Calculus of Variations and its application to Liquid Crystals

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Abstract

This thesis concerns the mathematical study of the calculus of variations and its application to liquid crystals. Throughout the thesis we will be looking to minimise integral functionals of the form

$$I(\mathbf{n}) = \int_{\Omega} F(x, \mathbf{n}, \nabla \mathbf{n})\, dx.$$

In the first chapter we examine vectorial problems in the calculus of variations with an additional pointwise constraint so that any admissible function $\mathbf{n} \in W^{1,1}(\Omega, M)$, and M is a manifold of suitable regularity. We formulate necessary and sufficient conditions for any given state $\mathbf{n}$ to be a strong or weak local minimiser of I. This is achieved using a nearest point projection mapping in order to use the more classical results which apply in the absence of a constraint. In the subsequent chapters we study various static continuum theories of liquid crystals. More specifically we look to explain a particular cholesteric fingerprint pattern observed by HP Labs. We begin in Chapter 2 by focusing on a specific cholesteric liquid crystal problem using the theory originally derived by Oseen and Frank [37, 76]. We find the global minimisers for general elastic constants amongst admissible functions which only depend on a single variable. Using the one-constant approximation for the Oseen-Frank free energy, we then show that these states are global minimisers of the three-dimensional problem if the pitch of the cholesteric liquid crystal is sufficiently long. Chapter 3 concerns the application of the results from the first chapter to the situations investigated in the second. The local stability of the one-dimensional states are quantified, analytically and numerically, and in doing so we unearth potential shortcomings of the classical Oseen-Frank theory.

In Chapter 4, we ascertain some equivalence results between the continuum theories of Oseen and Frank, Ericksen [33], and Landau and de Gennes [29]. We do so by proving lifting results, building on the work of Ball and Zarnescu [13], which relate the regularity of line and vector fields. The results prove to be interesting as they show that for a director theory to respect the head to tail symmetry of the liquid crystal molecules, the appropriate function space for the director field is $SBV^2\left(\Omega, \mathbb{S}^2\right)$. We take this idea and in the final chapter we propose a mathematical model of liquid crystals based upon the Oseen-Frank free energy but using special functions of bounded variation. We establish the existence of a minimiser, forms of the Euler-Lagrange equation, and find solutions of the

Euler-Lagrange equation in some simple cases. Finally we use our proposed model to re-examine the same problems from Chapter 2. By doing so we extend the analysis we were able to achieve using Sobolev spaces and predict the existence of multi-dimensional minimisers consistent with the known experimental properties of high-chirality cholesteric liquid crystals.

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Introduction

This thesis is devoted to better understanding liquid crystal systems through mathematical modelling and analysis. This is a very wide field in and of itself but my industrial sponsors, HP Labs, are particularly interested in an analytical explanation of certain liquid crystal patterns which, if understood, could improve display design. This interest provided a focus and direction for my mathematical analysis. There is a rich history of using continuum theories with energy functionals to model liquid crystals and we follow this approach. This thesis concerns the abstract study of the calculus of variations, the mathematical modelling of static liquid crystal problems, and the application of these models to predict liquid crystal behaviour.

0.1 Motivation

The central motivation of this work is to better understand liquid crystals as a step towards devices with improved optics so that a reflective, high resolution, colour display would be made possible. To this end, HP Labs were experimenting with the addition of chiral dopant to guest host zenithally bistable nematic (ZBN) devices. These ZBN devices are ones which have two optically distinct stable states that correspond to the 'on' and 'off' states of the pixel. If a liquid crystal display needs to be continually refreshed then this limits its maximum resolution. However having two stable states and a switching mechanism solves this problem. The ZBN device used by HP and shown in Figure 0.1 (Brown, Bryan-Bryan and Jones, U.S. Patent number 6,249,332) has a grating on the bottom of the cell to stabilise two states.

