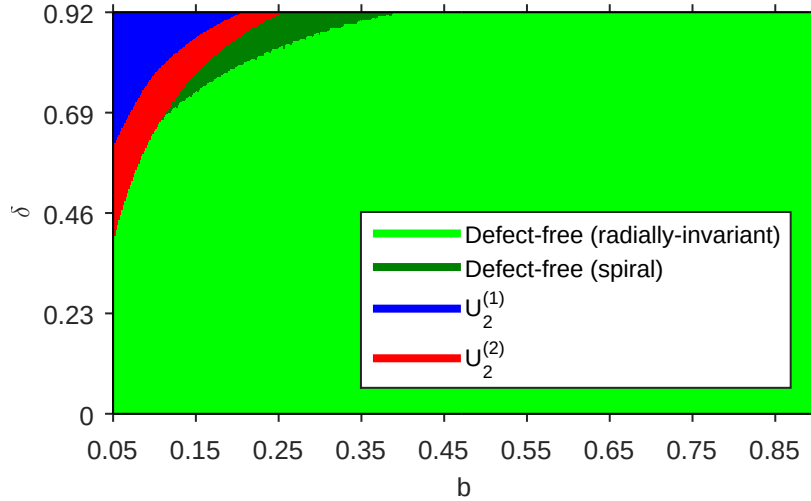


Figure 4.16: The parameter regions in the space (b, δ) which contain the minima of the regularized energies of the defect-free state, the spiral solution, the $U_2^{(1)}$ state and the $U_2^{(2)}$ state, with defect core size $\epsilon = 0.01$.

4.4.4 Equal Elastic Constants with Weak Anchoring

A second possible phenomenon which might stabilize boundary defects is the inclusion of weak anchoring effects. We consider the annular sector Ω_N , with weak anchoring on the edges at $r = b, 1$ and strong tangential anchoring on the edges at $\phi = 0, 2\pi/N$. Solutions equivalent to the U_2 state with strong anchoring are solutions of $\nabla^2\theta = 0$ subject to the boundary conditions

$$\frac{\partial\theta}{\partial\mathbf{v}} + \frac{\alpha}{2} \sin(2\theta - 2\theta_0) = 0 \quad \text{on } r = b, 1, \quad (4.145)$$

and $\theta = 0$ on $\phi = 0$ and $\theta = \frac{2\pi}{N} - \pi$ on $\phi = \frac{2\pi}{N}$. To investigate the effects of weak anchoring of the relative energies of the U_2 states and the defect-free state, we use COMSOL to solve the Laplace equation with boundary conditions (4.145) and evaluate the corresponding energy for given α and b .

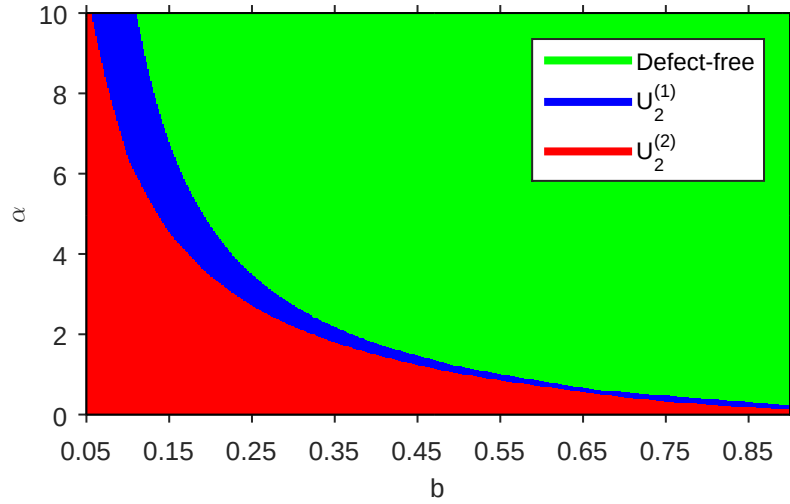


Figure 4.17: The parameter regions in the space (b, α) which contain the minima of the energies of the defect-free state, the $U_2^{(1)}$ state and the $U_2^{(2)}$ state.

In Figure 4.17, we plot a phase diagram which shows the values of b and α for which the energy is minimized by either the defect-free state, the $U_2^{(1)}$ state or the $U_2^{(2)}$ state. For large anchoring strengths, the defect-free state is energetically preferable unless b is extremely small. As the surface anchoring becomes weaker, states with

boundary defects become energetically preferable, even at relatively large values of the radius ratio b . Furthermore, the $U_2^{(1)}$ state is only energetically preferable to the $U_2^{(2)}$ state for a narrow region of the parameters shown in Figure 4.17, which is consistent with the experimental work on the *fd*-virus.

4.5 Summary

In this chapter, we have studied some problems related to nematic equilibria confined within two-dimensional annular domains with tangential anchoring using the Oseen-Frank and Landau-de Gennes theory.

We compute criteria for the stability of the defect-free state. We demonstrate that with both strong and weak anchoring, the defect-free state undergoes a supercritical bifurcation. We describe a spiral-like defect-free state, and show that this state is locally stable in the limit as $\delta \rightarrow 1$. We also show that the defect-free state is locally stable with respect to radial symmetry breaking perturbations, except when $\alpha = \frac{WR_{\text{outer}}}{K_3} < 1$.

Using the Landau-de Gennes theory, we derive two results on the stability of defect-free state. By adapting a result for the stability of radial critical points of the Ginzburg-Landau energy within a disk, we show that the defect-free state is locally stable in the low temperature limit ($\varepsilon^2 \rightarrow 0$). We then derive a condition on the global minimality of the defect-free state, independent of the parameter ε^2 .

We identify a number of possible equilibria with boundary defects in the Oseen-Frank theory. By considering the behaviour on a sector with the one-constant approximation, we derive expressions for the director field and Oseen-Frank energies. We show that the lowest energy equilibrium is the state with $+\frac{1}{2}$ defects on the outer boundary and $-\frac{1}{2}$ defects on the inner boundary. Equilibria with defects of both strengths on the same wall are always unstable due to the competing attractive and

repulsive forces acting on the defects. Our analytic estimates do not fully capture the behaviour of the experiments system and we discuss some possible parameter regimes which might explain this difference. For nematic liquid crystals with elastic constants $K_3 \gg K_1$, equilibria with boundary defects can have lower energy than the radially invariant defect-free state or the spiral-like defect-free state. The precise critical value of the ratio of $\frac{K_1}{K_3}$ is dependent on the defect core size ϵ . We also consider the effects of weak anchoring and suggest that this could allow for the formation of boundary defects. We believe that is it weak anchoring effects that allow for the formation of the equilibria found experimentally. The existence of multiple states with different numbers of boundary defects suggests that there are multiple stable equilibria, and it would be interesting to numerically study the range of local stability of these states.

Chapter 5

The Radial Hedgehog Defect in the Sixth Order Bulk Potential

5.1 Introduction

5.1.1 The Radial Hedgehog Defect

Three-dimensional spherical droplets with strong homeotropic anchoring have been extensively used as a prototype system to model the fine structure and stability of liquid crystal point defects without the effects of distortion from other defects or boundary conditions [119, 64, 120]. Using such a geometry, two competing defect structures have been identified in the Landau-de Gennes theory with a fourth order bulk potential; the radial hedgehog and the biaxial torus.

The structure of the radial hedgehog defect is described in [63], and closely resembles the point defect solution in the Oseen-Frank theory. In the nematic regime, the one-constant Landau-de Gennes energy with a fourth order bulk potential,

$$E[\mathbf{Q}] = \iiint_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + \frac{A}{2} \text{tr} \mathbf{Q}^2 + \frac{B}{3} \text{tr} \mathbf{Q}^3 + \frac{C}{4} (\text{tr} \mathbf{Q}^2)^2 \, d\Omega, \quad (5.1)$$

has a critical point of form

$$\mathbf{Q} = \sqrt{\frac{3}{2}} s(r) \left(\hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{\mathbf{I}_3}{3} \right), \quad (5.2)$$

where s is the solution to the differential equation

$$s'' + \frac{2s'}{r} - \frac{6s}{r^2} = -ts - 3s^2 + 2s^3, \quad (5.3)$$

and $t := \frac{27AC}{B^2}$ is the rescaled temperature [121]. On the boundary of a droplet with radius R , s satisfies $s(R) = \frac{3+\sqrt{9+8t}}{4}$ or, in the limiting case, $s(\infty) = \frac{3+\sqrt{9+8t}}{4}$ [122]. The director is aligned in the radial direction $\hat{\mathbf{r}}$ centred at the origin of droplet, as depicted in Figure 5.1a. The order parameter is zero at the origin and positive everywhere else, so the radial hedgehog is uniaxial except at the isotropic point at the origin. Solutions to Equation (5.3) are monotonically increasing [121] for $t > -1$, satisfy some upper and lower bounds [122] and are unique in several parameter regimes; including in the limit as $R \rightarrow \infty$ [123], in the limit as R and $t \rightarrow \infty$, and, more generally, for any finite $t > 0$ and finite R [121].

In [124], the authors showed that the radial hedgehog defect is not the global minimizer of the Landau-de Gennes energy in an infinite domain by constructing a lower energy solution with a ring disclination about the origin. Further numerical studies [64, 65, 120, 125, 126] and analytic work [122, 119] showed that the radial hedgehog is only stable for small droplets and temperatures close to the isotropic-nematic transition temperature, and described an alternative state referred to as the biaxial torus. The biaxial torus defect features uniaxial alignment along a single axis of symmetry through the origin, which is encircled by a disclination loop of strength $+\frac{1}{2}$. The disclination loop is surrounded by a torus-shaped region of biaxiality where the director rotates from alignment along the axis of symmetry to a radial alignment on the boundary [64], as shown in Figure 5.1b.

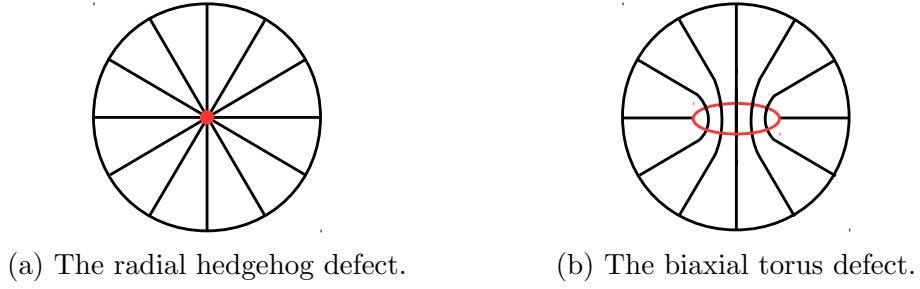


Figure 5.1: Sketches of the director field for radial hedgehog and biaxial torus defects, with defects shown in red.

5.1.2 Chapter Outline

As discussed above, the properties and stability of the radial hedgehog defect have been studied extensively using a fourth order bulk potential. In this chapter, we carry out the first investigation of the radial hedgehog defect using the sixth order bulk potential

$$\begin{aligned}
 f_B(\mathbf{Q}) = & \frac{A}{2}\text{tr}\mathbf{Q}^2 + \frac{B}{3}\text{tr}\mathbf{Q}^3 + \frac{C}{4}(\text{tr}\mathbf{Q}^2)^2 + \frac{D}{5}(\text{tr}\mathbf{Q}^2)(\text{tr}\mathbf{Q}^3) \\
 & + \frac{E}{6}(\text{tr}\mathbf{Q}^2)^3 + (F - E)(\text{tr}\mathbf{Q}^3)^2.
 \end{aligned} \tag{5.4}$$

This expansion is simplest form of the bulk potential which allows for biaxial critical points, although is only applicable to systems comprised of uniaxial molecules. Modelling of systems of biaxial molecules in the Landau-de Gennes framework requires a second tensor to account for the ordering of the short axes, and hence the Taylor expansion of the bulk potential contains coupling terms between the two tensors [127, 128]

In this chapter, we study the radial hedgehog defect using the sixth order bulk potential given in Equation (5.4). The choice of this potential allows us to more fully explore the behaviour of point defects in liquid crystals comprised of uniaxial molecules. In particular, this sixth order bulk potential allows us to control the effects of biaxiality on these systems via the parameters E and F , in contrast, the

more commonly used fourth order bulk potential allows for no such control over the formation of biaxial regions. This has particular relevance to the stability of the radial hedgehog, which, using the fourth order bulk potential, is the driving force behind the loss of stability and the formation of the biaxial torus defect.

This chapter is arranged as follows. In §5.2, we introduce the sixth order bulk potential and discuss some qualitative properties of the critical points of the bulk potential. In §5.3, we prove that the radial hedgehog defect is a critical point of the Landau-de Gennes energy with a sixth order bulk potential. We then show that the order parameter satisfies many of the properties identified using the fourth order bulk potential, subject to some constraints on the coefficients of the potential.

Finally, we investigate the local stability of the radial hedgehog in §5.4. We prove that the radial hedgehog is locally stable for small droplet size and temperatures close to the critical temperature at which the isotropic phase loses stability. To show that the radial hedgehog loses stability, we consider two classes of perturbations. We identify three parameter regimes governing the instability of the radial hedgehog, based on the ratio of the sixth order coefficients, and discuss the physical relevance of these regimes.

5.2 The Sixth Order Bulk Potential

The study of biaxial nematic phases is an active area of research in soft-matter physics, particularly in the design of new biaxial molecules (see the review articles in [129, 130, 131]). In a continuum framework, the Landau-de Gennes theory with a sixth order bulk potential is the simplest model for describing biaxial and uniaxial phases and studying phase transitions [36].

The sixth order bulk potential is the smallest order truncation of the Taylor expansion of bulk potential which allows for biaxial critical points [1, 132, 133]. The

sixth order bulk potential allows four possible phases: the isotropic phase (I), the biaxial phase (B), a uniaxial phase with positive order parameter (U_+), and a uniaxial phase with negative order parameter (U_-). In this chapter, we work with the most general form of the sixth order potential, namely

$$f_B(\mathbf{Q}) = \frac{A}{2}\text{tr}\mathbf{Q}^2 + \frac{B}{3}\text{tr}\mathbf{Q}^3 + \frac{C}{4}(\text{tr}\mathbf{Q}^2)^2 + \frac{D}{5}(\text{tr}\mathbf{Q}^2)(\text{tr}\mathbf{Q}^3) + \frac{E}{6}(\text{tr}\mathbf{Q}^2)^3 + (F - E)(\text{tr}\mathbf{Q}^3)^2. \quad (5.5)$$

A comprehensive study of the possible phases, their relative stability and the types of transitions using the sixth order bulk potential (5.5) is given in [36, 134, 135].

There are several possible simplifications of (5.5). In [132, 133], the authors show that the simplest bulk potential which allows for stable biaxial and uniaxial phases has the form

$$f_B(\mathbf{Q}) = \frac{A}{2}\text{tr}\mathbf{Q}^2 + \frac{B}{3}\text{tr}\mathbf{Q}^3 + \frac{C}{4}(\text{tr}\mathbf{Q}^2)^2 + \frac{F}{6}(\text{tr}\mathbf{Q}^3)^2. \quad (5.6)$$

By considering the A - B plane with fixed $C > 0$ and $F > 0$, the authors identify a first order isotropic-uniaxial transition and a second order uniaxial-biaxial transition.

A more complex potential of the form

$$f_B(\mathbf{Q}) = \frac{A}{2}\text{tr}\mathbf{Q}^2 + \frac{B}{3}\text{tr}\mathbf{Q}^3 + \frac{C}{4}(\text{tr}\mathbf{Q}^2)^2 + \frac{D}{5}(\text{tr}\mathbf{Q}^2)(\text{tr}\mathbf{Q}^3) + \frac{F}{6}(\text{tr}\mathbf{Q}^3)^2 \quad (5.7)$$

is discussed in [1]. For potentials of this form, a biaxial phase can occur if the coefficients satisfy $25CF > 6D^2$ and $A < 0$.

5.2.1 Non-dimensionalization

We define a rescaling of the Landau-de Gennes energy which we will use in the remainder of this chapter. We work with the one-constant approximation, so the

energy functional is

$$E[\mathbf{Q}] = \iiint_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + F_0 + \frac{A}{2} \text{tr} \mathbf{Q}^2 + \frac{B}{3} \text{tr} \mathbf{Q}^3 + \frac{C}{4} (\text{tr} \mathbf{Q}^2)^2 + \frac{D}{5} (\text{tr} \mathbf{Q}^2)(\text{tr} \mathbf{Q}^3) + \frac{E}{6} (\text{tr} \mathbf{Q}^2)^3 + (F - E)(\text{tr} \mathbf{Q}^3)^2 \, d\Omega. \quad (5.8)$$

The constant coefficient $F_0 > 0$ is chosen so that the bulk potential is greater than or equal to zero for any admissible $\mathbf{Q}$ -tensor. As in the fourth order potential [13], we assume that only the second order coefficient A is temperature dependent, with a linear relationship of the form

$$A = \alpha(T - T^*). \quad (5.9)$$

Here, T^* is the temperature at which the isotropic phase loses stability and α is some positive coefficient. In this chapter we will work below this critical temperature, and so $A < 0$. We restrict the fifth order coefficient D to be strictly negative, which ensures that the U_+ phase will have lower energy than the U_- phase for $A \ll 0$ [36]. For work on the radial hedgehog, we also assume that $B < 0$ and $C > 0$. The bulk potential must have a finite global minimizer, therefore, both E and F must be positive.

We introduce non-dimensionalized variables $\tilde{\mathbf{Q}}$ and $\tilde{\mathbf{x}}$, defined to be $\tilde{\mathbf{Q}} = \frac{\mathbf{Q}}{q}$ and $\tilde{\mathbf{x}} = \frac{\mathbf{x}}{\xi}$. In terms of the non-dimensionalized variables, the Landau-de Gennes energy is

$$E[\mathbf{Q}] = \iiint_{\tilde{\Omega}} \frac{L\xi\hat{q}^2}{2} |\nabla \tilde{\mathbf{Q}}|^2 + F_0 + \frac{A\hat{q}^2\xi^3}{2} \text{tr} \tilde{\mathbf{Q}}^2 + \frac{B\hat{q}^3\xi^3}{3} \text{tr} \tilde{\mathbf{Q}}^3 + \frac{C\hat{q}^4\xi^3}{4} (\text{tr} \tilde{\mathbf{Q}})^2 - \frac{|D|\hat{q}^5\xi^3}{5} (\text{tr} \tilde{\mathbf{Q}}^2)(\text{tr} \tilde{\mathbf{Q}}^3) + \frac{E\hat{q}^6\xi^3}{6} (\text{tr} \tilde{\mathbf{Q}}^2)^3 + (F - E)\hat{q}^6\xi^3 (\text{tr} \tilde{\mathbf{Q}}^3)^2 \, d\tilde{\mathbf{x}}. \quad (5.10)$$

We match the coefficients of fifth order term with $F\hat{q}^6\xi^3$,

$$\hat{q} = \frac{|D|}{\sqrt{6F}}, \quad (5.11)$$

and match the coefficients of the gradient term with $F\hat{q}^6\xi^3$ to derive a lengthscale,

$$\xi = \frac{6\sqrt{LF^3}}{|D|^2}. \quad (5.12)$$

The lengthscale ξ is related to the fourth order nematic correlation length $\xi_4 := \sqrt{\frac{27CL}{B^2}}$ defined in [64], by the factor $\frac{1}{|D|^2}\sqrt{\frac{2B^2F^3}{9C}}$. Multiplying $E[\mathbf{Q}]$ by $\sqrt{\frac{F}{L^3}}$, the dimensionless Landau-de Gennes energy is

$$\begin{aligned} \tilde{E}[\tilde{\mathbf{Q}}] = \iiint_{\tilde{\Omega}} \frac{1}{2} |\nabla \tilde{\mathbf{Q}}|^2 + \tilde{F}_0 - \frac{t_1}{2} \text{tr} \tilde{\mathbf{Q}}^2 - \frac{\sqrt{6}t_2}{3} \text{tr} \tilde{\mathbf{Q}}^3 + \frac{t_3}{4} (\text{tr} \tilde{\mathbf{Q}}^2)^2 \\ - \frac{\sqrt{6}}{5} \text{tr} \tilde{\mathbf{Q}}^2 \text{tr} \tilde{\mathbf{Q}}^3 + \frac{t_4}{6} (\text{tr} \tilde{\mathbf{Q}}^2)^3 + (1 - t_4) (\text{tr} \tilde{\mathbf{Q}}^3)^2 d\tilde{\mathbf{x}}, \end{aligned} \quad (5.13)$$

where we define the coefficients

$$t_1 := -\frac{36AF^3}{D^4}, \quad t_2 := -\frac{6BF^2}{|D|^3}, \quad t_3 := \frac{6CF}{D^2}, \quad t_4 := \frac{E}{F}. \quad (5.14)$$

The coefficient t_1 is the sixth order version of the rescaled temperature t from the fourth order potential. At all points in our study of the radial hedgehog, the coefficients $t_i > 0$ (for $i = 1, \dots, 4$). In the remainder of this chapter, we drop the tilde and all results are expressed in dimensionless variables.