In a guest host device, rod-like dye molecules are added to the nematic host. The dye molecules disperse throughout the sample and align themselves in the same direction as the host nematic molecules. The dye molecules absorb light passing through the liquid crystal layer depending on the polarisation of the light and the tilt of the dye molecule. Maximum absorption occurs when light is polarised parallel to the molecule and it has no tilt (incoming light is perpendicular to the dye molecule). If a display does not use polarised light then either two switchable layers of liquid crystal are required, or the dye molecules need to twist in order to absorb all polarisations of the light. Adding a chiral dopant to the ZBN device introduces such a twist. Additionally it flattens the tilt profile in Figure 0.1(b) which increases the absorption in the 'dark' state of the device. However the amount of chiral dopant added is critical. Too much can cause the vertical state to destabilise or unwanted textures, for example cholesteric fingers, to occur. At present numerical models are unable to explain the

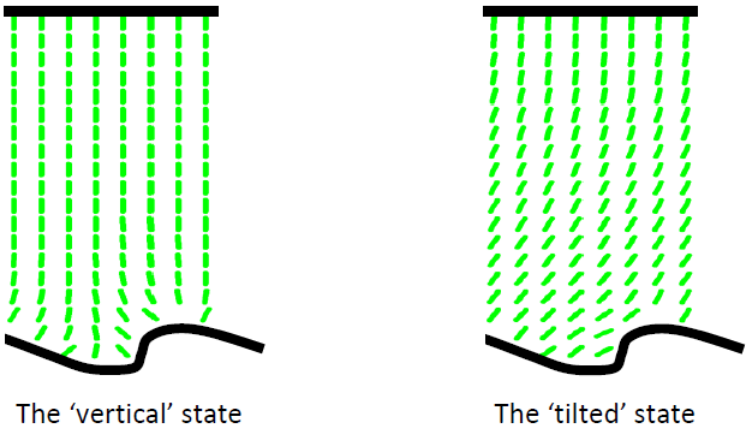


Figure 0.1: ZBN device - (courtesy Chris Newton, HP Labs)

existence of these textures. Therefore understanding the underlying structure and causes of these patterns would potentially be of great help in display design.

0.2 Calculus of Variations

The canonical problem which is studied in the calculus of variations is to minimise an integral functional. If $\Omega \subset \mathbb{R}^d$ is a bounded domain, where a domain is an open and connected set, then the aim is to minimise

$$I(\mathbf{n}) := \int_\Omega F(x, \mathbf{n}, \nabla \mathbf{n})\, dx \tag{0.1}$$

where $\mathbf{n} : \Omega \to \mathbb{R}^k$ and $F : \Omega \times \mathbb{R}^k \times \mathbb{R}^{k\times d} \to \mathbb{R}$ lie in some function space and some boundary conditions may also be applied on $\partial\Omega$. This covers a wide variety of both abstract and physical problems. For example, the shortest path $y(x)$ between two points $(x_1, y_1), (x_2, y_2) \in \mathbb{R}^2$ is given by minimisers of the arc length functional

$$I(y) = \int_{x_1}^{x_2} \sqrt{1 + y'(x)^2}\, dx,$$

with admissible functions $y \in C^1((x_1, x_2), \mathbb{R})$ such that $y(x_1) = y_1$ and $y(x_2) = y_2$. For a more physical example, in order to find solutions of Poisson's equation, $\triangle u = f$ in $\Omega \subset \mathbb{R}^3$, we can find minimisers of the energy functional

$$I(u) = \int_\Omega \frac{1}{2}|\nabla u(x)|^2 + f(x)u(x)\, dx,$$

where $u : \Omega \to \mathbb{R}$ lies in the Sobolev space $W^{1,2}(\Omega)$. Sobolev spaces are widely used as the appropriate function space in variational problems as they provide a natural extension of continuously differentiable functions which still give finite values for the functional I. They will be extensively used in this thesis so we recall their definition.

Definition 0.1 (Sobolev Spaces)**.** *Let $\Omega \subset \mathbb{R}^d$ be an open set. Then for $m \in \mathbb{N}$ and $1 \leqslant p \leqslant \infty$ we define*

$$W^{m,p}\left(\Omega, \mathbb{R}^k\right) := \left\{ \mathbf{u} \in L^p\left(\Omega, \mathbb{R}^k\right) \,\middle|\, D^\alpha \mathbf{u} \in L^p\left(\Omega, \mathbb{R}^k\right),\ \forall\, |\alpha| \leqslant m \right\}$$

where $D^\alpha \mathbf{u}$ is the distributional derivative with respect to the multi-index α.