5.2.2 Critical Points of the Sixth Order Potential

The most general form of the $\mathbf{Q}$ -tensor is

$$\mathbf{Q} = \sqrt{\frac{3}{2}} s \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}_3}{3} \right) + \sqrt{\frac{3}{2}} p \left(\mathbf{m} \otimes \mathbf{m} - \frac{\mathbf{I}_3}{3} \right), \quad (5.15)$$

where $\mathbf{n}$ and $\mathbf{m}$ are orthonormal eigenvectors and the order parameters s and p satisfy the following relations [32],

$$0 \leq p \leq \frac{s}{2} \quad \text{or} \quad \frac{s}{2} \leq p \leq 0. \quad (5.16)$$

The bulk potential can be expressed in terms of the order parameters s and p , since

$$\text{tr} \mathbf{Q}^2 = s^2 - ps + p^2, \quad (5.17)$$

$$\sqrt{6} \text{tr} \mathbf{Q}^3 = s^3 - \frac{3}{2}(sp^2 + ps^2) + p^3. \quad (5.18)$$

Alternatively, we can express the bulk potential in two parameters q and β , which are defined in [36]. Here, q and β are related to the order parameters by the relations

$$q^2 = s^2 - ps + p^2, \quad (5.19)$$

$$q^3(1 - \beta) = s^3 - \frac{3}{2}(sp^2 + ps^2) + p^3. \quad (5.20)$$

The parameter $\beta \in [0, 1]$ acts as measure of biaxiality, with $\beta = 0$ corresponding to a uniaxial state (where $p = 0$) and $\beta = 1$ corresponds to a state with maximum biaxiality, where $s = 2p$. The sign of the parameter q is taken to be the sign of s (and p , if the state is biaxial).

Following [36], we write the bulk potential in terms of q and β :

$$f_B(q, \beta) = g(q) + B(q)\beta + \frac{(1 - t_4)q^6\beta^2}{6}, \quad (5.21)$$

where

$$g(q) := -\frac{t_1 q^2}{2} - \frac{t_2 q^3}{3} + \frac{t_3 q^4}{4} - \frac{q^5}{5} + \frac{q^6}{6}, \quad (5.22)$$

$$B(q) := \frac{t_2 q^3}{3} + \frac{q^5}{5} + \frac{(t_4 - 1)q^6}{3}. \quad (5.23)$$

Here, $g(q)$ is the bulk potential for any purely uniaxial state, such as the radial hedgehog defect, and the remaining terms represent biaxial contributions to the potential. Stable phases are minimizers of $f_B(q, \beta)$, subject to the constraint that $0 \leq \beta \leq 1$. This constraint can be implemented by Karush-Kuhn-Tucker multipliers [136], or, by solving

$$\frac{\partial f_B}{\partial q} = 0 \quad \text{and} \quad \beta = 0, \quad (5.24)$$

$$\frac{\partial f_B}{\partial q} = \frac{\partial f_B}{\partial \beta} = 0, \quad (5.25)$$

$$\frac{\partial f_B}{\partial q} = 0 \quad \text{and} \quad \beta = 1, \quad (5.26)$$

and ignoring solutions when $\beta \notin [0, 1]$.

In [36], the authors show that $t_4 < 1$ is a necessary condition for a biaxial phase to be the global minimizer of f_B . If $0 < \beta < 1$, then by solving $\frac{\partial f_B}{\partial \beta} = 0$ the equilibrium value of the biaxiality parameter β_b must satisfy

$$B(q) + \frac{(1 - t_4)q^6}{3}\beta_b = 0. \quad (5.27)$$

Substituting β_b into the bulk potential,

$$f_B(q, \beta_b) = g(q) - \frac{(1 - t_4)q^6\beta_b^2}{6}, \quad (5.28)$$

the global minimizer will always be uniaxial if $t_4 > 1$.

Solving the equations (5.24)–(5.26) will give non-zero solutions in terms of roots

to a quartic polynomial. The roots of these quartic polynomials can, in principle, be expressed analytically; however, the expressions are difficult to work with. Instead, we either evaluate q and β numerically or use an asymptotic approximation in the limit as $t_1 \rightarrow \infty$. In Figure 5.2, we show the results of numerically calculating the global minimizers in order to highlight some key features of f_B . As expected, biaxial phases are global minimizers only if $t_4 < 1$. If $t_4 > 1$, the uniaxial phase (U_+) is the global minimizer for all $t_2 \geq 0$ (an analytic expression for the first order U_+ to U_- phase transition line is given in [36]). The isotropic phase ($q = 0$) is always a critical point and is a local minima if $t_1 < 0$. If $t_1 \ll 0$, the isotropic phase is the global minimizer. Below the isotropic-nematic transition ($t_1 > 0$), the isotropic phase is always a local maxima of the bulk potential.

5.2.3 The Low Temperature Limit

We derive some asymptotic approximations for the critical points of f_B in the low temperature limit as $t_1 \rightarrow \infty$. We assume throughout that the remaining coefficients t_2 , t_3 and t_4 remain $O(1)$.

If $\beta = 0$, non-zero critical points are solutions of

$$\frac{\partial f_B}{\partial q} = 0, \quad (5.29)$$

or, equivalently,

$$g'(s)/s = -t_1 - t_2 s + t_3 s^2 - s^3 + s^4 = 0. \quad (5.30)$$

In the limit as $t_1 \rightarrow \infty$, there are two non-zero critical points:

$$s_+ \sim t_1^{\frac{1}{4}} + \frac{1}{4} + t_1^{-\frac{1}{4}} \left(\frac{3}{32} - \frac{t_3}{4} \right) + O\left(t_1^{-\frac{1}{2}}\right), \quad (5.31)$$

$$s_- \sim -t_1^{\frac{1}{4}} + \frac{1}{4} - t_1^{-\frac{1}{4}} \left(\frac{3}{32} - \frac{t_3}{4} \right) + O\left(t_1^{-\frac{1}{2}}\right). \quad (5.32)$$

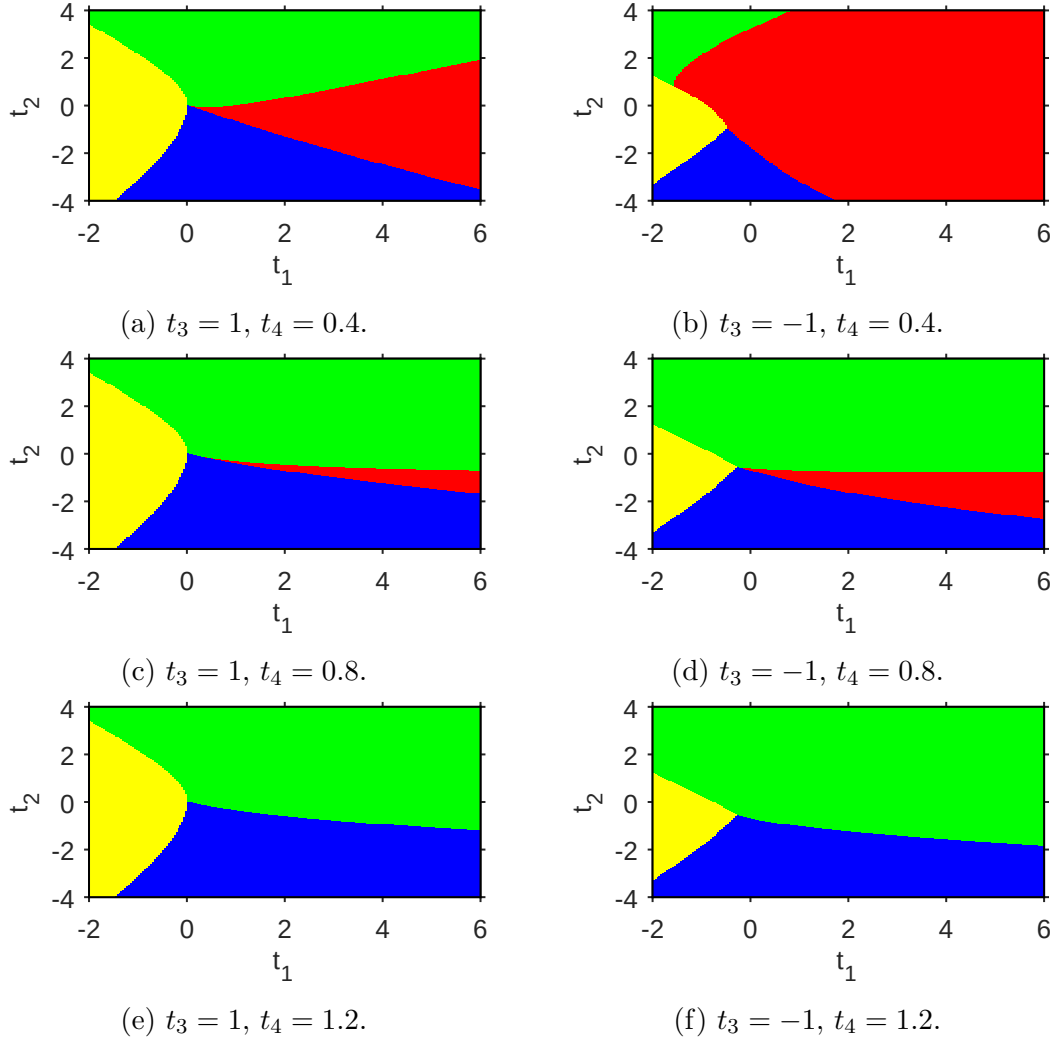


Figure 5.2: Global energy minimising phase of the bulk potential for fixed t_3 and t_4 , with the isotropic phase in yellow, the uniaxial U_+ phase in green, the uniaxial U_- phase in blue, and the biaxial phase in red.

The associated values of the bulk potential are

$$f_B(s_+, 0) \sim -\frac{t_1^{\frac{3}{2}}}{3} - \frac{t_1^{\frac{5}{4}}}{5} + O(t_1), \quad (5.33)$$

$$f_B(s_-, 0) \sim -\frac{t_1^{\frac{3}{2}}}{3} + \frac{t_1^{\frac{5}{4}}}{5} + O(t_1). \quad (5.34)$$

If $\beta \in (0, 1)$, we solve

$$\frac{\partial f_B}{\partial q} = \frac{\partial f_B}{\partial \beta} = 0. \quad (5.35)$$

There are two pairs of solutions:

$$q_+ \sim \frac{t_1^{\frac{1}{4}}}{t_4^{\frac{1}{4}}} - t_1^{-\frac{1}{4}} \left(\frac{t_3}{4t_4^{\frac{3}{4}}} + \frac{3}{50t_4^{\frac{3}{4}}(t_4 - 1)} \right) + O\left(t_1^{-\frac{3}{4}}\right), \quad (5.36)$$

$$\beta_+ \sim 1 - \frac{3t_4^{\frac{1}{4}}}{5(1 - t_4)} t_1^{-\frac{1}{4}} + O\left(t_1^{-\frac{3}{4}}\right), \quad (5.37)$$

$$q_- \sim -\frac{t_1^{\frac{1}{4}}}{t_4^{\frac{1}{4}}} + t_1^{-\frac{1}{4}} \left(\frac{t_3}{4t_4^{\frac{3}{4}}} + \frac{3}{50t_4^{\frac{3}{4}}(t_4 - 1)} \right) + O\left(t_1^{-\frac{3}{4}}\right), \quad (5.38)$$

$$\beta_- \sim 1 + \frac{3t_4^{\frac{1}{4}}}{5(1 - t_4)} t_1^{-\frac{1}{4}} + O\left(t_1^{-\frac{3}{4}}\right). \quad (5.39)$$

If $t_4 < 1$, then $\beta_- > 1$, and if $t_4 > 1$ then, $\beta_+ > 1$, and these solutions fail to satisfy constraint on β . The corresponding values of the bulk potential are

$$f_B(q_+, \beta_+) \sim -\frac{t_1^{\frac{3}{2}}}{3\sqrt{t_4}} + \left(\frac{t_3}{4t_4} + \frac{3}{50t_4(t_4 - 1)} \right) t_1 + O\left(t_1^{\frac{1}{2}}\right) \quad \text{if } t_4 < 1, \quad (5.40)$$

$$f_B(q_-, \beta_-) \sim -\frac{t_1^{\frac{3}{2}}}{3\sqrt{t_4}} + \left(\frac{t_3}{4t_4} + \frac{3}{50t_4(t_4 - 1)} \right) t_1 + O\left(t_1^{\frac{1}{2}}\right) \quad \text{if } t_4 > 1. \quad (5.41)$$

If $\beta = 1$, the solutions of $\frac{\partial f_B}{\partial q} = 0$ have exact solutions

$$\hat{q}_{\pm} = \pm \frac{\sqrt{t_4(-t_3 + \sqrt{4t_1 t_4 + t_3^2})}}{\sqrt{2}t_4} \sim \pm \left(\frac{t_1^{\frac{1}{4}}}{t_4^{\frac{1}{4}}} - \frac{t_3 t_1^{-\frac{1}{4}}}{4t_4^{\frac{3}{4}}} \right) + O\left(t_1^{-\frac{3}{4}}\right), \quad (5.42)$$

and the associated value of the bulk potential

$$f_B(\hat{q}_{\pm}, 1) = \frac{(-t_3 + \sqrt{4t_1 t_4 + t_3^2})(-8t_1 t_4 - t_3^2 + t_3 \sqrt{4t_1 t_4 + t_3^2})}{48t_4^2} \quad (5.43)$$

$$\sim -\frac{t_1^{\frac{3}{2}}}{3\sqrt{t_4}} + \frac{t_3 t_1}{4t_4} + O\left(t_1^{\frac{1}{2}}\right). \quad (5.44)$$

In the low temperature limit, the biaxial solution (q_+, β_+) will always be the global minimizer of the bulk potential if $t_4 < 1$. If $t_4 > 1$, the uniaxial state with positive order s_+ will be the global minimizer.

5.2.4 The Uniaxial Sixth Order Bulk Potential

Consider the uniaxial part of the sixth order bulk potential, defined by

$$g(s) := -\frac{t_1 s^2}{2} - \frac{t_2 s^3}{3} + \frac{t_3 s^4}{4} - \frac{s^5}{5} + \frac{s^6}{6}, \quad (5.45)$$

and the rescaled fourth order bulk potential, defined by

$$g_4(s) := -\frac{ts^2}{2} - s^3 + \frac{s^4}{2}, \quad (5.46)$$

where the reduced temperature $t := \frac{27AC}{B^2}$ [122]. The structure of the fourth order bulk potential is important in proving that the radial hedgehog order is bounded [119], monotonically increasing [121] and unique [121, 123]. Specifically, these properties are dependent on the fact that the fourth order potential has two minimizers when $t > 0$, $s_{\pm} = \frac{3 \pm \sqrt{9+8t}}{4}$, therefore, the fourth order potential is monotonically decreasing for $0 < s < s_+$ and monotonically increasing for $s_+ > s > \infty$.

Unlike the fourth order potential, the sixth order potential given in Equation (5.45) can have up to four non-zero critical points. The critical points are roots of the polynomial

$$s(-t_1 - t_2 s + t_3 s^2 - s^3 + s^4) = 0. \quad (5.47)$$

We work below the isotropic-nematic transition temperature ($t_1 > 0$), and, therefore, $g(s)$ always must have at least one positive and one negative minimizer. The positive minimizer s_+ is the global minimizer of g if $t_2 \geq 0$ [36].

On the interval $[0, \infty)$, a sixth order polynomial g can exhibit several distinct behaviours. If there are no other positive critical points, then g is monotonically decreasing for $s \in (0, s_+)$ and monotonically increasing for $s \in (s_+, \infty)$, as depicted in Figure 5.3a. If g has four critical points, then g is not necessary monotonically decreasing on $(0, s_+)$ and increasing on (s_+, ∞) , such as the potential shown in Fig-

ure 5.3b.

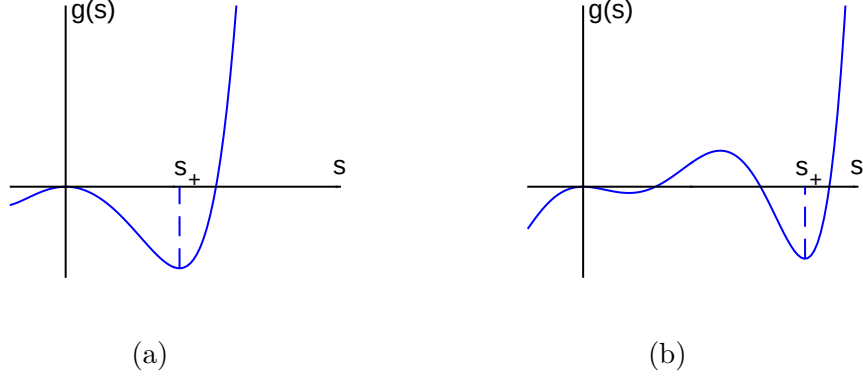


Figure 5.3: Possible behaviours of the uniaxial potential on $0 \leq s \leq \infty$.

We would like to extend many of the properties of the order parameter of the radial hedgehog with the fourth order potential and, therefore, look for some conditions on the number of roots of (5.47). Analytic expressions for the roots of a quartic polynomial exist [97], however, these expressions are impractical for identifying the global minimum of g . Instead, we consider the discriminant of the quartic polynomial $g'(s)/s$, namely

$$\begin{aligned}
\Delta := & -256t_1^3 + (-128t_3^2 - 192t_2 + 144t_3 - 27)t_1^2 \\
& + (-16t_3^4 - 144t_2^2t_3 + 80t_2t_3^2 + 4t_3^3 + 6t_2^2 - 18t_2t_3)t_1 \\
& - 4t_2^2t_3^3 - 27t_2^4 + 18t_2^3t_3 + t_2^2t_3^2 - 4t_2^3.
\end{aligned} \tag{5.48}$$

If the discriminant Δ of a quartic polynomial is less than zero, then the polynomial has two real roots and two complex roots [137]. We know that $g(s) \rightarrow \infty$ as $|s| \rightarrow \infty$ and has a local maximum at $s = 0$ if $t_1 > 0$, therefore, g must have at least one positive and one negative minimizer. Showing that the sixth order potential behaves as in Figure 5.3a is equivalent to showing that Δ defined in Equation (5.48) is less than zero for some coefficients t_1 , t_2 and t_3 .

In the low temperature limit, as $t_1 \rightarrow \infty$, $\Delta \sim -256t_1^3 < 0$. This agrees with our

asymptotic series expansions in §5.2.3, where we find two non-zero critical points of $g(s)$. Numerical inspection of Δ shows that $\Delta < 0$ for almost all values of t_1, t_2 and $t_3 \geq 0$. We define the region $\mathcal{D}$ to be the set

$$\mathcal{D} := \{(t_1, t_2, t_3) \in \mathbb{R}^3 : \Delta \geq 0, t_1 \geq 0, t_2 \geq 0, t_3 \geq 0\}. \quad (5.49)$$

In Figure 5.4, we plot $\mathcal{D}$ and use this graph to identify some upper bounds t_1^* , t_2^* and t_3^* such that for any $t_i > t_i^*$, $\Delta < 0$. The critical value t_1^* occurs on the plane $t_2 = 0$. Solving $\Delta = 0$, we see that $t_1^* = \frac{27}{4096}$. The critical values t_2^* and t_3^* occur on the plane $t_1 = 0$, and take the values $t_2^* = \frac{1}{27}$ and $t_3^* = \frac{1}{3}$.

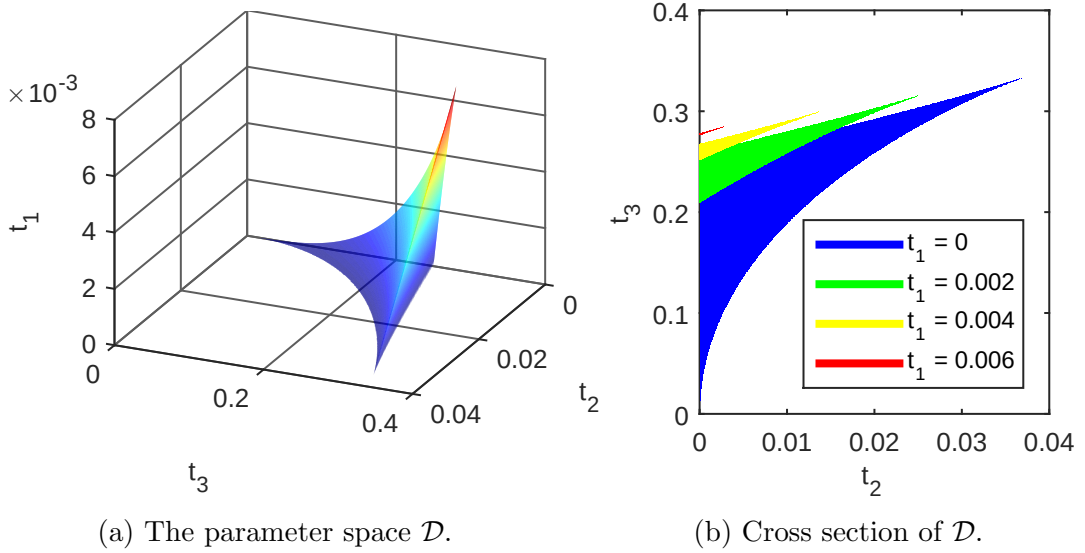


Figure 5.4: Parameter space $\mathcal{D}$ and cross-sections for fixed values of t_1 .