Sobolev spaces are also Banach spaces when equipped with the norm

$$\|\mathbf{u}\|_{m,p,\Omega} := \begin{cases} \sum_{|\alpha| \leqslant m} \|D^\alpha \mathbf{u}\|_{p,\Omega} & \text{if } p \in [1, \infty) \\ \\ \max_{|\alpha| \leqslant m} \|D^\alpha \mathbf{u}\|_{\infty,\Omega} & \text{if } p = \infty. \end{cases}$$

When there is no room for confusion we will drop the domain subscript Ω from our norm notation. Given a variational problem in the form of (0.1) there are a number of aspects which are studied. Firstly the existence of a minimiser is usually established through the direct method of the calculus of variations. It is here that the advantage of Sobolev functions become clear; for $1 < p < \infty$, $W^{m,p}\left(\Omega, \mathbb{R}^k\right)$ is reflexive so any bounded sequence contains a weakly convergent subsequence. Then Morrey [70, 71] showed that if the Lagrangian satisfies suitable growth conditions and quasiconvexity with respect to the gradient term, then

$$\inf \left\{ \int_\Omega F(x, \mathbf{n}, \nabla \mathbf{n})\, dx \,\middle|\, \mathbf{n} \in \mathbf{n}_0 + W_0^{1,p}\left(\Omega, \mathbb{R}^k\right) \right\}$$

admits a solution. In this thesis, proving the existence of a minimiser for our problems will usually be trivial because of this result. Our focus is more specifically on finding local and global minimisers which correspond to physically viable states. A global minimiser is simple to define. If $\mathbf{n}$ is an admissible function such that $I(\mathbf{n}) \leqslant I(\mathbf{m})$ for all admissible functions $\mathbf{m}$, then $\mathbf{n}$ is a global minimiser. Local minimisers are more subtle because they depend upon which metric is used to measure locality. Suppose that we are looking to minimise (0.1) over some set of admissible functions $\mathcal{A}$.

Definition 0.2 (Local minimiser)**.** *Let $1 \leqslant p \leqslant \infty$. Then $\mathbf{n} \in \mathcal{A}$ is a $W^{1,p}$-local minimiser (respectively L^p-local minimiser) if there exists some $\epsilon > 0$ such that*

$$I(\mathbf{n}) \leqslant I(\mathbf{m})$$

for all $\mathbf{m} \in \mathcal{A}$ such that $\|\mathbf{n} - \mathbf{m}\|_{1,p,\Omega} < \epsilon$ (respectively $\|\mathbf{n} - \mathbf{m}\|_{p,\Omega} < \epsilon$).

Henceforth we will refer to $W^{1,\infty}$ and L^∞ local minimisers as weak and strong local minimisers respectively. These are the most commonly used metrics in this field. The main technique in the calculus of variations is to take small perturbations of the given state $\mathbf{n}$ to test its stability. If we take some $\phi \in C_0^\infty\left(\Omega, \mathbb{R}^k\right)$, by which we mean a smooth function whose support is compactly contained in Ω, then $\mathbf{n} + t\phi \in \mathcal{A}$ for any t. If $\mathbf{n}$ is a global or local minimiser this means that $g(t) := I(\mathbf{n} + t\phi)$ has a local minimum at zero. Hence

$$\delta I(\mathbf{n})(\phi) := \frac{d}{dt} I(\mathbf{n} + t\phi)\bigg|_{t=0} = 0, \tag{0.2}$$

and

$$\delta I(\mathbf{n})(\phi, \phi) := \frac{d^2}{dt^2} I(\mathbf{n} + t\phi)\Big|_{t=0} \geqslant 0. \tag{0.3}$$

Equation (0.2) is the weak form of the Euler-Lagrange equation which is satisfied by any global or local minimiser. It is therefore a useful starting point to find any candidate minimisers. The strong form of the Euler-Lagrange equation is the following system of second order partial differential equations

$$F_{\mathbf{n}_i}(x, \mathbf{n}, \nabla\mathbf{n}) = \sum_{j=1}^{d} \frac{\partial}{\partial x_j} F_{\mathbf{n}_{i,j}}(x, \mathbf{n}, \nabla\mathbf{n}) \quad i = 1, \ldots, k.$$

The local minimiser conditions (0.2) and (0.3) have analogies to the study of critical points of one dimensional functions. A local minimum has a non-negative second derivative at a critical point, however the converse is not true in general. A stronger condition on the second derivative must be assumed. In the scalar case $d, k = 1$, Weierstrass was able to prove a strong local minimiser sufficiency result with the idea of a field of extremals. Hestenes [46] was able to extend Weierstrass' result to the case $d > 1$ with the following result.

Theorem 0.3. *[46] Let $\Omega \subset \mathbb{R}^d$ and suppose that $n \in C^1\left(\overline{\Omega}, \mathbb{R}\right)$. If n satisfies the Euler-Lagrange equation as well as the following three conditions*

- *Strong Legendre Condition: There exists some $\alpha > 0$ such that*

$$\sum_{i,j} F_{\nabla n_i, \nabla n_j}(x, n(x), \nabla n(x))\lambda_i\lambda_j \geqslant \alpha|\lambda|^2$$

  for all $\lambda \in \mathbb{R}^k$ and $x \in \overline{\Omega}$.

- *Positive Second Variation:*

$$\delta^2 I(n)(\phi, \phi) > 0$$

  for all $\phi \in C_0^\infty(\Omega)$ such that $\phi \neq 0$.

- *Strong Weierstrass Condition: There exists some $\epsilon > 0$ such that*

$$\mathcal{E}_F(x, m, \mathbf{u}, \mathbf{v}) := F(x, m, \mathbf{v}) - F(x, m, \mathbf{u}) - \sum_i F_{\mathbf{u}_i}(x, m, \mathbf{u})(\mathbf{v}_i - \mathbf{u}_i) \geqslant 0$$

  for all $|m - n| < \epsilon$, $|\mathbf{u} - \nabla n| < \epsilon$, $\mathbf{v} \in \mathbb{R}^d$ and $x \in \overline{\Omega}$.

Then n is a strong local minimiser of I.

Results which are equivalent to this one in the vectorial case when $d, k \geqslant 2$ have proved to be much harder to formulate. Taheri [89] did prove a such a result, however in order to do so he had to assume a strong convexity condition. In 2009 Grabovsky & Mengesha [41] were able to extend this and prove the vectorial analogue of the above theorem for C^1 domains. It is these ideas and results that we will be focusing on in Chapter 1 with the additional complication of constraints. The nature of variational problems is significantly altered when

a constraint is applied to the admissible functions. For example, suppose we were looking to minimise

$$I(\mathbf{n}) := \int_\Omega |\nabla \mathbf{n}(x)|^2 \, dx$$

over $\mathcal{A} := \left\{ \mathbf{v} \in W^{1,2}\left(\Omega, \mathbb{R}^k\right) \middle| \ \mathbf{v}(x) \in \mathbb{S}^{k-1} \text{ a.e.} \right\}$. Then if we took some $\phi \in C_0^\infty\left(\Omega, \mathbb{R}^k\right)$, $\mathbf{n} + t\phi$ will not, in general, satisfy the constraint $|\mathbf{n} + t\phi| = 1$. Therefore the set of possible variations is restricted. This alters both the first and second variations of the functional so that the unconstrained results cannot be applied to these situations. Even though constrained problems are studied in many areas such as liquid crystals or micromagnetics, the local stability of states, a very pertinent physical issue, has received little attention. In Chapter 1 we supplement the literature by formulating a new set of results giving necessary and sufficient conditions for strong and weak local minimisers for constrained vectorial problems. Many of the issues we consider in this part of the thesis are parallel to those encountered in the study of harmonic maps because of the pointwise constraint. Harmonic maps are stationary points (minimisers) of the functional

$$I(\mathbf{n}) := \int_M \|D\mathbf{n}\|^2 \, d\mu_N$$

where M and N are manifolds, $d\mu_N$ is the measure on N and $\mathbf{n} \in W^{1,2}(N, M)$. Smith [86] found the second variation of this functional using projections onto the manifolds to ensure that the constraints are satisfied. This is precisely the idea that we use in Chapter 1 for our local stability results.