The analytic form of s_+ is too unwieldy for use in our work and, for much of our analysis, it is sufficient to know that s_+ exists and can be evaluated numerically. However, at several points in our work, we require the use of an upper bound on s_+ . For a polynomial

$$p := a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0, \quad (5.50)$$

the Fujiwara bound [138] on the roots r is

$$|r| \leq 2 \max \left\{ \left| \frac{a_{n-1}}{a_n} \right|, \left| \frac{a_{n-2}}{a_n} \right|^{\frac{1}{2}}, \dots, \left| \frac{a_1}{a_n} \right|^{\frac{1}{n-1}}, \left| \frac{a_0}{2a_n} \right|^{\frac{1}{n}} \right\}. \quad (5.51)$$

Applying this bound to $g'(s)/s$, we see that s_+ is bounded by

$$s_+ \leq 2 \max \left\{ 1, |t_3|^{\frac{1}{2}}, |t_2|^{\frac{1}{3}}, \left(\frac{t_1}{2} \right)^{\frac{1}{4}} \right\}. \quad (5.52)$$

5.3 The Radial Hedgehog Defect

We consider the spherical droplet Ω with radius $R > 0$,

$$\Omega := \left\{ (x, y, z) \in \mathbb{R}^3 : 0 \leq \sqrt{x^2 + y^2 + z^2} \leq R \right\}. \quad (5.53)$$

We assume that strong anchoring holds on $\partial\Omega$. We impose radial Dirichlet conditions of

$$\mathbf{Q} = \sqrt{\frac{3}{2}} s_+ \left(\hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{\mathbf{I}_3}{3} \right) \quad \text{on } r = R, \quad (5.54)$$

where $\hat{\mathbf{r}}$ is the unit vector in the radial direction, $\mathbf{I}_3$ is the 3×3 identity matrix and s_+ is the global minimizer of the uniaxial part of the sixth order potential,

$$g(s) = -\frac{t_1 s^2}{2} - \frac{t_2 s^3}{3} + \frac{t_3 s^4}{4} - \frac{s^5}{5} + \frac{s^6}{6}. \quad (5.55)$$

5.3.1 Existence of the Radial Hedgehog

We first show that the Landau-de Gennes energy with a sixth order bulk potential,

$$\begin{aligned} E[\mathbf{Q}] = \iiint_{\Omega} & \frac{1}{2} |\nabla \mathbf{Q}|^2 + F_0 - \frac{t_1}{2} \text{tr} \mathbf{Q}^2 - \frac{\sqrt{6} t_2}{3} \text{tr} \mathbf{Q}^3 + \frac{t_3}{4} (\text{tr} \mathbf{Q}^2)^2 \\ & - \frac{\sqrt{6}}{5} \text{tr} \mathbf{Q}^2 \text{tr} \mathbf{Q}^3 + \frac{t_4}{6} (\text{tr} \mathbf{Q}^2)^3 + (1 - t_4) (\text{tr} \mathbf{Q}^3)^2 \, d\Omega, \end{aligned} \quad (5.56)$$

has a radial hedgehog critical point of the form (5.61).

We let $\mathbb{M}$ be the set of symmetric, traceless 3×3 matrices. We define an admissible space for the $\mathbf{Q}$ -tensors,

$$\mathcal{A} = \left\{ \mathbf{Q} \in W^{1,2}(\Omega, \mathbb{M}); \quad \mathbf{Q} = \sqrt{\frac{3}{2}} s_+ \left(\hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{\mathbf{I}_3}{3} \right) \quad \text{on } r = R \right\}, \quad (5.57)$$

where $W^{1,2}(\Omega, \mathbb{M})$ is the Sobolev space

$$W^{1,2}(\Omega, \mathbb{M}) := \{ M \in L^2(\Omega) : \partial_x M \in L^2(\Omega), M \in \mathbb{M} \}. \quad (5.58)$$

Critical points of (5.56) are solutions of the Euler-Lagrange equations,

$$\begin{aligned} \Delta \mathbf{Q}_{ij} = & \left(-t_1 + t_3 \text{tr} \mathbf{Q}^2 - \frac{2\sqrt{6}}{5} \text{tr} \mathbf{Q}^3 + t_4 (\text{tr} \mathbf{Q}^2)^2 \right) \mathbf{Q}_{ij} \\ & + \left(-t_2 \sqrt{6} - \frac{3\sqrt{6}}{5} \text{tr} \mathbf{Q}^2 + 6(1 - t_4) \text{tr} \mathbf{Q}^3 \right) \mathbf{Q}_{ik} \mathbf{Q}_{kj} + \lambda \delta_{ij}, \end{aligned} \quad (5.59)$$

where λ is a Lagrange multiplier to account for the tracelessness condition. Summing Equation (5.59) over $i, j = 1, 2, 3$, we calculate the Lagrange multiplier to be

$$\lambda = -\frac{\text{tr} \mathbf{Q}^2}{3} \left(-t_2 \sqrt{6} - \frac{3\sqrt{6}}{5} \text{tr} \mathbf{Q}^2 + 6(1 - t_4) \text{tr} \mathbf{Q}^3 \right). \quad (5.60)$$

Radial hedgehog critical points are solutions of the form

$$\mathbf{Q} = \sqrt{\frac{3}{2}} s(r) \left(\hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{\mathbf{I}_3}{3} \right), \quad (5.61)$$

where the order parameter s is in the admissible space [121]

$$\mathcal{A}_s = \{ s \in L^2([0, R]; dr), s' \in L^2([0, R]; r^2 dr), s(R) = s_+ \}. \quad (5.62)$$

We now define the radial hedgehog as follows.

Proposition 5.3.1. *A functional of the form*

$$E[s] = 4\pi \int_0^R \left(\frac{1}{2} s'^2 + \frac{3s^2}{r^2} + g(s) \right) r^2 dr, \quad (5.63)$$

defined for functions $s \in \mathcal{A}_s$, has a global minimizer which is the solution to the Euler-Lagrange equation,

$$s'' + \frac{2s'}{r} - \frac{6s}{r^2} = g'(s), \quad (5.64)$$

subject to $s(R) = s_+$. Then, the radial hedgehog state

$$\mathbf{Q} = \sqrt{\frac{3}{2}} s(r) \left(\hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{\mathbf{I}_3}{3} \right), \quad (5.65)$$

is a solution of Equation (5.59).

Proof. The admissible space $\mathcal{A}_s$ is non-empty, since the constant function $s(r) = s_+$ is in $\mathcal{A}_s$. The functional $E[s]$ is bounded below and is convex in s' , therefore $E[s]$ is weakly lower semi-continuous on $\mathcal{A}_s$ (Theorem 1 of §8.2 in [114]). Since the final term in $g(s)$ is positive, the functional $E[s]$ satisfies the coercivity condition of §8.2.2 in [114]. By direct methods in the calculus of variations [115], a global minimizer of $E[s]$ in $\mathcal{A}_s$ exists and is the solution to the Euler-Lagrange equation

$$s'' + \frac{2s'}{r} - \frac{6s}{r^2} = g'(s). \quad (5.66)$$

We substitute a $\mathbf{Q}$ -tensor of the form

$$\mathbf{Q} = \sqrt{\frac{3}{2}} s(r) \left(\hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{\mathbf{I}_3}{3} \right), \quad (5.67)$$

into the Euler-Lagrange equations (5.59), which are satisfied if $s(r)$ is the solution to Equation (5.64). □

Hereafter, we let s denote the global minimizer of $E[s]$. The function s must be analytic on $[0, R]$. The $\mathbf{Q}$ -tensor is continuous on Ω , therefore, s cannot be singular at the origin. This implies that $s(0) = s'(0) = 0$, so there is an isotropic point at the origin of Ω .

Next, we compute bounds on the order parameter s .

Proposition 5.3.2. *The function s satisfies the bounds*

$$0 \leq s(r) \leq s_+ \quad (5.68)$$

for all $r \in (0, R)$ if $\{t_1, t_2, t_3\} \notin \mathcal{D}$.

Proof. We first consider the lower bound on s . We assume for a contradiction that in some interval $A \subset [0, R]$, $s(r) < 0$. It follows that

$$E[|s|] - E[s] = -2 \int_A \left(\frac{t_2}{3} |s|^3 + \frac{1}{5} |s|^5 \right) r^2 dr < 0 \quad (5.69)$$

if $t_2 \geq 0$. Since s is the minimizer of $E[s]$, it follows that $E[|s|] - E[s] \geq 0$ and, hence, we have a contradiction.

To show that $s(r)$ is bounded above, we assume for a contradiction that the maximum of $s(r)$ occurs at some $r_* \in (0, R)$ and $s(r_*) > s_+$. Since r_* is a maximum $s''(r_*) \leq 0$ and $s'(r_*) = 0$, and it follows that,

$$g'(s(r_*)) + \frac{6s(r_*)}{r_*^2} \leq 0. \quad (5.70)$$

Since $s(r_*) > s_+$, $g'(s(r_*)) \geq 0$ if $g(s)$ is increasing on the interval (s_+, ∞) . Therefore, we have a contradiction as

$$g'(s(r_*)) + \frac{6s(r_*)}{r_*^2} > 0. \quad (5.71)$$

□

We have now shown that the radial hedgehog exists and the associated order parameter is bounded, subject to some constraints on the coefficients t_1 , t_2 and t_3 . A number of results follow immediately from previous work on the radial hedgehog in the fourth order potential:

- The order parameter $s(r) > 0$ for all $r > 0$ if $0 \leq s(r) \leq s_+$, so the radial hedgehog is uniaxial everywhere except at the origin. The proof follows identically to the Corollary to Proposition 2.1 in [119].
- The order parameter s is monotonically increasing on the interval $(0, R]$. This result follows identically to Proposition 3 in [121] and requires $0 \leq s(r) \leq s_+$.
- The order parameter s is unique if the potential g is decreasing on $[0, s_+]$ and $0 \leq s \leq s_+$. Theorem 4 in [121] is directly applicable to the sixth order potential, provided g has a single critical point in the interval $(0, \infty)$.

We next consider the behaviour of s near the isotropic point at $r = 0$.

Proposition 5.3.3. *If s is a minimizer of $E[s]$, with $0 \leq s \leq s_+$, then as $r \rightarrow 0$,*

$$s \sim a_2 r^2 \left(1 - \frac{t_1 r^2}{14} + o(r^2) \right). \quad (5.72)$$

Proof. Using a Taylor expansion about $r = 0$, we let

$$s(r) = \sum_{n=0}^{\infty} a_n r^n. \quad (5.73)$$

By substituting into Equation (5.64) and comparing coefficients, we see that

$$a_0 = a_1 = a_3 = a_5 = 0, \quad (5.74)$$

$$a_2 = -\frac{14a_4}{t_1}, \quad (5.75)$$

where a_2 is some arbitrary, non-zero constant. $\square$

The first two non-zero terms in this expansion are identical to the expansion for the order parameter with a fourth order bulk potential [119].

5.3.2 Bounds on the Order Parameter

We now derive some bounds on the order parameter s , which are useful in proving that the radial hedgehog may be an unstable critical point of the Landau-de Gennes energy. This bound follows similarly to results in [109, 116].

Proposition 5.3.4. *If g is decreasing on $[0, s_+]$, then the function s is bounded from below by the solution to the differential equation*

$$h'' + \frac{2h'}{r} - \frac{6h}{r^2} = 0, \quad (5.76)$$

subject to boundary conditions $h(0) = 0$ and $h(R) = s_+$. Equation (5.76) subject to these boundary conditions has the unique solution

$$h(r) = \frac{s_+ r^2}{R^2}. \quad (5.77)$$

Proof. We assume for a contradiction that for some $r_* \in (0, R)$, $s(r_*) - h(r_*) < 0$.

Therefore, there must exist some R_1, R_2 such that $0 \leq R_1 < r_* < R_2 \leq R$ and

$$s(R_1) - h(R_1) = 0, \quad (5.78)$$

$$s'(R_1) - h'(R_1) < 0, \quad (5.79)$$

$$s(R_2) - h(R_2) = 0, \quad (5.80)$$

$$s'(R_2) - h'(R_2) > 0. \quad (5.81)$$

Multiplying (5.64) by $r^2 h$ and (5.76) by $r^2 s$, subtracting the resulting equations and

integrating over (R_1, R_2) , we find that

$$\int_{R_1}^{R_2} h(r^2 s')' - s(r^2 h')' dr = \int_{R_1}^{R_2} g'(s) h r^2 dr. \quad (5.82)$$

The right-hand side of (5.82) is always negative since $g' < 0$ on $r \in (0, R)$. Integrating by parts, the left-hand side is

$$R_2^2 s(R_2)(s'(R_2) - h'(R_2)) - R_1^2 s(R_1)(s'(R_1) - h'(R_1)) > 0, \quad (5.83)$$

and hence we have a contradiction. Equation (5.76) with the boundary conditions $h(0) = 0$ and $h(R) = s_+$ is an Euler differential equation, with solution

$$h(r) = \frac{s_+ r^2}{R^2}. \quad (5.84)$$

□

Unfortunately, the lower bound (5.77) underestimates s considerably, as seen in Figure 5.5. In the following Proposition, we derive an improved lower bound which better captures the behaviour of s . This result is similar to the bounds derived for the fourth order bulk potential in [122, 119, 139]. From [140], for the system

$$N[s] := s'' + \frac{2s'}{r} - \frac{6s}{r^2} - g'(s) \quad (5.85)$$

with $s(0) = 0$ and $s(R) = s_+$, if there exist functions α and β such that

$$N[\alpha] \geq 0, \quad N[\beta] \leq 0, \quad (5.86)$$

and $\alpha(0) \leq 0 \leq \beta(0)$ and $\alpha(R) \leq s_+ \leq \beta(R)$, then

$$\alpha(r) \leq s(r) \leq \beta(r), \quad (5.87)$$

where $N[s] = 0$, $s(0) = 0$ and $s(R) = s_+$.

Proposition 5.3.5. *The function $s(r)$ is bounded from below by*

$$\frac{s_+ r^2}{r^2 + \lambda_{\max}^2} \leq s(r). \quad (5.88)$$

where $\lambda_{\max}$ is the maximum of

$$\left\{ \sqrt{\frac{14}{t_1}}, \sqrt{\frac{34}{4t_1 + s_+ t_2}}, \sqrt{\frac{26}{-t_3 s_+^2 + 3t_2 s_+ + 6t_1}}, \sqrt{\frac{6}{s_+^3 - 2t_3 s_+^2 + 3t_2 s_+ + 4t_1}} \right\}. \quad (5.89)$$

If $t_1 \geq \max \left\{ 2, 2t_3^2, 2t_2^{\frac{4}{3}} \right\}$ then

$$\lambda_{\max} = \sqrt{\frac{14}{t_1}}. \quad (5.90)$$

Proof. As in [122, 119, 139], we consider a function of the form

$$\alpha(r) = \frac{s_+ r^2}{r^2 + \lambda^2}. \quad (5.91)$$

The boundary conditions are satisfied immediately, as $\alpha(0) = 0$ and $\alpha(R) \leq s_+$.

Substituting α into (5.85), we find that

$$N[\alpha] = -\frac{s_+ r^2}{(r^2 + \lambda^2)^5} (\lambda^6 C_1 + r^2 \lambda^4 C_2 + r^4 \lambda^2 C_3 + r^6 C_4), \quad (5.92)$$

where

$$C_1 := 14 - \lambda^2 t_1, \quad (5.93)$$

$$C_2 := 34 - \lambda^2 (4t_1 + s_+ t_2), \quad (5.94)$$

$$C_3 := 26 - \lambda^2 (-t_3 s_+^2 + 3t_2 s_+ + 6t_1), \quad (5.95)$$

$$C_4 := 6 - \lambda^2 (s_+^3 - 2t_3 s_+^2 + 3t_2 s_+ + 4t_1). \quad (5.96)$$

For $N[\alpha] \geq 0$, we must have $C_i \leq 0$ for all $i = 1, \dots, 4$, or equivalently,

$$\lambda \geq \lambda_{\max} \equiv \max \left\{ \sqrt{\frac{14}{t_1}}, \sqrt{\frac{34}{4t_1 + s_+ t_2}}, \sqrt{\frac{26}{-t_3 s_+^2 + 3t_2 s_+ + 6t_1}}, \sqrt{\frac{6}{s_+^3 - 2t_3 s_+^2 + 3t_2 s_+ + 4t_1}} \right\}. \quad (5.97)$$

Finally, we show that with some constraints on the relative magnitude of t_1 , $\lambda_{\max} = \sqrt{\frac{14}{t_1}}$. For any t_1 , it follows immediately that

$$\frac{14}{t_1} - \frac{34}{4t_1 + s_+ t_2} > 0. \quad (5.98)$$

To prove the second relation, we assume that

$$\left(\frac{t_1}{2}\right)^{\frac{1}{4}} = \max \left\{ 1, |t_3|^{\frac{1}{2}}, |t_2|^{\frac{1}{3}}, \left(\frac{|t_1|}{2}\right)^{\frac{1}{4}} \right\}, \quad (5.99)$$

and, therefore, by the Fujiwara bound given in §5.2.4, $\left(\frac{t_1}{2}\right)^{\frac{1}{2}} \geq t_3$ and $4\left(\frac{t_1}{2}\right)^{\frac{1}{2}} \geq s_+^2$.

Then, $2t_1 > t_3 s_+^2$ and

$$\frac{14}{t_1} - \frac{26}{-t_3 s_+^2 + 3t_2 s_+ + 6t_1} = \frac{2(29t_1 + 21t_2 s_+ - 7t_3 s_+^2)}{t_1(6t_1 + 3t_2 s_+ - t_3 s_+^2)} > 0, \quad (5.100)$$

since $6t_1 - t_3 s_+^2 \geq 4t_1 > 0$ and $29t_1 - 7t_3 s_+^2 \geq 15t_1 > 0$.

Finally, we show that

$$\frac{14}{t_1} - \frac{6}{s_+^3 - 2t_3 s_+^2 + 3t_2 s_+ + 4t_1} \geq 0, \quad (5.101)$$

or equivalently

$$\frac{2(7s_+^3 - 14t_3 s_+^2 + 21s_+ t_2 + 25t_1)}{t_1(s_+^3 - 2t_3 s_+^2 + 3t_2 s_+ + 4t_1)} \geq 0. \quad (5.102)$$

If $2t_1 \geq t_3 s_+^2$, then

$$s_+^3 - 2t_3 s_+^2 + 3t_2 s_+ + 4t_1 \geq s_+^3 + 3t_2 s_+ > 0, \quad (5.103)$$

and it suffices to show

$$(7s_+^3 - 14t_3 s_+^2 + 21t_2 s_+ + 25t_1) \geq 0. \quad (5.104)$$

We make the substitution $s_+^3 = s_+^4 + t_3 s_+^2 - t_2 s_+ - t_1$, thus,

$$(7s_+^4 - 7t_3 s_+^2 + 14t_2 s_+ + 18t_1) \geq (7s_+^4 s_+^2 + 14t_2 s_+ + 4t_1) > 0. \quad (5.105)$$

Hence, for $t_1 \geq \max \left\{ 2, 2t_3^2, 2t_2^{\frac{4}{3}} \right\}$, $\lambda_{\max} = \sqrt{\frac{14}{t_1}}$. $\square$

To show that s is bounded from above by a similar function is considerably harder, as any bounding function β must satisfy $\beta(R) \geq s_+$, for which we do not have a useful analytic form. If we work in an infinite domain ($R \rightarrow \infty$), then we can define a function

$$\beta(r) := \frac{s_+ r^2}{r^2 + \lambda_{\min}^2}, \quad (5.106)$$

where $\lambda_{\min}$ is the minimum of the set given in (5.89). For some sufficiently large t_1 , $\lambda_{\min} = \sqrt{\frac{6}{s_+^3 - 2t_3 s_+^2 + 3t_2 s_+ + 4t_1}}$. Then, $N[\beta] \leq 0$ for all r and satisfies the condition at infinity $\beta(\infty) = s_+$. Based on these bounds, we estimate that the core of radial hedgehog scales with $t_1^{-\frac{1}{2}}$ in the low temperature limit.

In Figure 5.5, we plot the lower bounds (5.77) and (5.88) and a numerically computed solution for s . We see that both bounds underestimate s , although the function defined in Proposition 5.3.5 captures the behaviour of s far better.