0.3 Functions of Bounded Variation

As well as deciding on an appropriate form for the Lagrangian, a second major aspect of variational models is the need to specify the regularity of the admissible functions. The importance of this choice is often overlooked, and in Chapter 4 we will consider the appropriate function space for some liquid crystal energy functionals. In the course of our investigations it became clear that the spaces of functions of bounded variation are a natural choice for some liquid crystal variational problems. We recommend [5] for an excellent overview of the basic aspects of these spaces but here we will only introduce the elements relevant to this thesis.

Definition 0.4 (Bounded Variation)**.** *Let $u \in L^1(\Omega)$ for some open set $\Omega \subset \mathbb{R}^d$. Then $u \in BV(\Omega)$ if and only if there exists some $\mathbb{R}^d$-valued Borel measure $Du = (D_1 u, \ldots, D_d, u)$ such that*

$$\int_\Omega u \frac{\partial \phi}{\partial x_i} \, dx = -\int_\Omega \phi dD_i u$$

for all $\phi \in C_0^\infty(\Omega)$ and $i = 1, \ldots, d$.

This space is a Banach space when equipped with the norm

$$\|u\|_{BV} := \int_\Omega |u(x)| \, dx + \sup \left\{ \int_\Omega u \nabla \cdot \phi \, dx \middle| \ \phi \in C_0^1\left(\Omega, \mathbb{R}^d\right), \ \|\phi\|_\infty \leqslant 1 \right\}.$$

It is clear from Definitions 0.4 and 0.1 that functions of bounded variation are a generalisation of Sobolev functions. Therefore

$$W^{1,1}(\Omega) \subset BV(\Omega).$$

However, even though these functions are more general than Sobolev functions, they do share many of the properties of Sobolev spaces which are necessary for use in variational problems. They have appropriate embedding and trace theorems.

Theorem 0.5 (BV embedding)**.** *Let $\Omega \subset \mathbb{R}^d$ be a domain of sufficient regularity (Lipschitz is sufficient). Then there is a continuous embedding $BV(\Omega) \hookrightarrow L^{\frac{d}{d-1}}(\Omega)$ and for every $1 \leqslant p < \frac{d}{d-1}$ the embedding $BV(\Omega) \hookrightarrow L^p(\Omega)$ is compact.*

Theorem 0.6 (Traces in BV)**.** *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and $u \in BV(\Omega)$. Then there exists some $u_{\partial\Omega} \in L^1(\partial\Omega)$ such that for $\mathcal{H}^{d-1}$ almost every $x \in \partial\Omega$*

$$\lim_{r\to 0} r^{-d} \int_{\Omega\cap B(x,r)} |u(y) - u_{\partial\Omega}|\, dy = 0$$

and $\|u_{\partial\Omega}\|_{1,\partial\Omega} \leqslant C\|u\|_{BV}$ where C only depends on Ω.

Even more importantly, due to the Radon-Nikodym theorem, the derivative of a BV function can be written as $Du = D^a u + D^s u$ where $D^a u$, often written $\nabla u \mathcal{L}^d$, is the absolutely continuous part of the derivative with respect to the d-dimensional Lebesgue measure. Furthermore the singular part of the derivative can be decomposed into two further components $D^s u = D^j u + D^c u = (u_+ - u_-)\nu_u \mathcal{H}^{d-1} \lfloor S_u + D^c u$ where: S_u is the approximate discontinuity set of u; u_+ and u_- are the limits approaching from either side; and ν_u is the vector normal to S_u. We will not focus on the Cantor part of the derivative $D^c u$ since we will be using the subset of BV called special functions of bounded variation (SBV).