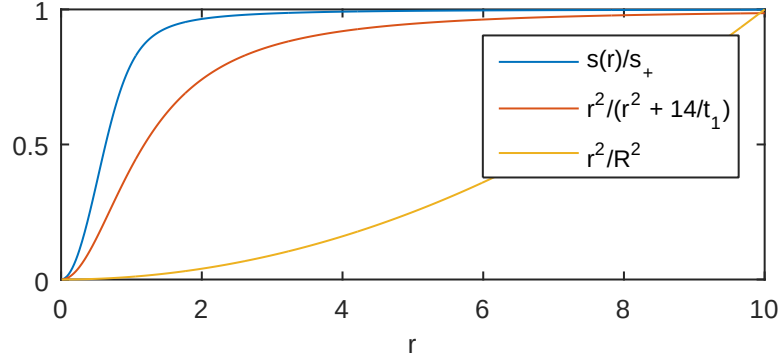


Figure 5.5: Normalized solution for s and lower bounds for $R = 10$, $t_1 = 10$, $t_2 = 1$ and $t_3 = 1$.

5.4 Some Results on the Stability and Instability of the Radial Hedgehog Defect

In this final section, we discuss the stability of the radial hedgehog. We first show that the radial hedgehog is locally stable for small radii. We then use two classes of perturbation to show that the radial hedgehog is unstable for a wide range of bulk potential coefficients and droplet radii.

5.4.1 The Second Variation

For some arbitrary critical point $\mathbf{Q}$ and perturbation $\mathbf{H}$, the second variation is

$$\begin{aligned}
\delta^2 E = & \iiint_{\Omega} |\nabla \mathbf{H}|^2 - t_1 \text{tr} \mathbf{H}^2 - 2\sqrt{6} t_2 \text{tr} \mathbf{Q} \mathbf{H}^2 + t_3 (\text{tr} \mathbf{H}^2 \text{tr} \mathbf{Q}^2 + 2(\text{tr} \mathbf{Q} \mathbf{H})^2) \\
& - \frac{2\sqrt{6}}{5} (3\text{tr} \mathbf{H}^2 \mathbf{Q} \text{tr} \mathbf{Q}^2 + 6\text{tr} \mathbf{Q}^2 \mathbf{H} \text{tr} \mathbf{Q} \mathbf{H} + \text{tr} \mathbf{H}^2 \text{tr} \mathbf{Q}^3) \\
& + t_4 ((\text{tr} \mathbf{Q}^2)^2 \text{tr} \mathbf{H}^2 + 4\text{tr} \mathbf{Q}^2 (\text{tr} \mathbf{Q} \mathbf{H})^2) \\
& + 2(1 - t_4) (6\text{tr} \mathbf{Q}^3 \text{tr} \mathbf{Q} \mathbf{H}^2 + 9(\text{tr} \mathbf{Q}^2 \mathbf{H})^2) \, d\Omega.
\end{aligned} \tag{5.107}$$

Any critical point of the Landau-de Gennes energy will be unstable if the second variation is negative for some admissible perturbation. For the radial hedgehog solution,

the second variation can be simplified by the use of a basis introduced in [141]. We define the orthonormal vectors

$$\mathbf{n} = (\sin(\theta) \cos(\phi), \sin(\theta) \sin(\phi), \cos(\theta)), \quad (5.108)$$

$$\mathbf{m} = (\cos(\theta) \cos(\phi), \cos(\theta) \sin(\phi), -\sin(\theta)), \quad (5.109)$$

$$\mathbf{p} = (-\sin(\phi), \cos(\phi), 0), \quad (5.110)$$

and then define five orthonormal tensors

$$\mathbf{E}_{ij} := \left(\mathbf{n}_i \mathbf{n}_j - \frac{\delta_{ij}}{3} \right), \quad \mathbf{F}_{ij} := \mathbf{n}_i \mathbf{m}_j + \mathbf{m}_i \mathbf{n}_j, \quad (5.111)$$

$$\mathbf{G}_{ij} := \mathbf{n}_i \mathbf{p}_j + \mathbf{p}_i \mathbf{n}_j, \quad \mathbf{X}_{ij} := \mathbf{m}_i \mathbf{p}_j + \mathbf{p}_i \mathbf{m}_j, \quad (5.112)$$

$$\mathbf{Y}_{ij} := \mathbf{m}_i \mathbf{m}_j - \mathbf{p}_i \mathbf{p}_j. \quad (5.113)$$

Then, any arbitrary perturbation can be expressed as a linear combination of these tensors, i.e.

$$\mathbf{H} = v_0(r, \theta, \phi) \mathbf{E} + v_1(r, \theta, \phi) \mathbf{F} + v_2(r, \theta, \phi) \mathbf{G} + v_3(r, \theta, \phi) \mathbf{X} + v_4(r, \theta, \phi) \mathbf{Y}, \quad (5.114)$$

where $v_i(R, \theta, \phi) = 0$ for $i = 0, \dots, 4$. By analogy with [116, 141],

$$\delta^2 E = \iiint_{\Omega} |\nabla \mathbf{H}|^2 + \frac{2v_0^2}{3} g_1(s) + 2(v_1^2 + v_2^2) g_2(s) + 2(v_3^2 + v_4^2) g_3(s) \, d\Omega, \quad (5.115)$$

where

$$g_1(s) := (-t_1 - 2t_2 s + 3t_3 s^2 - 4s^3 + 5s^4) \equiv g''(s), \quad (5.116)$$

$$g_2(s) := (-t_1 - t_2 s + t_3 s^2 - s^3 + s^4) \equiv \frac{g'(s)}{s}, \quad (5.117)$$

$$g_3(s) := \left(-t_1 + 2t_2 s + t_3 s^2 + \frac{4s^3}{5} + (3t_4 - 2)s^4 \right). \quad (5.118)$$

5.4.2 Local Stability for Small Droplet Radii

Following the methodology in Proposition 3.4 of [119], we show that the radial hedgehog state is locally stable for small values of t_1 and R . We make use of the following Lemmas.

Lemma 5.4.1. *For any 3×3 tensor $\mathbf{H}$ satisfying $\mathbf{H}_{ij} = 0$ on $r = 1$,*

$$\int_0^1 |\nabla \mathbf{H}|^2 r^2 \, dr \geq \int_0^1 \frac{1}{4} \text{tr} \mathbf{H}^2 \, dr, \quad (5.119)$$

Proof. We first note that

$$|\nabla \mathbf{H}|^2 \geq \sum_{i,j=1}^3 \left(\frac{\partial \mathbf{H}_{ij}}{\partial r} \right)^2. \quad (5.120)$$

We then apply the inequality from [142] to each term $\mathbf{H}_{ij}$; for any function $h(r)$ such that $h(1) = 0$,

$$\int_0^1 r^2 h'^2 \, dr \geq \frac{1}{4} \int_0^1 h^2 \, dr. \quad (5.121)$$

□

Lemma 5.4.2. *If $\mathbf{Q}$ is the radial hedgehog tensor and the coefficients $\{t_1, t_2, t_3\} \notin \mathcal{D}$, then for any tensor $\mathbf{H}$ the following inequalities hold:*

$$\sqrt{6} \text{tr} \mathbf{Q} \mathbf{H}^2 \leq s_+ \text{tr} \mathbf{H}^2, \quad (5.122)$$

$$0 \leq (\text{tr} \mathbf{Q} \mathbf{H})^2 \leq s_+^2 \text{tr} \mathbf{H}^2, \quad (5.123)$$

$$0 \leq \sqrt{6} (\text{tr} \mathbf{Q}^2 \mathbf{H}) (\text{tr} \mathbf{Q} \mathbf{H}) \leq s_+^3 \text{tr} \mathbf{H}^2, \quad (5.124)$$

$$0 \leq (\text{tr} \mathbf{Q}^2 \mathbf{H})^2 \leq \frac{s_+^4 \text{tr} \mathbf{H}^2}{6}. \quad (5.125)$$

Proof. We express the tensor $\mathbf{H}$ in terms of the linear combination introduced in

Equation (5.114). Therefore,

$$\mathrm{tr}\mathbf{H}^2 = \frac{2v_0^2}{3} + 2(v_1^2 + v_2^2 + v_3^2 + v_4^2), \quad (5.126)$$

and

$$\sqrt{6}\mathrm{tr}\mathbf{Q}\mathbf{H}^2 = s(2v_0^2 + 3v_1^2 + 3v_2^2 - 6v_3^2 - 6v_4^2). \quad (5.127)$$

Subtracting $\mathrm{str}\mathbf{H}^2$, we see that

$$\sqrt{6}\mathrm{tr}\mathbf{Q}\mathbf{H}^2 - \mathrm{str}\mathbf{H}^2 = -s(v_1^2 + v_2^2 + 4(v_3^2 + v_4^2)) \leq 0. \quad (5.128)$$

If $\{t_1, t_2, t_3\} \notin \mathcal{D}$, then s is bounded by s_+ and

$$\sqrt{6}\mathrm{tr}\mathbf{Q}\mathbf{H}^2 \leq \mathrm{str}\mathbf{H}^2 \leq s_+\mathrm{tr}\mathbf{H}^2. \quad (5.129)$$

The other results follow immediately,

$$(\mathrm{tr}\mathbf{Q}\mathbf{H})^2 = \frac{2s^2v_0^2}{3} \leq s^2\mathrm{tr}\mathbf{H}^2 \leq s_+^2\mathrm{tr}\mathbf{H}^2, \quad (5.130)$$

$$\sqrt{6}(\mathrm{tr}\mathbf{Q}^2\mathbf{H})(\mathrm{tr}\mathbf{Q}\mathbf{H}) = s^3\mathrm{tr}\mathbf{H}^2 \leq s_+^3\mathrm{tr}\mathbf{H}^2, \quad (5.131)$$

$$(\mathrm{tr}\mathbf{Q}^2\mathbf{H})^2 = \frac{s^4v_0^2}{9} \leq \frac{s^4\mathrm{tr}\mathbf{H}^2}{6} \leq \frac{s_+^4\mathrm{tr}\mathbf{H}^2}{6}. \quad (5.132)$$

□

Proposition 5.4.3. *The radial hedgehog state is locally stable if*

$$R^2 < \begin{cases} (4(t_1 + 2t_2s_+ + 4s_+^2))^{-1} & \text{if } t_4 < 1, \\ (4(t_1 + 2t_2s_+ + 4s_+^2 + \frac{5}{2}(t_4 - 1)s_+^4))^{-1} & \text{if } t_4 \geq 1. \end{cases} \quad (5.133)$$

Proof. We introduce the rescaled variable $\tilde{r} = \frac{r}{R}$ and consider Equation (5.107).

Applying the inequalities from Lemma 5.4.2, we see that if $t_4 < 1$, then

$$\delta^2 E \geq \int_0^{2\pi} \int_0^\pi \int_0^1 \{|\nabla \mathbf{H}|^2 - \text{tr} \mathbf{H}^2 R^2 h\} \sin(\theta) \tilde{r}^2 d\tilde{r} d\theta d\phi, \quad (5.134)$$

where

$$h := \begin{cases} t_1 + 2t_2 s_+ + 4s_+^2 & \text{if } t_4 < 1, \\ (t_1 + 2t_2 s_+ + 4s_+^2 + \frac{5}{2}(t_4 - 1)s_+^4) & \text{if } t_4 \geq 1. \end{cases} \quad (5.135)$$

Using the result from Lemma 5.4.1 and that $r \leq 1$, it follows that

$$\delta^2 E \geq \int_0^{2\pi} \int_0^\pi \int_0^1 \left\{ \frac{1}{4} \text{tr} \mathbf{H}^2 - \text{tr} \mathbf{H}^2 R^2 h \right\} \sin(\theta) d\tilde{r} d\theta d\phi, \quad (5.136)$$

By comparing the coefficients of $\text{tr} \mathbf{H}^2$, we derive the inequalities in Equation (5.133). $\square$

The radial hedgehog is locally stable if the droplet radius is sufficiently small, which is in agreement with the analytic estimates and numerical work using the fourth order potential [64, 119]. In the limit as $t_1 \rightarrow \infty$, this condition on the radius scales like $\frac{1}{t_1}$.

5.4.3 Instability for $0 < t_4 < 1$

We now show that the radial hedgehog is unstable for $t_4 < 1$, and some suitably large t_1 and R , by considering a perturbation similar to one identified in Theorem 2.4 of [141]. In this parameter regime, biaxial phases can be the global minimizer of the bulk potential. This motivates our choice of perturbation, which aims to create a large region of biaxiality within Ω .

We consider the perturbation

$$\mathbf{H} = v(r) \sin^2(\theta) \mathbf{X}, \quad (5.137)$$

with $v(0) = v(R) = 0$ and associated second variation

$$\delta^2 E = \frac{32\pi}{15} \int_0^R \left(v'^2 + \frac{4v^2}{r^2} + v^2 g_3(s) \right) r^2 dr. \quad (5.138)$$

We make use of Hardy's decomposition trick and set $v = sw$, with $w(0) = w(R) = 0$.

Then,

$$\int_0^R r^2 v'^2 dr = \int_0^R r^2 (s'w + sw')^2 dr = \int_0^R r^2 (w^2 s'^2 + 2ss'ww' + s^2 w'^2) dr. \quad (5.139)$$

Considering the first term, we see that

$$\begin{aligned} \int_0^R r^2 s'^2 w^2 dr &= r^2 s s' w^2 \Big|_0^R - \int_0^R s (r^2 s' w^2)' dr \\ &= - \int_0^R r^2 s s'' w^2 + r^2 s s' w w' + 2r s s' w^2 dr. \end{aligned} \quad (5.140)$$

Therefore, we have

$$\int_0^R r^2 v'^2 dr = \int_0^R r^2 \left(s^2 w'^2 - \frac{2s^2}{r^2} - s g'(s) \right) dr, \quad (5.141)$$

and the second variation simplifies to

$$\delta^2 E = \int_0^R r^2 s^2 \left(w'^2 - \frac{2w^2}{r^2} + 3s w^2 \left(t_2 + \frac{3}{5} s^2 + (t_4 - 1) s^3 \right) \right) dr. \quad (5.142)$$

We note that the coefficient of the largest power of s in (5.142) is negative for any $t_4 < 1$. For any $t_4 < 1$, then, for suitably large R , we can always find some $r_0 \in (0, R)$ such that for all $r > r_0$, $t_2 + \frac{3}{5} s^2 + (t_4 - 1) s^3 < 0$. We can derive an estimate for r_0 using the bounds for $s(r)$ derived in Proposition 5.77:

$$t_2 + \frac{3}{5} s^2 + (t_4 - 1) s^3 \leq t_2 + \frac{3}{5} s_+^2 + (t_4 - 1) s_+^3 \left(\frac{r^2}{r^2 + \frac{14}{t_1}} \right)^3. \quad (5.143)$$

Hence, a possible choice for r_0 is

$$r_0 = \sqrt{\frac{14}{t_1} \frac{\left(\frac{t_2 + \frac{3}{5}s_+^2}{(1-t_4)s_+^3}\right)^{\frac{1}{3}}}{1 - \left(\frac{t_2 + \frac{3}{5}s_+^2}{(1-t_4)s_+^3}\right)^{\frac{1}{3}}}} > 0. \quad (5.144)$$

We now consider the term

$$\int_0^R r^2 s^2 \left(w'^2 - \frac{2w^2}{r^2} \right) dr \leq s_+^2 \int_0^R r^2 \left(w'^2 - \frac{2w^2}{r^2} \left(\frac{r^2}{r^2 + \frac{14}{t_1}} \right)^2 \right) dr. \quad (5.145)$$

For suitably large R and t_1 , we can always pick some r_1 such that for all $r > r_1$,

$$2 \left(\frac{r^2}{r^2 + \frac{14}{t_1}} \right)^2 \geq \frac{3}{2}. \quad (5.146)$$

Solving, we define $r_1 := \sqrt{\frac{14\sqrt{3}}{t_1(2-\sqrt{3})}}$. Therefore, we define $r_2 := \max\{r_0, r_1\}$ and construct a function w on the interval (r_2, R) such that

$$\int_{r_2}^R r^2 w'^2 - \frac{3w^2}{2} dr < 0. \quad (5.147)$$

By experimentation, we find the function

$$w = \begin{cases} 0 & \text{if } 0 \leq r < r_2, \\ \sqrt{\frac{r_2}{r}} \sin \left(\pi \frac{\log\left(\frac{r}{r_2}\right)}{\log\left(\frac{R}{r_2}\right)} \right) & \text{if } r_2 \leq r < R, \end{cases} \quad (5.148)$$

for which

$$\int_{r_2}^R r^2 w'^2 - \frac{3w^2}{2} dr = \frac{r_2}{8} \frac{(4\pi^2 - 5(\ln(R))^2 + 10\ln(R)\ln(r_2) - 5(\ln(r_2))^2)}{\ln(R) - \ln(r_2)}. \quad (5.149)$$

Therefore, the second variation is less than zero for

$$R > r_2 e^{\frac{2\pi}{\sqrt{5}}} = 16.6087 r_2. \quad (5.150)$$

The condition (5.150) allows us to calculate explicit values of the droplet radius for which the radial hedgehog defect is unstable. For example, setting $t_1 = 10$, $t_2 = 1$, $t_3 = 1$ and $t_4 = 0.5$, we have $r_0 = 5.0149$ and $r_1 = 3.0083$ and, therefore, the radial hedgehog will be unstable for droplet radius $R > 83.2910$. Since s_+ is an increasing function of t_1 , which scales with $t_1^{\frac{1}{4}}$, both r_0 and r_1 are decreasing functions of t_1 . Therefore, we expect the critical droplet radius for instability to decrease with increasing t_1 .

We can improve on the estimate (5.150) by numerically finding minimizers of Equation (5.138), by solving

$$v'' + \frac{2v'}{r} - \frac{4v}{r^2} = v g_3(s), \quad (5.151)$$

subject to $v(0) = v'(0) = v(R) = 0$ and the constraint that

$$\int_0^R r^2 v^2 dr = 1. \quad (5.152)$$

In Figure 5.6, we plot computed regions of instability in the R - t_1 plane, given in the shaded regions. Decreasing t_4 from 1 allows instabilities to occur for increasingly small values of t_1 and R . We also see that boundary of these instability regions as $R \rightarrow \infty$ approximately correspond to the values of t_1 for which the biaxial phase becomes the global minimizer of f_B (see Figure 5.2).

The ease with which we are able to find perturbations which induce instability makes sense physically. Any perturbation of the form given in Equation (5.137) to the radial hedgehog will create a region of biaxiality in Ω . As we discussed in §5.2.2,

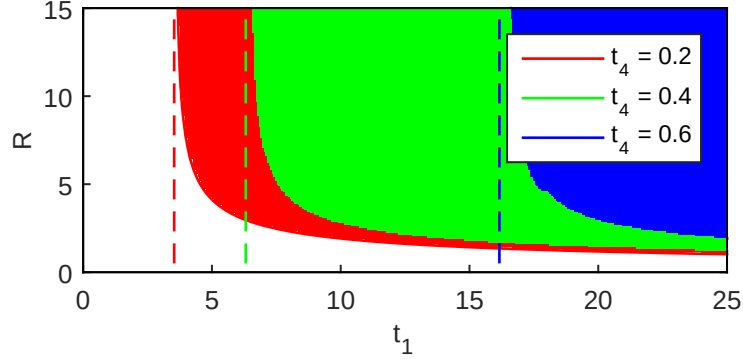


Figure 5.6: Numerically calculated regions of instability (shaded region) using Equation (5.151) and value of t_1 for which the biaxial phase becomes the global minimizer of f_B (dashed line) for $t_2 = 1$, $t_3 = 2$ and variable t_4 .

a biaxial phase is the global minimizer of the bulk potential for $t_4 < 1$ and large t_1 and so, by creating a biaxial region, we are moving the bulk potential towards a lower energy phase. We note that our choice of perturbation preserves the isotropic point at $r = 0$, since minimizers of (5.138) must be continuous on Ω . We would expect this isotropic point to vanish as the radial hedgehog becomes unstable. We also observe that in this parameter regime of $t_4 < 1$ and large t_1 , strong uniaxial radial anchoring conditions on $\partial\Omega$ will not be the global minimizer of the bulk potential. Instead, it would be physically realistic to apply a biaxial anchoring on $\partial\Omega$, which is beyond the scope of this chapter.

5.4.4 Instability for $t_4 > 1$

We now show that the radial hedgehog becomes unstable for some $t_4 > 1$ as t_1 and R become large but finite. We seek a perturbation which is non-zero at $r = 0$. We consider a perturbation used in [122, 119] of the form

$$\mathbf{H} = \sqrt{\frac{3}{2}} p(r) \left(\mathbf{z} \otimes \mathbf{z} - \frac{\mathbf{I}_3}{3} \right), \quad (5.153)$$

where $\mathbf{z} = (0, 0, 1)$ is the unit vector in z -direction. The associated second variation is

$$\delta^2 E = \int_0^R \left\{ p'^2 + p^2 \left(-t_1 + \frac{7t_3 s^2}{5} - \frac{22s^3}{25} + \frac{3}{5}(2t_4 + 1)s^4 \right) \right\} r^2 dr, \quad (5.154)$$

and minimizers must satisfy

$$p'' + \frac{2p'}{r} = p \left(-t_1 + \frac{7t_3 s^2}{5} - \frac{22s^3}{25} + \frac{3}{5}(2t_4 + 1)s^4 \right), \quad (5.155)$$

subject to $p'(0) = 0$ and $p(R) = 0$. We briefly remark on the suitability of this perturbation tensor. In [122, 119], the authors choose such a perturbation in order to mimic the structure of the biaxial torus defect. Specifically, this perturbation removes the singularity at the centre of Ω and replaces it with a uniaxial line in the z -axis, surrounded by a biaxial region. This perturbation is successfully used to prove the instability of the radial hedgehog with a fourth order potential in the low temperature limit and infinite domain ($t \rightarrow \infty$, $R \rightarrow \infty$) [122], and with large, but finite, t and R in [119]. Furthermore, in [141] the authors show local stability of the radial hedgehog reduces to proving the non-negativity of the functionals Φ_i , for $i \in \mathbb{N}$, defined to be

$$\Phi_0[v_0] := \frac{2}{3} \int_0^R \left\{ |v_0'|^2 + \frac{6v_0^2}{r^2} + g_1(s)v_0^2 \right\} r^2 dr, \quad (5.156)$$

$$\begin{aligned} \Phi_i[v_0, v_1, v_2] := \int_0^R \left\{ \frac{\lambda_i}{3} |v_0'|^2 + |v_1'|^2 + (\lambda_i - 2)|v_2'|^2 + \frac{1}{r^2} \left(\frac{\lambda_i(\lambda_i + 6)}{3} v_0^2 + (\lambda_i + 4)v_1^2 \right. \right. \\ \left. \left. + (\lambda_i - 2)^2 v_2^2 - 4\lambda_i v_0 v_1 + 4(\lambda_i - 2)v_1 v_2 \right) \right. \\ \left. + \frac{\lambda_i}{3} g_1(s)v_0^2 + g_2(s)v_1^2 + (\lambda_i - 2)g_3(s)v_2^2 \right\} r^2 dr, \end{aligned} \quad (5.157)$$

where $\lambda_i := i(i + 1)$ and the functions v_0 , v_1 and v_2 belong to the space

$$H^1(R) = \{v \in L^2([0, R]; dr) : v' \in L^2([0, R]; r^2 dr), v(R) = 0\}. \quad (5.158)$$

In [141], the authors work with a fourth order bulk potential and show that $\Phi_i \geq 0$ for all $i \geq 3$ if Φ_0, Φ_1 and $\Phi_2 \geq 0$. We note, as in [116], that this proof is dependent only on gradient terms of the the Landau-de Gennes energy and, therefore, can be naturally generalized to the sixth order bulk potential. The non-negativity of Φ_0 and Φ_1 is immediate from Theorem 2.4 and Proposition 4.1 of [141]. We do not attempt to show that $\Phi_2 \geq 0$, but observe if the minimizers of Φ_2 are to be non-zero at $r = 0$, then they must satisfy the relations

$$48v_0 - 24v_1 = 0, \quad 20v_1 + 16v_2 - 24v_0 = 0, \quad 16v_1 + 32v_2 = 0, \quad (5.159)$$

which has a single solution $v_0 = -v_2, v_1 = -2v_2, v_2 \in H^1(R)$. The functional Φ_2 simplifies to

$$\Phi_2[-v_2, -2v_2, v_2] = \int_0^R \{10|v_2'|^2 + (2g_1(s) + 4g_2(s) + g_3(s))v_2^2\} r^2 dr, \quad (5.160)$$

where

$$2g_1(s) + 4g_2(s) + g_3(s) = 10 \left(-t_1 + \frac{7t_3s^2}{5} - \frac{22s^3}{25} + \frac{3}{5}(2t_4 + 1)s^4 \right). \quad (5.161)$$

Therefore, analysis of the minimizers of the functional (5.154) is a first step in constructing a general proof of the local stability of the radial hedgehog defect.

We solve Equation (5.155) numerically using MATLAB's boundary value problem solvers [143]. Some solutions are shown in Figure 5.7. We compute critical values of $R^c(t_1, t_2, t_3, t_4)$, such that for all $R > R^c$, $\delta^2 E < 0$. For fixed t_2, t_3 and t_4 , this defines a stability curve in the R - t_1 plane. We show the results of such computations in Figure 5.8. It is interesting to note that as t_4 increases, we require large t_1 and R for the radial hedgehog to become unstable. This is explored further in the following section. This perturbation is also suitable for values of $t_4 < 1$, and extends the range

of instability found in Figure 5.6.

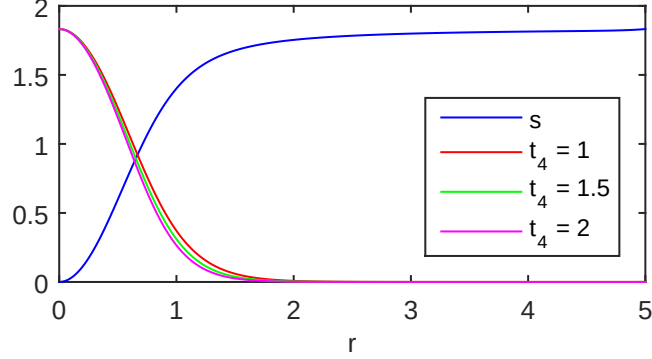


Figure 5.7: Radial hedgehog solution $s(r)$ and perturbations $p(r)$ for $t_1 = 10$, $t_2 = 1$, $t_3 = 2$, $R = 5$ and variable t_4 .

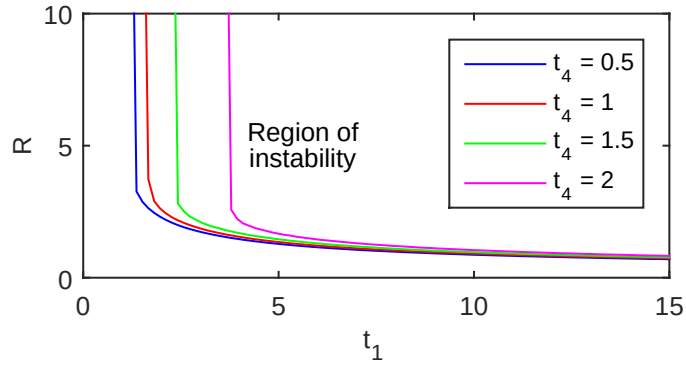


Figure 5.8: Critical value R^c for $t_2 = 1$, $t_3 = 2$ and variable t_4 .

5.4.5 Instability in the Low Temperature Limit

In the previous section we numerically demonstrated that the radial hedgehog is unstable for perturbations of the form

$$\mathbf{H} = \sqrt{\frac{3}{2}} p(r) \left(\mathbf{z} \otimes \mathbf{z} - \frac{\mathbf{I}_3}{3} \right), \quad (5.162)$$

for a wide range of parameters, provided t_4 is kept small. In this section, we explore the dependence on t_4 in more detail by working in the low temperature limit $t_1 \rightarrow \infty$.

We follow the procedure in [139, 122] used to study the effect of elastic anisotropy on the instability of the radial hedgehog with a fourth order potential.

We assume that the coefficients t_2 , t_3 and t_4 remain $O(1)$. From our bounds in Proposition 5.77, we know that for $t_1 \gg \max\{1, t_2, t_3\}$, the size of the defect core scales with $O\left(t_1^{-\frac{1}{2}}\right)$. Using this scaling as a guide, we introduce the rescaled radius $\hat{r} := \sqrt{t_1}r$ and rescaled order parameter $\hat{s}(\hat{r}) := \frac{s(r)}{s_+}$. From Equation (5.31), we know that $s_+ \sim t_1^{\frac{1}{4}}$. Taking the limit $t_1 \rightarrow \infty$, the governing equation for $\hat{s}$ is

$$\hat{s}'' + \frac{2\hat{s}'}{\hat{r}} - \frac{6\hat{s}}{\hat{r}^2} = -\hat{s} + \hat{s}^5, \quad (5.163)$$

subject to $\hat{s}(0) = 0$ and $\hat{s}(\hat{R}) = 1$, which is referred to as the ‘limiting rescaled problem’ [122].

We rewrite the second variation from Equation (5.154) in terms of $\hat{r}$, $\hat{s}$, $\hat{R} := \sqrt{t_1}R$ and $\hat{p} := \frac{p}{s_+}$ and take the limit $t_1 \rightarrow \infty$:

$$\delta^2 E \sim \delta^2 \hat{E} := \int_0^{\hat{R}} \hat{r}^2 \hat{p}'^2 + \hat{r}^2 \hat{p}^2 \left(-1 + \frac{3}{5}(2t_4 + 1)\hat{s}^4 \right) d\hat{r}. \quad (5.164)$$

In the limit as $\hat{R} \rightarrow \infty$, the function $\hat{s}$ is bounded above and below by

$$\frac{\hat{r}^2}{\hat{r}^2 + 14} \leq \hat{s}(\hat{r}) \leq \frac{\hat{r}^2}{\hat{r}^2 + \frac{3}{2}}. \quad (5.165)$$

This can be shown by considering the maxima and minima of the set given in (5.89) and taking the limit $t_1 \rightarrow \infty$. Using the upper bound, we find that

$$\delta^2 E < \int_0^\infty \hat{r}^2 \hat{p}'^2 + \hat{r}^2 \hat{p}^2 \left(-1 + \frac{3}{5}(2t_4 + 1) \left(\frac{\hat{r}^2}{\hat{r}^2 + \frac{3}{2}} \right)^4 \right) d\hat{r}. \quad (5.166)$$

By experimentation, we find that for a function

$$\hat{p}(r) = \frac{1}{(\hat{r}^2 + 3)^2}, \quad (5.167)$$

the second variation $\delta^2 \hat{E} < 0$ for all $t_4 < 1.016$. This estimate agrees with the behaviour identified for small t_4 in §5.4.3.

We are now interested to see if we can extend the range of t_4 for which $\delta^2 \hat{E} < 0$. By rearranging and normalizing (5.164), we derive an instability condition:

$$\lambda(t_4) := \inf_{\hat{p}} \frac{\int_0^{\hat{R}} \hat{r}^2 \hat{p}'^2 + \frac{3}{5}(2t_4 + 1) \hat{r}^2 \hat{p}^2 \hat{s}^4 d\hat{r}}{\int_0^{\hat{R}} \hat{p}^2 \hat{r}^2 d\hat{r}} < 1, \quad (5.168)$$

where $\hat{p}'(0) = 0$ and $\hat{p}(\hat{R}) = 0$.

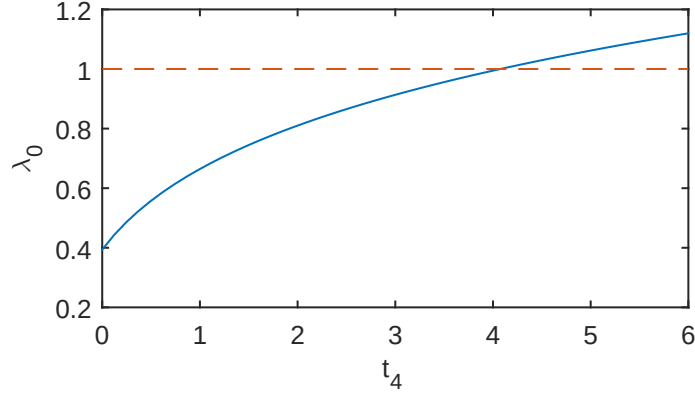
The extremal to the problem (5.168) is the solution to the eigenvalue problem

$$\hat{p}'' + \frac{2\hat{p}'}{\hat{r}} + \hat{p} \left(\lambda - \frac{3}{5}(2t_4 + 1) \hat{s}^4 \right) = 0, \quad (5.169)$$

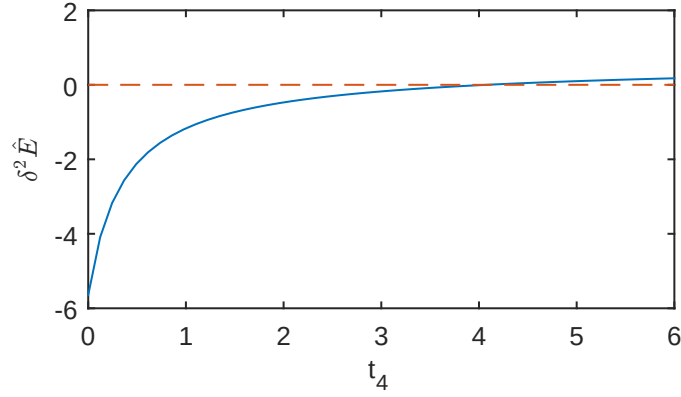
subject to $\hat{p}'(0) = 0$ and $\hat{p}(\hat{R}) = 0$. If the minimum eigenvalue $\lambda_0 < 1$, then the radial hedgehog solution will be unstable.

Using MATLAB's boundary value problem solvers [143], we can evaluate λ_0 for given t_4 and $\hat{R}$. In Figure 5.9, we plot computed values of λ_0 and $\delta^2 \hat{E}$ for $\hat{R} = 100$. We see that there is a critical value $t_4^c \approx 4$, such that for all $t_4 < t_4^c$, $\lambda_0(t_4) < 1$.

Using a bisection root-finding method, we can derive an estimate for t_4^c and the dependence on $\hat{R}$. In Figure 5.10, we plot the computed t_4^c in terms of $\hat{R}$ in the bisection method root-finder using a tolerance of 10^{-3} . The critical value t_4^c converges to a constant value $t_4^c = 4.07$, improving on the analytic bound of 1.016. This critical value is independent of $\hat{R}$ as $\hat{R} \rightarrow \infty$.



(a) Minimum eigenvalues λ_0 .



(b) Second variation evaluated for eigenfunction $\hat{p}_0$.

Figure 5.9: Numerically computed lowest eigenvalue of Equation (5.169), and second variation evaluated for the associated eigenfunction for $\hat{R} = 100$.

5.4.6 Discussion of the Role of t_4 on the Stability of the Radial Hedgehog

We have observed that for moderately large values of t_4 we are unable to find perturbations of the form given in Equation 5.153 that cause the radial hedgehog defect to lose stability. We now provide some justification for this behaviour.

For the fourth order potential, the loss of stability of the radial hedgehog is driven by the fact that the isotropic core is a local maximum of the bulk potential. Replacing the isotropic point with a line disclination replaces the isotropic core with a uniaxial region at the origin, surrounded by a torus of biaxiality where the director rotates from

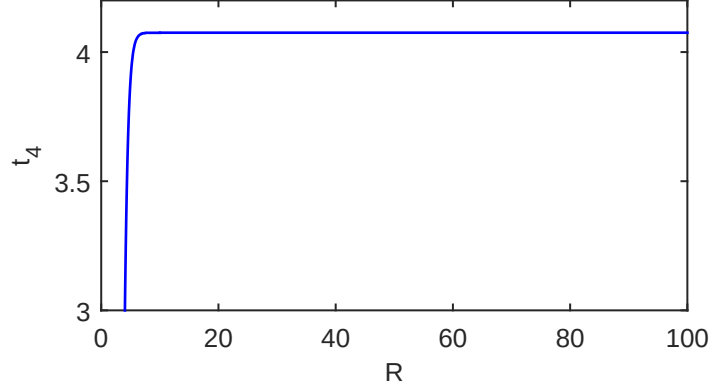


Figure 5.10: Estimate of t_4^c in terms of R .

a vertical alignment along the z -axis to the radial direction. Numerical studies of the biaxial torus show that regions of maximum biaxiality occur about the disclination [64, 126]. In terms of the order parameter h and the biaxiality parameter β introduced in §5.2.2, the fourth order potential is

$$g_4(h, \beta) = -\frac{th^2}{2} - h^3(1 - \beta) + \frac{h^4}{2}, \quad (5.170)$$

This potential has a global minimizer at $h_+ = \frac{3+\sqrt{9+8t}}{4}$ and $\beta = 0$. In the low temperature limit, the difference in the bulk potential between an isotropic point and the uniaxial minimum is

$$\Delta_{IU} = g_4(0, 0) - g_4(h_+, 0) \sim \frac{t^2}{8} + \frac{t^{\frac{3}{2}}}{\sqrt{8}} + O(t), \quad (5.171)$$

and the difference between the uniaxial minimum and the state with maximum biaxiality ($\beta = 1$) is

$$\Delta_{BU} = g_4\left(\sqrt{\frac{t}{2}}, 1\right) - g_4(h_+, 0) \sim \frac{t^{\frac{3}{2}}}{\sqrt{8}} + O(t). \quad (5.172)$$

The contribution to the Landau-de Gennes energy from a small biaxial region is negligible compared to the contribution from an isotropic point.

From §5.2.3, we know that the equivalent differences in the sixth order potential are

$$\Delta_{IU} = f_B(0, 0) - f_B(s_+, 0) \sim \frac{t_1^{\frac{3}{2}}}{3} + \frac{t_1^{\frac{5}{4}}}{5} + O(t_1), \quad (5.173)$$

and

$$\Delta_{BU} = f_B(\hat{q}_+, 1) - f_B(s_+, 0) \sim \frac{t_1^{\frac{3}{2}}}{3} \left(1 - \frac{1}{\sqrt{t_4}}\right) + \frac{t_1^{\frac{5}{4}}}{5} + O(t_1). \quad (5.174)$$

Unlike the fourth order potential, regions of maximum biaxiality have a contribution to the energy which is the same order of magnitude as the isotropic point. For large t_4 , this will require biaxial regions in Ω to be as small as possible. We suggest that it is this phenomenon which allows the radial hedgehog defect to regain local stability under certain classes of perturbations for large t_4 .

5.5 Summary

In this chapter, we have studied the properties of the radial hedgehog defect using the Landau-de Gennes theory with a sixth order potential. We have proven that the radial hedgehog defect is a critical point of Landau-de Gennes energy. By imposing some constraints on the coefficients of the bulk potential, we show the properties of the order parameter derived with the fourth potential generalize to the sixth order potential. Our solution includes the root of a quartic equation; we show that theory on the number of roots and bounds on roots of polynomials can be used to avoid working with explicit expressions for these roots.

We study the instability of the radial hedgehog under two classes of perturbations and identify three important parameter regions. For $t_4 < 1$, we prove that the radial hedgehog is unstable for suitably large R and t_1 by defining a perturbation which creates a large region of biaxiality. For $t_4 > 1$, we use a specific perturbation

motivated by previous work. We numerically calculate regions of instability in terms of the droplet radius R , rescaled temperature t_1 and sixth order coefficient t_4 . By analogy with [122], we consider the low temperature limit and find that the radial hedgehog is stable under this perturbation for some critical value of $t_4 \approx 4.07$. This stability under this class of perturbations does not guarantee the local stability of the radial hedgehog under all perturbations. This problem would be best addressed numerically using an approach similar to [64] in which the authors identify local and global minimizers of the Landau-de Gennes energy with a fourth order bulk potential in a droplet. It would be interesting to investigate if the biaxial torus defect is a local minima using a sixth order potential with large t_4 , or if new defect structures will emerge in this theory.

Chapter 6

Conclusions and Future Work

6.1 Conclusions

The aim of this thesis has been to explore multistability in simple geometries and understand the properties of defects in confinement. Through our work on liquid crystals in confinement, we gained insights into the role of defects, elastic anisotropy, geometrical aspect ratios and surface anchoring conditions on different equilibria. In our final problem, related to the fine structure of point defects, we carried out one of the first studies on the properties and stability of the radial hedgehog defect in the Landau-de Gennes theory with a sixth order bulk potential.

In Chapter 2, we study nematic equilibria in rectangular wells. This is motivated by bistability in shallow square wells. We derive exact analytic expressions for the director and Oseen-Frank energies of the three equilibria in the one-constant approximation. These expressions for energy separate the logarithmic contribution from the corner defects and a normalized energy due to the distortion of the liquid crystals in the bulk. We generalize these expressions for the director and energy to consider states with defects located inside the rectangle. We examine the energy landscape of a state with a $\pm\frac{1}{2}$ strength internal defect and identify some important features.

Applying these energy expressions to the problem of switching between different equilibria, we are able to identify two distinct energy minimizing pathways for an internal defect to move through the rectangle. Finally, we consider equilibria with unequal constants and derive an expression for the energies of the two lowest energy states in the small rectangular aspect ratio limit. We find that the diagonal state is the global energy minimum in the limit as the rectangular aspect ratio goes to zero; the difference between this state and the nearest low energy minimum is exponentially small.

In Chapter 3, we study the stability of the uniform state in a semi-infinite rectangular domain with weak tangential anchoring. We derive a condition on the loss of stability of the uniform state in terms of the extrapolation length and channel size. We demonstrate that the loss of stability is a supercritical bifurcation for all ratios of the elastic constants. In the one-constant approximation, we derive an asymptotic approximation to the energy in the large anchoring strength limit. This takes advantage of virtual defect solutions in the corner of the channels. We complete the bifurcation diagram using COMSOL, and cannot find any coexistence of an equilibrium with defect structures at the corners of the channel and the uniform state. We then apply our condition on the loss of stability to estimate an upper bound on the extrapolation length for the *fd*-virus.