Proposition 0.7. *[5, Prop. 4.2] Let $u \in BV(\Omega)$. Then the following are equivalent*

- *$u \in SBV(\Omega)$*
- *$D^s u$ is concentrated on a Borel set which is σ-finite with respect to $\mathcal{H}^{d-1}$*
- *$D^c u = 0$*

We will be using this closed subspace of BV because SBV functions can be thought of as piecewise Sobolev functions in the following sense.

Proposition 0.8. *[5, Prop. 4.4] Let $\Omega \subset \mathbb{R}^d$ be a bounded domain. Let $K \subset \mathbb{R}^d$ be closed and $\mathcal{H}^{d-1}(\Omega \cap K) < \infty$. If $u \in W^{1,1}(\Omega \setminus K) \cap L^\infty(\Omega \setminus K)$ then $u \in SBV(\Omega)$ and $\mathcal{H}^{d-1}(S_u \setminus K) = 0$.*

The final property that we will note here about SBV functions is their compactness property [5, Theorem 4.8]. This is particularly important in the direct method of the calculus of variations as it ensures that minimisers exist given an appropriate Lagrangian. With the addition of some technicalities, the essence of [5, Theorem 4.8] is that a bounded sequence

$\left(u_j\right) \subset SBV(\Omega)$ such that $\|u_j\|_\infty$ is also uniformly bounded has a weakly* convergent subsequence, converging to some $u \in SBV(\Omega)$.

In recent years a number of physical problems have been studied using SBV functions. Free discontinuity problems such as the Mumford-Shah image segmentation functional have been studied with SBV functions [3]. Another free-discontinuity problem involving brittle fracture has also come into the SBV sphere of influence [15]. This is natural given that the essence of fracture is to create discontinuities which cannot be modelled by Sobolev functions alone. In the later chapters we will be interested in formulating liquid crystal energies using SBV functions. Ambrosio [5] proposed a variational formulation for solving the problem of finding the shape and structure of a droplet of liquid crystal in another fluid. However we will go further and show that SBV functions naturally arise from the existing continuum models of liquid crystals. Furthermore they have the potential to shed new light on the widely studied problems of liquid crystals as well as our own industrially motivated problem.

0.4 The Mathematics of Liquid Crystals

One of the basic scientific tenets which is taught in schools is that there are three distinct phases of matter: solid, liquid and gas. However this is far from being the complete story. In 1888 the Austrian scientist Reinitzer noted two distinct melting points for cholesteryl benzoate upon heating [80]. Above the first melting point a cloudy liquid formed, which became a clear one above the second melting point. This began the early investigation into substances which exhibit this intermediary phase behaviour. Vorländer (see [83] for a translation) made the crucial connection between the two melting points and rod-like molecules in the first decade of the twentieth century. This was a vital observation for the mathematical modelling of liquid crystals for reasons which will become apparent below. In 1922 Friedel [38] was able to categorise liquid crystals into three groups which are pictorially represented in Figure 0.2.

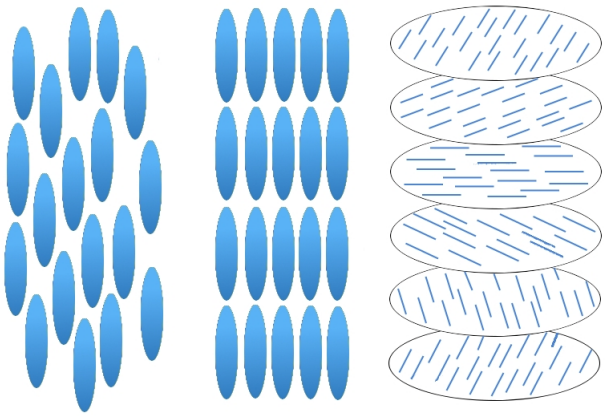


Figure 0.2: Nematic, smectic, and cholesteric phases

- **Nematic Liquid Crystals**: Nematic liquid crystal molecules have orientational ordering as they prefer to lie parallel to each other along some common axis. However there is no positional ordering so the molecules can flow over each other as a liquid.
- **Cholesteric Liquid Crystals**: Cholesteric liquid crystals, also called chiral nematic liquid crystals, are similar to nematics but the molecules prefer to form a slight angle with their nearest neighbours. Therefore they naturally form a helical structure by twisting perpendicular to a fixed axis.
- **Smectic Liquid Crystals**: Smectics have a degree of positional order not exhibited by the other two. The molecules form in individual liquid-like layers but they all have some orientational ordering within each layer like nematics and cholesterics.