In Chapter 4, we consider some problems related to nematic equilibria confined to an annulus. This is motivated by experiments on the nematic phases of *fd*-virus, which show the development of boundary defects for thick annuli. We study the defect-free state and calculate conditions for the loss of stability in the Oseen-Frank theory. We then consider a related problem in the Landau-de Gennes theory, and derive a condition for the local stability and global minimality of the defect-free state. Finally, we consider equilibria with boundary defects and calculate the associated one-constant Oseen-Frank energies. Here, we find that this theoretical treatment of

boundary defects is not sufficient to capture the experimentally observed behaviour, and we briefly introduce two possible parameter regimes, unequal elastic constants and weak anchoring, which could resolve this difference.

In Chapter 5, we study the radial hedgehog defect in the Landau-de Gennes theory with a sixth order bulk potential. The radial hedgehog defect is an example of a point defect, which has been widely studied using the fourth order bulk potential. We introduce the sixth order bulk potential and highlight some important properties of the critical points of the potential. We then show that the radial hedgehog is a critical point of the Landau-de Gennes energy with a sixth order bulk potential. Subject to some constraints on the coefficients of the bulk potential, we find that the order parameter of the radial hedgehog satisfies many of the properties derived with the fourth order bulk potential. We show that the radial hedgehog is locally stable for temperatures close to the critical temperatures and small droplet radii. We then consider the instability of the radial hedgehog defect. We identify three key parameter regimes based on the ratio of the sixth order coefficients of the bulk potential, denoted by the parameters E and F . If the sixth order coefficients satisfy $E < F$, then we induce an instability using a perturbation which creates a large region of biaxiality. If the sixth order coefficients satisfy $E > F$, then we make use of a perturbation which has been successful in predicting instability with the fourth order bulk potential. Using computational methods, we predict that the existence of some critical value of the ratio $\frac{E}{F} \approx 4$ for which this perturbation fails to induce instability. Physically, this ratio corresponds to biaxial structures and isotropic regions having comparable energy costs.

6.2 Future Work

The simplest extension to our work in Chapter 2 concerns our expressions for states with internal defects. These expressions can be generalized to include multiple internal defects by the introduction of a second discontinuity and branch cut. A more significant question concerns the role of elastic anisotropy on these defects, which might give a deeper understanding into why equilibria with only $-\frac{1}{2}$ strength defects are found experimentally using the *fd*-virus. Though this is difficult to implement analytically, numerical methods may offer more success. We note that our analytic expressions for the one-constant director field should make excellent initial conditions for computer simulations of this problem.

There are several natural extensions of our work in Chapter 3. Restricting the domain to a finite rectangular well instead of the semi-infinite domain may allow for multiple bifurcation points, as we expect perturbations corresponding to the lower energy diagonal state to occur for smaller values of α than the perturbations corresponding to the higher energy U_1 and U_2 states. An extension that might allow for the reported bistability is to include the effects of an order parameter and study a similar stability problem in the Landau-de Gennes theory.

Our work on the annular wells (Chapter 4) offers up several potential directions for studying equilibria with boundary defects. Our solutions based on annular sectors indicate that systems with weak anchoring or strong elastic anisotropy ($K_3 > K_1$) can support multiple stable equilibria. While we suggest that the weak anchoring behaviour might allow us to interpret the experimental work on the *fd*-virus, system with a strong elastic anisotropy offers the possibility of genuine multistability even in the strong anchoring limit for a wide range of annulus radii.

Finally, we consider some extensions to our work on the radial hedgehog defect in Chapter 5. Many of the properties and instability results in this chapter can be immediately generalized to systems with elastic anisotropy. We would expect that

a significantly larger splay elastic constant would reduce the critical temperature or droplet radius required to induce instability. Beyond this immediate extension, our work on the radial hedgehog opens up several important areas for further research on the fine structure of defects in the Landau-de Gennes theory. The sixth order coefficients allow the radial hedgehog to recover local stability under a particular class of perturbations, and it is obvious to ask if this behaviour holds under all perturbations. This question would most likely have to be answered numerically using an approach similar to [64], using a finite-element method to identify critical points and describe the bifurcation diagram. It would also be interesting to know if the biaxial torus defect remains a stable equilibrium for large values of t_4 , or if the preferential uniaxial ordering in this regime causes this defect to become unstable. If this behaviour holds, it would be interesting to investigate the structure of line disclinations using the sixth order theory. Similarly to point defects, line disclinations in the fourth order bulk potential are also reported to have biaxial internal structures. In §5.4.3, we noted that for $t_4 < 1$, the strong uniaxial anchoring conditions on the boundary of the droplet may not be the global minimizer of the bulk potential. Instead, a biaxial anchoring condition may be energetically preferable. The choice of anchoring conditions, as well as the structure of defects in biaxial nematics, has yet to be discussed. Our final open question concerns the values of the coefficients of the sixth order potential. So far, we have only been able to identify one set of coefficients in [132]. Unfortunately, these values fail to distinguish between the two sixth order coefficients, and in our variables correspond to $t_4 < 1$. We therefore believe it would be important to experimentally determine the values of the sixth order coefficients, particularly if numerical simulations demonstrate that the radial hedgehog defect is stable for large t_4 .

Appendix A

Expressions for Energies of States with Internal Defects

In this appendix, we give some further details on evaluating the Oseen-Frank energy of an equilibria within a rectangular well with an internal defect located at the point $(x, y) = (x_1, y_1)$.

A.1 Series Expansions

Here, we list the series which arise from evaluating terms (2) and (3) from Equation (2.80) in §2.3.2. The integrals in term (2) are:

$$\int_{C_1} \frac{\partial h}{\partial n} ds \sim \frac{m}{2} \ln \left(\frac{x_1^2 + y_1^2}{y_1^2 + (x_1 - 1)^2} \right) + O(\epsilon), \quad (\text{A.1})$$

$$\int_{C_2} \frac{\partial h}{\partial n} ds \sim \frac{m}{2} \ln \left(\frac{y_1^2 + (x_1 - 1)^2}{(x_1 - 1)^2 + (y_1 - \lambda)^2} \right) + O(\epsilon), \quad (\text{A.2})$$

$$\int_{C_3} \frac{\partial h}{\partial n} ds \sim \frac{m}{2} \ln \left(\frac{(x_1 - 1)^2 + (y_1 - \lambda)^2}{(y_1 - \lambda)^2 + x_1^2} \right) + O(\epsilon), \quad (\text{A.3})$$

$$\int_{C_4} \frac{\partial h}{\partial n} ds \sim \frac{m}{2} \ln \left(\frac{(y_1 - \lambda)^2 + x_1^2}{x_1^2 + y_1^2} \right) + O(\epsilon). \quad (\text{A.4})$$

The integrals in (3) can be evaluated exactly using the series expressions for the

functions g_i :

$$\int_{C_1} \frac{\partial g_1}{\partial n} ds = \sum_{n=1}^{\infty} A_n (1 - (-1)^n) \cos(n\pi\epsilon) \coth(n\pi\lambda), \quad (\text{A.5})$$

$$\int_{C_2} \frac{\partial g_1}{\partial n} ds = \sum_{n=1}^{\infty} A_n (-1)^n \left(\frac{\cosh(n\pi(\lambda - \epsilon)) - \cosh(n\pi\epsilon)}{\sinh(n\pi\lambda)} \right), \quad (\text{A.6})$$

$$\int_{C_3} \frac{\partial g_1}{\partial n} ds = \sum_{n=1}^{\infty} A_n (-1 + (-1)^n) \cos(n\pi\epsilon) \operatorname{csch}(n\pi\lambda), \quad (\text{A.7})$$

$$\int_{C_4} \frac{\partial g_1}{\partial n} ds = \sum_{n=1}^{\infty} -A_n \left(\frac{\cosh(n\pi(\lambda - \epsilon)) - \cosh(n\pi\epsilon)}{\sinh(n\pi\lambda)} \right), \quad (\text{A.8})$$

$$\int_{C_1} \frac{\partial g_2}{\partial n} ds = \sum_{n=1}^{\infty} -B_n \left(\frac{\cosh\left(\frac{n\pi(1-\epsilon)}{\lambda}\right) - \cosh\left(\frac{n\pi\epsilon}{\lambda}\right)}{\sinh\left(\frac{n\pi}{\lambda}\right)} \right), \quad (\text{A.9})$$

$$\int_{C_2} \frac{\partial g_2}{\partial n} ds = \sum_{n=1}^{\infty} B_n (1 - (-1)^n) \cos\left(\frac{n\pi\epsilon}{\lambda}\right) \coth\left(\frac{n\pi}{\lambda}\right), \quad (\text{A.10})$$

$$\int_{C_3} \frac{\partial g_2}{\partial n} ds = \sum_{n=1}^{\infty} B_n (-1)^n \left(\frac{\cosh\left(\frac{n\pi(1-\epsilon)}{\lambda}\right) - \cosh\left(\frac{n\pi\epsilon}{\lambda}\right)}{\sinh\left(\frac{n\pi}{\lambda}\right)} \right), \quad (\text{A.11})$$

$$\int_{C_4} \frac{\partial g_2}{\partial n} ds = \sum_{n=1}^{\infty} B_n (-1 + (-1)^n) \cos\left(\frac{n\pi\epsilon}{\lambda}\right) \operatorname{csch}\left(\frac{n\pi}{\lambda}\right), \quad (\text{A.12})$$

$$\int_{C_1} \frac{\partial g_3}{\partial n} ds = \sum_{n=1}^{\infty} C_n (-1 + (-1)^n) \cos(n\pi\epsilon) \operatorname{csch}(n\pi\lambda) \quad (\text{A.13})$$

$$\int_{C_2} \frac{\partial g_3}{\partial n} ds = \sum_{n=1}^{\infty} C_n (-1)^n \left(\frac{\cosh(n\pi(\lambda - \epsilon)) - \cosh(n\pi\epsilon)}{\sinh(n\pi\lambda)} \right), \quad (\text{A.14})$$

$$\int_{C_3} \frac{\partial g_3}{\partial n} ds = \sum_{n=1}^{\infty} C_n (1 - (-1)^n) \cos(n\pi\epsilon) \coth(n\pi\lambda), \quad (\text{A.15})$$

$$\int_{C_4} \frac{\partial g_3}{\partial n} ds = \sum_{n=1}^{\infty} -C_n \left(\frac{\cosh(n\pi(\lambda - \epsilon)) - \cosh(n\pi\epsilon)}{\sinh(n\pi\lambda)} \right), \quad (\text{A.16})$$

$$\int_{C_1} \frac{\partial g_4}{\partial n} ds = \sum_{n=1}^{\infty} -D_n \left(\frac{\cosh\left(\frac{n\pi(1-\epsilon)}{\lambda}\right) - \cosh\left(\frac{n\pi\epsilon}{\lambda}\right)}{\sinh\left(\frac{n\pi}{\lambda}\right)} \right), \quad (\text{A.17})$$

$$\int_{C_2} \frac{\partial g_4}{\partial n} ds = \sum_{n=1}^{\infty} D_n (-1 + (-1)^n) \cos\left(\frac{n\pi\epsilon}{\lambda}\right) \operatorname{csch}\left(\frac{n\pi}{\lambda}\right), \quad (\text{A.18})$$

$$\int_{C_3} \frac{\partial g_4}{\partial n} ds = \sum_{n=1}^{\infty} D_n (-1)^n \left(\frac{\cosh\left(\frac{n\pi(1-\epsilon)}{\lambda}\right) - \cosh\left(\frac{n\pi\epsilon}{\lambda}\right)}{\sinh\left(\frac{n\pi}{\lambda}\right)} \right), \quad (\text{A.19})$$

$$\int_{C_4} \frac{\partial g_4}{\partial n} ds = \sum_{n=1}^{\infty} D_n (1 - (-1)^n) \cos\left(\frac{n\pi\epsilon}{\lambda}\right) \coth\left(\frac{n\pi}{\lambda}\right). \quad (\text{A.20})$$

These integrals can be evaluated numerically for some values of x_1 , y_1 , λ and ϵ , or can be further simplified by considering the asymptotic behaviour as $\epsilon \rightarrow 0$ and using the functions s_1 and s_2 defined in (2.32) and (2.38). Using Equation (A.5) as an example, we first define the limiting Fourier coefficients

$$A_e := \lim_{n \rightarrow \infty} 2n A_{2n}, \quad A_o := \lim_{n \rightarrow \infty} (2n+1) A_{2n+1}, \quad (\text{A.21})$$

then, using the odd limit (A_o),

$$\int_{C_1} \frac{\partial g_1}{\partial n} ds = \sum_{n=1}^{\infty} A_n (1 - (-1)^n) \cos(n\pi\epsilon) \coth(n\pi\lambda), \quad (\text{A.22})$$

$$\begin{aligned} & \sim 2 \sum_{n=0}^{\infty} \left(A_{2n+1} - \frac{A_o}{2n+1} \right) \coth((2n+1)\pi\lambda) \\ & + A_o \left(\log\left(\frac{2}{\pi\epsilon}\right) + s_1(\lambda) \right) + O(\epsilon^2). \end{aligned} \quad (\text{A.23})$$

A.2 Asymptotic Expression of the Energy

Here, we list the asymptotic expression of the Oseen-Frank energy used in §2.3.3 to calculate the contour plots and energy barriers, with $a_1 = a_3 = 0$, $a_2 = a_4 = \frac{\pi}{2}$ and $s = -\frac{1}{2}$.

We first define two additional series expansions

$$s_3(\lambda) := \sum_{n=1}^{\infty} \frac{\coth(2n\pi\lambda) - 1}{n}, \quad (\text{A.24})$$

$$s_4(\lambda) := \sum_{n=1}^{\infty} \frac{\text{csch}(2n\pi\lambda)}{n}, \quad (\text{A.25})$$

and define the remaining limiting Fourier coefficients B_o , B_e , C_o , C_e , D_o and D_e analogously to (A.21).

The normalized energy is

$$E[\theta]/K \sim \frac{1}{2} (E_1 + E_2 + E_3 + E_4 + E_5) + O(\epsilon), \quad (\text{A.26})$$

where

$$E_1 := \pi \left(\ln \left(\frac{2\lambda}{\pi} \right) + s_1 \left(\frac{1}{\lambda} \right) - s_2 \left(\frac{1}{\lambda} \right) \right), \quad (\text{A.27})$$

$$\begin{aligned} E_2 := & \frac{\pi}{4} \left(\sum_{n=0}^{\infty} \left(\frac{A_o + C_o}{2n+1} - A_{2n+1} - C_{2n+1} \right) (\coth((2n+1)\pi\lambda) - \text{csch}((2n+1)\pi\lambda)) \right. \\ & + (A_o + C_o) \left(-\ln \left(\frac{2}{\pi\epsilon} \right) - s_1(\lambda) + s_2(\lambda) \right) \\ & - \sum_{n=0}^{\infty} \left(\frac{B_o + D_o}{2n+1} - B_{2n+1} - D_{2n+1} \right) \left(\coth \left(\frac{(2n+1)\pi}{\lambda} \right) - \text{csch} \left(\frac{(2n+1)\pi}{\lambda} \right) \right) \\ & \left. + (B_o + D_o) \left(\ln \left(\frac{2\lambda}{\pi\epsilon} \right) + s_1 \left(\frac{1}{\lambda} \right) - s_2 \left(\frac{1}{\lambda} \right) \right) \right), \end{aligned} \quad (\text{A.28})$$

$$E_3 := \frac{\pi}{2} \ln \left(\frac{\sqrt{(\lambda - y_1)^2 + x_1^2}}{\epsilon} \right), \quad (\text{A.29})$$

$$E_4 := \frac{\pi}{4} \ln \left(\sqrt{\frac{x_1 + y_1^2}{x_1^2 + (\lambda - y_1)^2}} \right) + \frac{\pi}{4} \ln \left(\sqrt{\frac{(x_1 - 1)^2 + (\lambda - y_1)^2}{(x_1 - 1)^2 + y_1^2}} \right), \quad (\text{A.30})$$

$$\begin{aligned}
E_5 := & \pi \left(\sum_{n=1}^{\infty} \frac{A_n (\cos(n\pi x_1) \cosh(n\pi(\lambda - y_1)) - 1)}{\sinh(\lambda n\pi)} \right. \\
& + \frac{B_n (\cosh(\frac{n\pi x_1}{\lambda}) \cos(\frac{n\pi y_1}{\lambda}) + (-1)^{n+1})}{\sinh(\frac{n\pi}{\lambda})} \\
& + \frac{C_e}{2} \left(\ln\left(\frac{1}{2\pi\epsilon}\right) + s_3(\lambda) \right) + \frac{C_o}{2} \left(\ln\left(\frac{2}{\pi\epsilon}\right) + s_1(\lambda) \right) \\
& + \sum_{n=1}^{\infty} \left(C_{2n} - \frac{C_e}{2n} \right) \coth(2n\pi\lambda) + \sum_{n=0}^{\infty} \left(C_{2n+1} - \frac{C_o}{2n+1} \right) \coth((2n+1)\pi\lambda) \\
& - \sum_{n=1}^{\infty} \frac{C_n \cos\left(\frac{n\pi x_1 \sqrt{(\lambda-y_1)^2 + x_1^2}}{\sqrt{\lambda^2 - 2\lambda y_1 + x_1^2 + y_1^2}}\right) \cosh\left(n\pi \left(\lambda - \frac{\sqrt{(\lambda-y_1)^2 + x_1^2}(\lambda-y_1)}{\sqrt{\lambda^2 - 2\lambda y_1 + x_1^2 + y_1^2}}\right)\right)}{\sinh(\lambda n\pi)} \\
& - \sum_{n=1}^{\infty} \frac{D_n \left(e^{-\frac{n\pi(x_1-y_1 i)}{\lambda}} + e^{-\frac{n\pi(x_1+y_1 i)}{\lambda}} \right) \left(\coth\left(\frac{n\pi}{\lambda}\right) - e^{\frac{2n\pi x_1}{\lambda}} + e^{\frac{2n\pi x_1}{\lambda}} \coth\left(\frac{n\pi}{\lambda}\right) + 1 \right)}{4} \\
& - \sum_{n=1}^{\infty} \left(-D_{2n} + \frac{D_e}{2n} \right) \coth\left(\frac{2n\pi}{\lambda}\right) - \sum_{n=0}^{\infty} \left(D_{2n+1} - \frac{D_o}{2n+1} \right) \coth\left(\frac{(2n+1)\pi}{\lambda}\right) \\
& + \frac{D_e}{2} \left(\ln\left(\frac{\lambda}{2\pi\epsilon}\right) + s_3\left(\frac{1}{\lambda}\right) \right) - \frac{D_o}{2} \left(\ln\left(\frac{2\lambda}{\pi\epsilon}\right) + s_1\left(\frac{1}{\lambda}\right) \right), \tag{A.31}
\end{aligned}$$

$$\begin{aligned}
E_6 := & \pi \left(\sum_{n=0}^{\infty} \frac{2 \cos\left(\frac{\pi y_1 (2n+1)}{\lambda}\right) \coth\left(\frac{\pi (2n+1)}{\lambda}\right) + \operatorname{csch}\left(\frac{\pi y_1 (2n+1)}{\lambda}\right)}{2n+1} \right. \\
& + \sum_{n=0}^{\infty} 2 \cos\left(\frac{\pi y_1 (2n+1)}{\lambda}\right) \left(\sinh\left(\frac{\pi x_1 (2n+1)}{\lambda}\right) \right. \\
& \quad \left. \left. - \coth\left(\frac{\pi (2n+1)}{\lambda}\right) \cosh\left(\frac{\pi x_1 (2n+1)}{\lambda}\right) \right) \right. \\
& \quad \left. - \left(\ln\left(\frac{2\lambda}{\pi\epsilon}\right) + s_1(\lambda) \right) \right). \tag{A.32}
\end{aligned}$$

We now provide some brief tests of this expression of the energy. The total defect strength is $\frac{5}{4}$ and, therefore, we expect the energy to scale with $\frac{5}{4}\pi \ln\left(\frac{1}{\epsilon}\right)$ for any x_1, y_1 and λ . Due to the nature of the limiting Fourier coefficients, we are unable to prove this. However, numerical evaluation of Equation (A.26) shows that this scaling law holds.

For square wells (with $\lambda = 1$), the director field is uniform on the lines C_5 and C_6 about the branch cut when the internal defect is on the line $(x_1, 1 - x_1)$. Therefore,

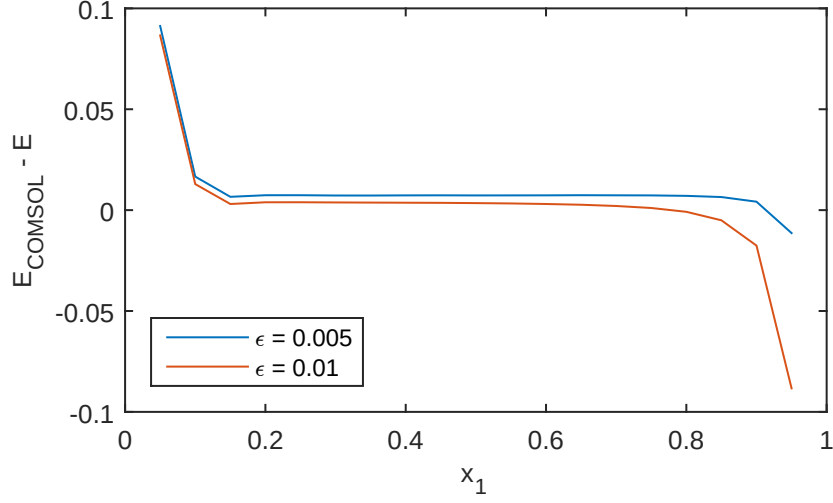


Figure A.1: Comparison between the asymptotic expression for the energy (Equation (A.26)) and energy calculated using COMSOL, with $\lambda = 1$ and the internal defect constrained to the line $(x_1, 1 - x_1)$.

we can solve for θ using COMSOL (see Appendix B) and evaluate the associated energy. In Figure A.1, we see that there is a close agreement between our expression for the energy and the numerically evaluated energy from COMSOL. As the internal defect approaches the corners, we find that this agreement breaks down, although the error remains $O(\epsilon)$. We also expect square wells to exhibit symmetry about the line $y_1 = 1 - x_1$, so $E(x_1, y_1) = E(1 - y_1, 1 - x_1)$. Numerical evaluation of (A.26) shows this relation holds for $\lambda = 1$.

Appendix B

COMSOL

In this appendix, we provide a brief overview of COMSOL, a commercially available finite element method solver [144]. We make use of COMSOL to gain insights into problems where the nonlinearity of the governing equations makes it difficult to make analytic progress, such as elastic anisotropy or weak anchoring conditions.

For the rectangular and annular sector problems with elastic anisotropy or weak anchoring, we create a domain Ω using COMSOL's shape drawing. If we implement strong anchoring conditions, we introduce arcs in each corner as shown in Figure B.1. This has the effect of improving the resolution of the mesh near the defects, and allows us to evaluate the regularized energy with defects removed.

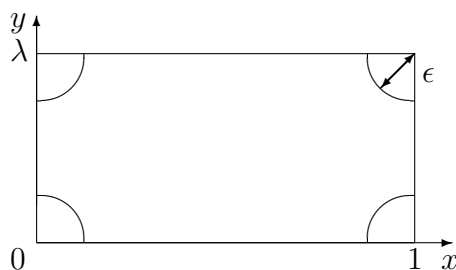


Figure B.1: The rectangular domain Ω for meshing.

We use COMSOL's default mesh algorithms, which have a number of preset element sizes. For our work in the thesis, we typically use COMSOL's 'Finer' mesh,

with a minimum element size 1.25×10^{-4} and a maximum element size of 0.037. We demonstrate the suitability of this mesh size by solving the one-constant strong anchoring problem in a rectangle and comparing with our analytic results. As we see in Figure B.2, the accuracy of our analytic expressions and COMSOL's results is on the order of the defect size ϵ . The only time when this has a significant impact on our work is when comparing our exponentially small difference in the D and U_1 states in §2.4.3, where we must ensure that our defect size $\epsilon < \exp\left(\frac{1}{\lambda}\right)$.

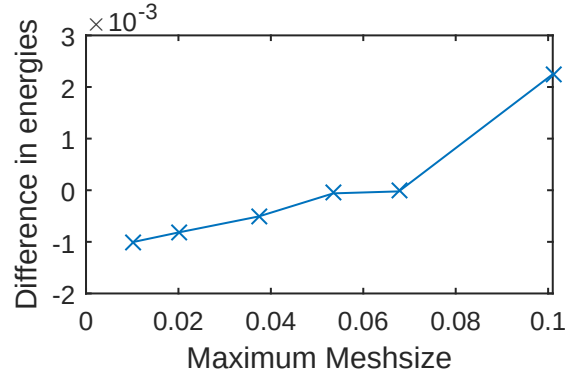


Figure B.2: Comparison of estimate of Oseen-Frank energy of the diagonal state rectangle with $\lambda = 0.4$ and $\epsilon = 0.005$ versus maximum mesh size.

Appendix C

Hardy's Decomposition Trick

In this appendix, we provide a brief summary of Hardy's decomposition trick [116], which we use in the study of the second variation of the Landau-de Gennes energy about the defect-free state in an annulus (§4.3) and the radial hedgehog point defect (§5.4.3).

C.1 The Defect-Free State in an Annulus

We define s to be the solution to the differential equation

$$s'' + \frac{s'}{r} - \frac{4s}{r^2} = g'(s), \tag{C.1}$$

subject to $s(1) = s(b) = \frac{1}{\sqrt{2}}$, where g is a polynomial in terms of s . We are interested in simplifying the functional

$$I[v] := \int_b^1 \left(v'^2 + \frac{av^2}{r^2} + v^2 f(s) \right) r \, dr, \tag{C.2}$$

where v is subject to $v(1) = v(b) = 0$, f is a polynomial in terms of s and $a \in \mathbb{R}$. We let $v(r) = s(r)V(r)$, where $V(1) = V(b) = 0$, and consider

$$\int_b^1 v'^2 r \, dr = \int_b^1 (s'V + sV')^2 r \, dr \quad (\text{C.3})$$

$$= \int_b^1 (s'^2 V^2 + 2ss'VV' + s^2 V'^2) r \, dr. \quad (\text{C.4})$$

We consider the first term in (C.4) and integrate by parts

$$\int_b^1 s'^2 V^2 r \, dr = r s s' V^2 \Big|_b^1 - \int_b^1 V^2 s s' + 2r s s' V V' + r s s'' V^2 \, dr. \quad (\text{C.5})$$

Therefore, using Equation (C.1) we find that the functional $I[v]$ simplifies to

$$I[sV] = \int_b^1 s^2 V'^2 r - r s V^2 \left(s'' + \frac{s'}{r} \right) + \frac{a s^2 V^2}{r} + s^2 V^2 f(s) r \, dr \quad (\text{C.6})$$

$$= \int_b^1 s^2 V'^2 r + \frac{(a-4)s^2 V^2}{r} + (f(s) - s g'(s)) s^2 V^2 r \, dr. \quad (\text{C.7})$$

C.2 The Radial Hedgehog Defect

We define s to be the solution to the ordinary differential equation

$$s'' + \frac{2s'}{r} - \frac{6s}{r^2} = g'(s), \quad (\text{C.8})$$

subject to $s(R) = s_+$ and $s(0) = 0$, where s_+ is a local minimizer of the polynomial g . We then consider the functional

$$I[v] := \int_0^R \left(v'^2 + \frac{a v^2}{r^2} + v^2 f(s) \right) r^2 \, dr, \quad (\text{C.9})$$

where v is subject to $v(R) = v(0) = 0$, f is a polynomial in terms of s and $a \in \mathbb{R}$.

We let $v(r) = s(r)V(r)$, where $V(R) = V(0) = 0$, and consider

$$\int_0^R v'^2 r^2 \, dr = \int_0^R (s'V + sV')^2 r^2 \, dr \quad (\text{C.10})$$

$$= \int_0^R (s'^2 V^2 + 2ss'VV' + s^2 V'^2) r^2 \, dr. \quad (\text{C.11})$$

We consider the first term in (C.11) and integrate by parts

$$\int_0^R s'^2 V^2 r^2 \, dr = r s s' V^2 \Big|_0^R - \int_0^R 2r V^2 s s' + 2r^2 s s' V V' + r^2 s s'' V^2 \, dr. \quad (\text{C.12})$$

Therefore, using Equation (C.8) we find that the functional $I[v]$ simplifies to

$$I[sV] = \int_0^R s^2 V'^2 r^2 - r^2 s V^2 \left(s'' + \frac{2s'}{r} \right) + a s^2 V^2 + s^2 V^2 f(s) r^2 \, dr \quad (\text{C.13})$$

$$= \int_0^R s^2 V'^2 r^2 + (a - 6) s^2 V^2 + (f(s) - s g'(s)) s^2 V^2 r^2 \, dr. \quad (\text{C.14})$$

Appendix D

Summary of Integrals for Regularized Annular Sectors

Here, we list the asymptotic approximations for the integrals about the edges of the regularized annular sector Ω_N discussed in § 4.4.2.

The integrals from the arcs γ_i are:

$$\int_{\gamma_1} \theta \frac{\partial \theta}{\partial v} ds \sim -\frac{2a_1}{\pi^2} ((a_0 + a_2)\pi + a_1) \epsilon + O(\epsilon^2), \quad (\text{D.1})$$

$$\int_{\gamma_2} \theta \frac{\partial \theta}{\partial v} ds \sim \frac{2(\pi^2 a_0 + a_1 N + 2a_2 \pi)(a_0 \pi N + a_2 \pi N - 2a_2 \pi - a_1 N) \epsilon}{N^2 \pi^2} + O(\epsilon^2), \quad (\text{D.2})$$

$$\int_{\gamma_3} \theta \frac{\partial \theta}{\partial v} ds \sim \frac{2(a_0 \pi N + a_4 \pi N + 2a_4 \pi + a_3 N)(a_3 N + \pi^2 a_0 + 2a_4 \pi) \epsilon}{N^2 \pi^2 b} + O(\epsilon^2), \quad (\text{D.3})$$

$$\int_{\gamma_4} \theta \frac{\partial \theta}{\partial v} ds \sim -\frac{2a_3}{\pi^2 b} ((a_0 + a_4)\pi - a_3) \epsilon + O(\epsilon^2). \quad (\text{D.4})$$

The integrals about the edge C_3 are:

$$\int_{C_3} \frac{\partial f_1}{\partial v} ds = \frac{s_1(N, b)}{2\pi} - \frac{s_2(N, b)}{2\pi} - \frac{2}{\pi} \ln \left(\frac{4}{N\epsilon} \right) + \frac{\epsilon}{\pi} + O(\epsilon^2), \quad (\text{D.5})$$

$$\int_{C_3} \frac{\partial f_2}{\partial v} ds = \frac{s_3(N, b)}{2N} - \frac{s_4(N, b)}{2N} - \frac{4}{N} \ln \left(\frac{2}{N\epsilon} \right) + \left(\frac{2-N}{N} \right) \epsilon + O(\epsilon^2), \quad (\text{D.6})$$

$$\int_{C_3} \frac{\partial f_3}{\partial v} ds = \frac{s_1(N, b)}{2\pi} - \frac{s_2(N, b)}{2\pi} - \frac{2}{\pi} \ln \left(\frac{4b}{N\epsilon} \right) - \frac{\epsilon}{\pi b} + O(\epsilon^2), \quad (\text{D.7})$$

$$\int_{C_3} \frac{\partial f_4}{\partial v} ds = \frac{s_3(N, b)}{2N} - \frac{s_4(N, b)}{2N} - \frac{4}{N} \ln \left(\frac{2b}{N\epsilon} \right) - \left(\frac{N+2}{N} \right) \epsilon + O(\epsilon^2). \quad (\text{D.8})$$

The integrals about the edge C_2 are:

$$\int_{C_2} \frac{\partial f_1}{\partial v} ds = -\frac{s_1(N, b)}{\pi} + \frac{4}{\pi} \ln \left(\frac{4}{N\epsilon} \right) + O(\epsilon^2), \quad (\text{D.9})$$

$$\int_{C_2} \frac{\partial f_2}{\partial v} ds = -\frac{s_1(N, b)}{N} + \frac{4}{N} \ln \left(\frac{4}{N\epsilon} \right) + O(\epsilon^2), \quad (\text{D.10})$$

$$\int_{C_2} \frac{\partial f_3}{\partial v} ds = \frac{s_2(N, b)}{\pi} + O(\epsilon^2), \quad (\text{D.11})$$

$$\int_{C_2} \frac{\partial f_4}{\partial v} ds = \frac{s_2(N, b)}{N} + O(\epsilon^2), \quad (\text{D.12})$$

$$\int_{C_2} \phi \frac{\partial f_1}{\partial v} ds = -\frac{s_1(N, b)}{N} + \frac{4}{N} \ln \left(\frac{4}{N\epsilon} \right) + O(\epsilon^2), \quad (\text{D.13})$$

$$\int_{C_2} \phi \frac{\partial f_2}{\partial v} ds = -\frac{\pi}{N^2} s_3(N, b) + \frac{8\pi}{N^2} \ln \left(\frac{2}{N\epsilon} \right) + \frac{4\epsilon}{N} + O(\epsilon^2), \quad (\text{D.14})$$

$$\int_{C_2} \phi \frac{\partial f_3}{\partial v} ds = \frac{s_2(N, b)}{N} + O(\epsilon^2), \quad (\text{D.15})$$

$$\int_{C_2} \phi \frac{\partial f_4}{\partial v} ds = \frac{\pi}{N^2} s_4(N, b) + O(\epsilon^2). \quad (\text{D.16})$$

The integrals about the edge C_4 are:

$$\int_{C_4} \frac{\partial f_1}{\partial v} ds = \frac{s_2(N, b)}{\pi} + O(\epsilon^2), \quad (\text{D.17})$$

$$\int_{C_4} \frac{\partial f_2}{\partial v} ds = \frac{s_2(N, b)}{N} + O(\epsilon^2), \quad (\text{D.18})$$

$$\int_{C_4} \frac{\partial f_3}{\partial v} ds = -\frac{s_1(N, b)}{\pi} + \frac{4}{\pi} \ln \left(\frac{4b}{N\epsilon} \right) O(\epsilon^2), \quad (\text{D.19})$$

$$\int_{C_4} \frac{\partial f_4}{\partial v} ds = -\frac{s_1(N, b)}{N} + \frac{4}{N} \ln \left(\frac{4b}{N\epsilon} \right) O(\epsilon^2), \quad (\text{D.20})$$

$$\int_{C_4} \phi \frac{\partial f_1}{\partial v} ds = \frac{s_2(N, b)}{N} + O(\epsilon^2), \quad (\text{D.21})$$

$$\int_{C_4} \phi \frac{\partial f_2}{\partial v} ds = \frac{\pi}{N^2} s_4(N, b) + O(\epsilon^2), \quad (\text{D.22})$$

$$\int_{C_4} \phi \frac{\partial f_3}{\partial v} ds = -\frac{s_1(N, b)}{N} + \frac{4}{N} \ln \left(\frac{4b}{N\epsilon} \right) + O(\epsilon^2), \quad (\text{D.23})$$

$$\int_{C_4} \phi \frac{\partial f_4}{\partial v} ds = -\frac{\pi}{N^2} s_3(N, b) + \frac{8\pi}{N^2} \ln \left(\frac{2b}{N\epsilon} \right) + \frac{4\epsilon}{Nb} + O(\epsilon^2). \quad (\text{D.24})$$

Bibliography

- [1] P. G. de Gennes and J. Prost. *The Physics of Liquid Crystals*, volume 83 of *International Series of Monographs on Physics*. Oxford University Press, Second edition, 1998.
- [2] E. G. Virga. *Variational Theories for Liquid Crystals*. Applied Mathematics. Taylor & Francis, 1995.
- [3] A. M. Fox. *Optical Properties of Solids*. Oxford Master Series in Condensed Matter Physics. Oxford University Press, 2001.
- [4] H. Maeda and Y. Maeda. Liquid crystal formation in suspensions of hard rodlike colloidal particles: Direct observation of particle arrangement and self-ordering behavior. *Phys. Rev. Lett.*, 90:018303, Jan 2003.
- [5] S. Chandrasekhar, B. K. Sadashiva, and K. A. Suresh. Liquid crystals of disc-like molecules. *Pramana*, 9(5):471–480, 1977.
- [6] E. van den Pol, D. M. E. Thies-Weesie, A. V. Petukhov, D. V. Byelov, and G. J. Vroege. Uniaxial and biaxial liquid crystal phases in colloidal dispersions of board-like particles. *Liq. Cryst.*, 37(6–7):641–651, 2010.
- [7] F. Reinitzer. Contributions to the knowledge of cholesterol. *Liq. Cryst.*, 5(1):7–18, 1989.

- [8] Michael J. Stephen and Joseph P. Straley. Physics of liquid crystals. *Rev. Mod. Phys.*, 46:617–704, Oct 1974.
- [9] T. E. Strzelecka, M. W. Davidson, and R. L. Rill. Multiple liquid crystal phases of DNA at high concentrations. *Nature*, 331:457–460, February 1988.
- [10] F. C. Bawden, N. W. Pirie, J. D. Bernal, and I. Fankuchen. Liquid crystalline substances from virus-infected plants. *Nature*, 138:1051–1052, 1936.
- [11] Z. Dogic and S. Fraden. Ordered phases of filamentous viruses. *Curr. Opin. Colloid Interface Sci.*, 11(1):47–55, 2006.
- [12] A. H. Lewis, I. Garlea, J. Alvarado, O. J. Dammone, P. D. Howell, A. Majumdar, B. M. Mulder, M. P. Lettinga, G. H. Koenderink, and D. G. A. L. Aarts. Colloidal liquid crystals in rectangular confinement: theory and experiment. *Soft Matter*, 10:7865–7873, 2014.
- [13] N. J. Mottram and C. J. P. Newton. Introduction to Q-tensor theory. Technical report, University of Strathclyde, 2014.
- [14] E. B. Priestly. Liquid crystal mesophases. In E. B. Priestly, P. J. Wojtowicz, and P. Sheng, editors, *Introduction to Liquid Crystals*. Plenum Press, 1975.
- [15] P. Oswald and P. Pieranski. *Smectic and Columnar Liquid Crystals: Concepts and Physical Properties Illustrated by Experiments*. Liquid Crystals Book Series. Taylor & Francis, 2005.
- [16] E. Grelet. Hexagonal order in crystalline and columnar phases of hard rods. *Phys. Rev. Lett.*, 100:168301, Apr 2008.
- [17] I. W. Stewart. *The Static and Dynamic Continuum Theory of Liquid Crystals: A Mathematical Introduction*. Liquid Crystals Book Series. Taylor & Francis, 2004.

- [18] G. W. Gray and S. M. Kelly. Liquid crystals for twisted nematic display devices. *J. Mater. Chem.*, 9:2037–2050, 1999.
- [19] M. Oh-e and K. Kondo. Electro-optical characteristics and switching behavior of the in-plane switching mode. *Appl. Phys. Lett.*, 67(26):3895–3897, 1995.
- [20] D. W. Berreman and W. R. Heffner. New bistable liquid-crystal twist cell. *J. Appl. Phys.*, 52(4):3032–3039, 1981.
- [21] E. Willman, F. A. Fernandez, R. James, and S. E. Day. Switching dynamics of a post-aligned bistable nematic liquid crystal device. *J. Display Technol.*, 4(3):276–281, Sept 2008.
- [22] A. Majumdar, C. J. P. Newton, J. M. Robbins, and M. Zyskin. Topology and bistability in liquid crystal devices. *Phys. Rev. E*, 75:051703, May 2007.
- [23] A. Raisch and A. Majumdar. Order reconstruction phenomena and temperature-driven dynamics in a 3D zenithally bistable device. *EPL*, 107(1):16002, 2014.
- [24] T. J. Spencer, C. M. Care, R. M. Amos, and J. C. Jones. Zenithal bistable device: Comparison of modeling and experiment. *Phys. Rev. E*, 82:021702, Aug 2010.
- [25] C. W. Oseen. The theory of liquid crystals. *Trans. Faraday Soc.*, 29:883–899, 1933.
- [26] F. C. Frank. I. liquid crystals. on the theory of liquid crystals. *Discuss. Faraday Soc.*, 25:19–28, 1958.
- [27] R. Hardt, D. Kinderlehrer, and F.-H. Lin. Existence and partial regularity of static liquid crystal configurations. *Commun. Math. Phys.*, 105(4):547–570, 1986.

- [28] H. Brezis, J.-M. Coron, and E. H. Lieb. Harmonic maps with defects. *Commun. Math. Phys.*, 107(4):649–705, 1986.
- [29] I. Haller. Elastic Constants of the Nematic Liquid Crystalline Phase of p-Methoxybenzylidene-p-n-Butylaniline (MBBA). *J. Chem. Phys.*, 57:1400–1405, August 1972.
- [30] A. Rapini and M. Papoular. Distorsion d’une lamelle nématique sous champ magnétique conditions d’ancrage aux parois. *J. Phys., Colloq.*, 30:54–56, Nov-Dec 1969.
- [31] J. L. Ericksen. Liquid crystals with variable degree of orientation. *Arch. Rational Mech. Anal.*, 113(2):97–120, 1991.
- [32] A. Majumdar and A. Zarnescu. Landau-de Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond. *Arch. Rational Mech. Anal.*, 196(1):227–280, 2010.
- [33] H. Mori, E. C. Gartland Jr., J. R. Kelly, and P. J. Bos. Multidimensional director modeling using the Q tensor representation in a liquid crystal cell and its application to the π cell with patterned electrodes. *Jpn. J. Appl. Phys.*, 38(1R):135, 1999.
- [34] P. J. Wojtowicz, P. Sheng, and E. B. Priestley. *Introduction to Liquid Crystals*. Springer, 1975.
- [35] J. M. Ball and A. Majumdar. Nematic liquid crystals: from Maier-Saupe to a continuum theory. *Mol. Cryst. Liq. Cryst.*, 525(1):1–11, 2010.
- [36] D. Allender and L. Longa. Landau–de Gennes theory of biaxial nematics reexamined. *Phys. Rev. E*, 78(1):011704, 2008.

- [37] T. A. Davis and E. C. Gartland Jr. Finite element analysis of the Landau-de Gennes minimization problem for liquid crystals. *SIAM J. Numer. Anal.*, 35(1):336–362, 1998.
- [38] K. R. Daly, G. D’Alessandro, and M. Kaczmarek. An efficient Q-tensor-based algorithm for liquid crystal alignment away from defects. *SIAM J. Appl. Math.*, 70(8):2844–2860, 2010.
- [39] S. Bartels and A. Raisch. Simulation of Q-tensor fields with constant orientational order parameter in the theory of uniaxial nematic liquid crystals. In Michael Griebel, editor, *Singular Phenomena and Scaling in Mathematical Models*, pages 383–412. Springer International Publishing, 2014.
- [40] C. Luo, A. Majumdar, and R. Erban. Multistability in planar liquid crystal wells. *Phys. Rev. E*, 85:061702, Jun 2012.
- [41] C. Tsakonas, A. J. Davidson, C. V. Brown, and N. J. Mottram. Multistable alignment states in nematic liquid crystal filled wells. *Appl. Phys. Lett.*, 90(11):111913, 2007.
- [42] M. Nobili and G. Durand. Disorientation-induced disordering at a nematic-liquid-crystal/solid interface. *Phys. Rev. A*, 46:R6174–R6177, Nov 1992.
- [43] A. Majumdar. The Landau-de Gennes theory of nematic liquid crystals: Uniaxiality versus Biaxiality. *Comm. Pure. Appl. Anal.*, 11(3):1303–1337, May 2012.
- [44] F. Bethuel, H. Brézis, and F. Hélein. *Ginzburg-Landau Vortices*. Progress in Nonlinear Differential Equations and Their Applications Series. Birkhäuser, 1994.

- [45] G. P. Alexander, B. G. Chen, E. A. Matsumoto, and R. D. Kamien. *Colloquium* : Disclination loops, point defects, and all that in nematic liquid crystals. *Rev. Mod. Phys.*, 84:497–514, Apr 2012.
- [46] W. F. Brinkman and P. E. Cladis. Defects in liquid crystals. *Phys. Today*, 35(5):48–54, 1982.
- [47] H.-R. Trebin. Classification of defects in liquid crystals. In O. D. Lavrentovich, P. Pasini, C. Zannoni, and S. Žumer, editors, *Defects in Liquid Crystals: Computer Simulations, Theory and Experiments*, volume 43 of *NATO Science Series*, pages 1–16. Springer Netherlands, 2001.
- [48] M. Kleman and O. D. Lavrentovich. Topological point defects in nematic liquid crystals. *Philos. Mag.*, 86(25-26):4117–4137, 2006.
- [49] Y.-K. Kim, S. V. Shiyankovskii, and O. D. Lavrentovich. Morphogenesis of defects and tactoids during isotropic–nematic phase transition in self-assembled lyotropic chromonic liquid crystals. *J. Phys. Condens. Matter*, 25(40):404202, 2013.
- [50] M. J. Bowick, L. Chandar, E. A. Schiff, and A. M. Srivastava. The cosmological Kibble mechanism in the laboratory-string formation in liquid-crystals. *Science*, 263(5149):943–945, 1994.
- [51] N. J. Mottram and S. J. Hogan. Disclination core structure and induced phase change in nematic liquid crystals. *Phil. Trans. R. Soc. A*, 355(1731):2045–2064, 1997.
- [52] N. J. Mottram and T. J. Sluckin. Defect-induced melting in nematic liquid crystals. *Liq. Cryst.*, 27(10):1301–1304, 2000.

- [53] I. I. Smalyukh, Y. Lansac, N. A. Clark, and R. P. Trivedi. Three-dimensional structure and multistable optical switching of triple-twisted particle-like excitations in anisotropic fluids. *Nat. Mater.*, 9(2):139–145, 2010.
- [54] D. J. Broer. Liquid crystals: Defects dictated. *Nat. Mater.*, 9:99–100, 2010.
- [55] B. F. de Oliveira, P. P. Avelino, F. Moraes, and J. C. R. E. Oliveira. Nematic liquid crystal dynamics under applied electric fields. *Phys. Rev. E*, 82(4):041707, 2010.
- [56] R. Cohen, R. Hardt, D. Kinderlehrer, S.-Y. Lin, and M. Luskin. Minimum Energy Configurations for Liquid Crystals: Computational Results. In J.L. Ericksen and David Kinderlehrer, editors, *Theory and Applications of Liquid Crystals*, volume 5 of *The IMA Volumes in Mathematics and Its Applications*, pages 99–121. Springer New York, 1987.
- [57] Frédéric Hélein. Minima de la fonctionnelle energie libre des cristaux liquides. *C. R. Acad. Sci. Paris*, 305:565–568, 1987.
- [58] R. Cohen and M. Taylor. Weak stability of the map $x/|x|$ for liquid crystal functionals. *Commun. Part. Diff. Eq.*, 15(5):675–692, 1990.
- [59] A. Majumdar, J. M. Robbins, and M. Zyskin. Elastic energy of liquid crystals in convex polyhedra. *J. Phys. A*, 38(34):7595, 2005.
- [60] A. Majumdar, J. M. Robbins, and M. Zyskin. Energies of s^2 -valued harmonic maps on polyhedra with tangent boundary conditions. In *Annales de l’Institut Henri Poincaré (C) Analyse non linéaire*, volume 25, pages 77–103, 2008.
- [61] M. Kleman. Defects in liquid crystals. *Rep. Prog. Phys.*, 52(5):555, 1989.
- [62] P. E. Cladis and M. Kleman. Non-singular disclinations of strength $s = +1$ in nematics. *J. Phys.-Paris*, 33(5–6):591–598, 1972.

- [63] N. Schopohl and T. J. Sluckin. Hedgehog structure in nematic and magnetic systems. *J. Phys.-Paris*, 49(7):1097–1101, 1988.
- [64] S. Mkaddem and E. C. Gartland Jr. Fine structure of defects in radial nematic droplets. *Phys. Rev. E*, 62(5):6694, 2000.
- [65] A. Sonnet, A. Kilian, and S. Hess. Alignment tensor versus director: Description of defects in nematic liquid crystals. *Phys. Rev. E*, 52:718–722, Jul 1995.
- [66] Y. Yi, M. Nakata, A. R. Martin, and N. A. Clark. Alignment of liquid crystals by topographically patterned polymer films prepared by nanoimprint lithography. *Appl. Phys. Lett.*, 90(16):163510, 2007.
- [67] M. S. e Silva, J. Alvarado, J. Nguyen, N. Georgoulia, B. M. Mulder, and G. H. Koenderink. Self-organized patterns of actin filaments in cell-sized confinement. *Soft Matter*, 7(22):10631–10641, 2011.
- [68] A. J. Davidson and N. J. Mottram. Conformal mapping techniques for the modelling of liquid crystal devices. *Eur. J. Appl. Math.*, 23:99–119, 2012.
- [69] H. Kusumaatmaja. Surveying the free energy landscapes of continuum models: Application to soft matter systems. *J. Chem. Phys*, 142(12):–, 2015.
- [70] H. Kusumaatmaja and A. Majumdar. Free energy pathways of a multistable liquid crystal device. *Soft Matter*, 11:4809–4817, 2015.
- [71] S. Kralj and A. Majumdar. Order reconstruction patterns in nematic liquid crystal wells. *Proc. R. Soc. A*, 470(2169):20140276, 2014.
- [72] J. Z. Y. Chen. Structure of two-dimensional rods confined by a line boundary. *Soft Matter*, 9:10921–10930, 2013.

- [73] M. González-Pinto, Y. Martínez-Ratón, and E. Velasco. Liquid-crystal patterns of rectangular particles in a square nanocavity. *Phys. Rev. E*, 88:032506, Sep 2013.
- [74] T. Geigenfeind, S. Rosenzweig, M. Schmidt, and D. de las Heras. Confinement of two-dimensional rods in slit pores and square cavities. *J. Chem. Phys.*, 142(17):174701, 2015.
- [75] O. J. Dammone. *Confinement of Colloidal Liquid Crystals*. PhD thesis, University College, University of Oxford, 2013.
- [76] J. Alvarado. *Biological polymers: confined, bent, and driven*. PhD thesis, VU University Amsterdam, 2013.
- [77] Z. Dogic and S. Fraden. Ordered phases of filamentous viruses. *Curr. Opin. Colloid Interface Sci.*, 11(1):47–55, 2006.
- [78] E. Barry, D. Beller, and Z. Dogic. A model liquid crystalline system based on rodlike viruses with variable chirality and persistence length. *Soft Matter*, 5:2563–2570, 2009.
- [79] O. J. Dammone, I. Zacharoudiou, R. P. A. Dullens, J. M. Yeomans, M. P. Lettinga, and D. G. A. L. Aarts. Confinement induced splay-to-bend transition of colloidal rods. *Phys. Rev. Lett.*, 109(10):108303, Sept 2012.
- [80] J. Alvarado, B. M. Mulder, and G. H. Koenderink. Alignment of nematic and bundled semiflexible polymers in cell-sized confinement. *Soft Matter*, 10:2354–2364, 2014.
- [81] Z. Dogic and S. Fraden. Cholesteric phase in virus suspensions. *Langmuir*, 16(20):7820–7824, 2000.
- [82] A. E. Danese. *Advanced Calculus*, volume 1. Allyn and Bacon, 1965.

- [83] A. Jeffrey and D. Zwillinger. *Table of Integrals, Series, and Products*. Elsevier Science, 2000.
- [84] C. F. Van Loan and K.-Y. D. Fan. *Insight through computing: a MATLAB introduction to computational science and engineering*. SIAM, 2010.
- [85] F. L. Pedrotti, S. J. Pedrotti, and L. S. Pedrotti. *Introduction to Optics*. Prentice-Hall International, Second edition, 1996.
- [86] S. H. Lee, S. L. Lee, and H. Y. Kim. Electro-optic characteristics and switching principle of a nematic liquid crystal cell controlled by fringe-field switching. *Appl. Phys. Letters*, 73(20):2881–2883, Nov 16 1998.
- [87] P. Prinsen and P. van der Schoot. Shape and director-field transformation of tactoids. *Phys. Rev. E*, 68(2):021701, 2003.
- [88] F. P. da Costa, M. Grinfeld, N. J. Mottram, and J. T. Pinto. Uniqueness in the freedericksz transition with weak anchoring. *J. Differ. Equations*, 246(7):2590–2600, 2009.
- [89] I. C. Garlea and B. M. Mulder. Defect structures mediate the isotropic-nematic transition in strongly confined liquid crystals. *Soft Matter*, 11:608–614, 2015.
- [90] R. Haberman. *Applied Partial Differential Equations: with Fourier series and boundary value problems*, volume 4. Pearson Prentice Hall, 2004.
- [91] J. F. Toland. The Peierls-Nabarro and Benjamin-Ono Equations. *J. Funct. Anal.*, 145(1):136 – 150, 1997.
- [92] A. Bogi, P. Martinot-Lagarde, I. Dozov, and M. Nobili. Anchoring screening of defects interaction in a nematic liquid crystal. *Phys. Rev. Lett.*, 89(22):225501, 2002.

- [93] C. Blanc, A. Vella, M. Nobili, and P. Martinot-Lagarde. Role of surface effects on the formation and the dynamics of defects in a nematic cell with a planar anchoring. *Mol. Cryst. Liq. Cryst.*, 438(1):175–1739, 2005.
- [94] M. Kurzke. Boundary vortices in thin magnetic films. *Calc. Var. Partial. Dif.*, 26(1):1–28, 2006.
- [95] P. Prinsen and P. van der Schoot. Continuous director-field transformation of nematic tactoids. *Eur. Phys. J. E Soft Matter*, 13(1):35–41, 2004.
- [96] P. Oswald and P. Pieranski. *Nematic and Cholesteric Liquid Crystals: Concepts and Physical Properties Illustrated by Experiments*. Liquid Crystals Book Series. Taylor & Francis, 2005.
- [97] M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions: With Formulas, Graphs, and Mathematical Tables*. Applied Mathematics Series. Dover Publications, 1964.
- [98] R. P. Cowburn and M. E. Welland. Micromagnetics of the single-domain state of square ferromagnetic nanostructures. *Phys. Rev. B*, 58:9217–9226, Oct 1998.
- [99] D. A. Goode and G. Rowlands. Analytically modelling the effects of interaction between two or more rectangular nanomagnets. *J. Magn. Magn. Mater.*, 296(1):46 – 56, 2006.
- [100] V. V. Slastikov. A note on configurational anisotropy. *Proc. R. Soc. A*, 466(2123):3167–3179, 2010.
- [101] F. Bethuel, H. Brezis, B. D. Coleman, and F. Hélein. Bifurcation analysis of minimizing harmonic maps describing the equilibrium of nematic phases between cylinders. *Arch. Ration. Mech. Anal.*, 118(2):149–168, 1992.

- [102] P. Palffy-Muhoray, A. Sparavigna, and A. Strigazzi. Saddle-splay and mechanical instability in nematics confined to a cylindrical annular geometry. *Liq. Crystals*, 14(4):1143–1151, 1993.
- [103] P. J. Barratt and B. R. Duffy. Weak-anchoring effects on a Freedericksz transition in an annulus. *Liq. Cryst.*, 19(1):57–63, 1995.
- [104] P. J. Barratt and B. R. Duffy. Freedericksz transitions in nematic liquid crystals in annular geometries. *J. Phys. D Appl. Phys.*, 29(6):1551, 1996.
- [105] P. J. Barratt and B. R. Duffy. The effect of splay-bend elasticity on Freedericksz transitions in an annulus. *Liq. Cryst.*, 26(5):743–751, 1999.
- [106] R. Teixeira de Souza, J. C. Dias, R. S. Mendes, and L. R. Evangelista. Critical exponents for Fréedericksz transition in nematics between concentric cylinders. *Physica A*, 389(5):945–950, 2010.
- [107] G. Bevilacqua and G. Napoli. Periodic splay-twist Fréedericksz transition for nematics confined between two concentric cylinders. *Phys. Rev. E*, 81:031707, Mar 2010.
- [108] T.-W. Pan. Existence and multiplicity of radial solutions describing the equilibrium of nematic liquid crystals on annular domains. *J. Math. Anal. Appl.*, 245(1):266–281, 2000.
- [109] D. Golovaty and L. Berlyand. On uniqueness of vector-valued minimizers of the Ginzburg-Landau functional in annular domains. *Calc. Var. Partial Dif.*, 14(2):213–232, 2002.
- [110] L. Berlyand and K. Voss. Symmetry breaking in annular domains for a Ginzburg-Landau superconductivity model. In *IUTAM Symposium on Me-*

- chanical and Electromagnetic Waves in Structured Media*, volume 91 of *Solid Mechanics and Its Applications*, pages 189–200. Springer Netherlands, 2002.
- [111] L. Berlyand and P. Mironescu. Ginzburg-Landau minimizers with prescribed degrees. Capacity of the domain and emergence of vortices. *J. Funct. Anal.*, 239(1):76–99, 2006.
 - [112] L. Berlyand and P. Mironescu. Ginzburg-Landau minimizers with prescribed degrees: dependence on domain. *C. R. Acad. Sci. Paris Sér. I Math.*, 337(6):375–380, 2003.
 - [113] O. V. Manyuhina, K. B. Lawlor, M. C. Marchetti, and M. J. Bowick. Viral nematics in confined geometries. *Soft Matter*, 11:6099–6105, 2015.
 - [114] L. C. Evans. *Partial Differential Equations*. Graduate Studies in Mathematics. American Mathematical Society, First edition, 1998.
 - [115] B. Dacorogna. *Direct Methods in the Calculus of Variations*, volume 78. Springer Science & Business Media, 2007.
 - [116] G. Canevari, M. Ramaswamy, and A. Majumdar. Radial symmetry on three-dimensional shells in the Landau-de Gennes theory. *Phys. D*, 314:18–34, 2016.
 - [117] P. Mironescu. On the stability of radial solutions of the Ginzburg-Landau equation. *J. Funct. Anal.*, 130(2):334–344, 1995.
 - [118] D. S. Mitrinovic, J. Pecaric, and A. M. Fink. *Inequalities involving functions and their integrals and derivatives*, volume 53. Springer Science & Business Media, 2012.
 - [119] A. Majumdar. The radial-hedgehog solution in Landau-de Gennes theory for nematic liquid crystals. *Eur. J. Appl. Math.*, 23(01):61–97, 2012.

- [120] R. Rosso and E. G. Virga. Metastable nematic hedgehogs. *J. Phys. A: Math. Gen.*, 29(14):4247, 1996.
- [121] X. Lamy. Some properties of the nematic radial hedgehog in the Landau-de Gennes theory. *J. Math. Anal. Appl.*, 397(2):586–594, 2013.
- [122] E. C. Gartland Jr. and S. Mkaddem. Instability of radial hedgehog configurations in nematic liquid crystals under Landau-de Gennes free-energy models. *Phys. Rev. E*, 59(1):563, 1999.
- [123] R. Ignat, L. Nguyen, V. Slastikov, and A. Zarnescu. Uniqueness results for an ODE related to a generalized Ginzburg-Landau model for liquid crystals. *SIAM J. Math. Anal.*, 46(5):3390–3425, 2014.
- [124] E. Penzenstadler and H.-R. Trebin. Fine structure of point defects and soliton decay in nematic liquid crystals. *J. Phys. France*, 50(9):1027–1040, May 1989.
- [125] C. Chiccoli, P. Pasini, F. Semeria, and C. Zannoni. Monte Carlo simulations of model nematic droplets. *Mol. Cryst. Liq. Cryst.*, 212(1):197–204, 1992.
- [126] S. Kralj, E. G. Virga, and S. Žumer. Biaxial torus around nematic point defects. *Phys. Rev. E*, 60(2):1858, 1999.
- [127] G. De Matteis, A. M. Sonnet, and E. G. Virga. Landau theory for biaxial nematic liquid crystals with two order parameter tensors. *Continuum Mech. Thermodyn.*, 20(6):347–374, 2008.
- [128] G. R. Luckhurst. *Biaxial nematic liquid crystals: theory, simulation and experiment*. John Wiley & Sons, 2015.
- [129] G. R. Luckhurst. Biaxial nematic liquid crystals: fact or fiction? *Thin Solid Films*, 393:40 – 52, 2001. Proceedings from the 4th International Conference on Nano-Molecular Electronics.

- [130] C. Tschierske and D. J. Photinos. Biaxial nematic phases. *J. Mater. Chem.*, 20:4263–4294, 2010.
- [131] G. R. Luckhurst. Liquid crystals: A missing phase found at last? *Nature*, 430(6998):413–414, 2004.
- [132] E. F. Gramsbergen, L. Longa, and W. H. de Jeu. Landau theory of the nematic-isotropic phase transition. *Phys. Rep.*, 135(4):195–257, 1986.
- [133] S. Singh. Phase transitions in liquid crystals. *Phys Rep.*, 324(2–4):107–269, 2000.
- [134] D. W. Allender, M. A. Lee, and N. Hafiz. Landau theory of biaxial and uniaxial nematic liquid crystals. *Mol. Cryst. Liq. Cryst.*, 124(1):45–52, 1985.
- [135] D. W. Allender and M. A. Lee. Landau theory of biaxial nematic liquid crystals. *Mol. Cryst. Liq. Cryst.*, 110(1-4):331–339, 1984.
- [136] Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge University Press, 2004.
- [137] E. L. Rees. Graphical discussion of the roots of a quartic equation. *Am. Math. Monthly*, 29(2):51–55, 1922.
- [138] A. van der Sluis. Upperbounds for roots of polynomials. *Numer. Math.*, 15(3):250–262, 1970.
- [139] E. C. Gartland Jr. and S. Mkaddem. On the local instability of radial hedgehog configurations in nematic liquid crystals under Landau-de Gennes free-energy models. Technical Report ICM-199807-0005, Kent State University, 1998.
- [140] S. R. Bernfeld and V. Lakshmikantham. *An Introduction to Nonlinear Boundary Value Problems*. Mathematics in Science and Engineering. Elsevier Science, 1974.

- [141] R. Ignat, L. Nguyen, V. Slastikov, and A. Zarnescu. Stability of the melting hedgehog in the Landau-de Gennes theory of nematic liquid crystals. *Arch. Rational Mech. Anal.*, 215(2):633–737, 2013.
- [142] D. P. Chi and G. H. Park. Weak-stability of $x/|x|$ and symmetries of liquid crystals. *J. Korean Math. Soc.*, 29:251–260, 1992.
- [143] L. F. Shampine, J. Kierzenka, and M. W. Reichelt. *Solving boundary value problems for ordinary differential equations in MATLAB with bvp4c*, 2000.
- [144] COMSOL. *Introduction to COMSOL Multiphysics*, 5.1 edition, 2016.