These three categories should not be viewed as an absolute classification because some liquid crystals can behave like two or more types. For example, a nematic liquid crystal can be made chiral with the addition of a chiral dopant. The pitch of the resulting chiral nematic depends on the amount of dopant added to the system, more dopant results in shorter cholesteric pitch. There are a number of different types of smectic liquid crystal but we shall not focus on that because we are principally interested in nematic and cholesteric liquid crystals in this work. Cholesteric liquid crystal molecules prefer to form a slight angle to their nearest neighbours because they are enantiomorphic, which means they are not invariant upon reflection. This encourages them to form the helical pattern shown in Figure 0.2 and the periodicity of the pattern is called the cholesteric pitch. Even though they are enantiomorphic they are still modelled as rigid rods for the purposes of the mathematical models. The actual length of liquid crystal molecules is in the region of 20Å$= 2 \times 10^{-9}$m.

There are two main mechanisms for inducing liquid crystal behaviours. The most common uses changes in temperature to induce the mesophase; these are called *thermotropic liquid crystals*. However some liquid crystal phases can be induced by changing the concentration of molecules in a solvent; these are called *lyotropic liquid crystals*. In this thesis we will only consider thermotropic liquid crystals and unless stated otherwise we will be assuming that the temperature is fixed and below the nematic-isotropic transition temperature.

One of the reasons that liquid crystals are interesting to study from a mathematical point of view is the rich array of defects and structures that can form under certain experimental conditions. There are the Schlieren textures [74] which form when a nematic is cooled from above the transition temperature. They consist of defects with strengths $s = \pm\frac{1}{2}, \pm 1$ which spontaneously form and interact with each other. For cholesterics the situation is even more complex; at least four different kinds of cholesteric finger patterns have been characterised [77, 85] and they can occur with suitably frustrated boundary conditions or an applied electric field. In addition, if the cholesteric pitch is short, there are structures called blue phases which can occur close to the transition temperature and these have some form of cubic symmetry as well as a defect lattice throughout the substance. Within the last decade, Smalyukh and his research group have identified further stable cholesteric structures called torons [1] which can be induced with diffracted laser beams. From a mathematical point of view there is

a significant literature for nematic liquid crystals and the relative simplicity of the energy Lagrangian ensures that they are reasonably well understood. However much less attention has been given over to the study of cholesteric liquid crystals using tools from the calculus of variations. A central goal of this thesis is to try and rectify this knowledge asymmetry and bring the understanding of cholesteric and nematic liquid crystals closer to parity.

Mathematical Modelling

The mathematical study of liquid crystals has given rise to many different theories in attempts to describe the energy of the systems in the best possible way. We will be interested in the macroscopic continuum theories of Oseen-Frank, Ericksen, Landau-de Gennes and the Q-tensor theory. Beginning chronologically, Oseen [76] and Frank [37] developed a theory where the anisotropic axis of the molecules was the variable with which to describe the energy of the system. Their theory is based around the following coarse-graining approach: at each point in the sample, consider the ball B given by

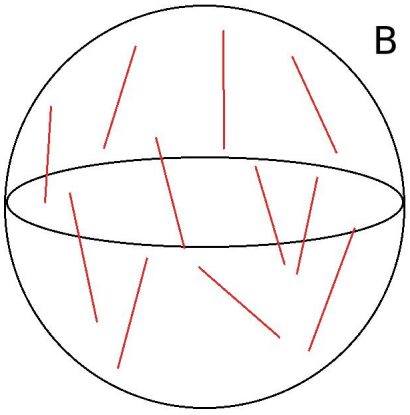


Figure 0.3: Constructing a director field

$$B := \left\{ \, y \in \mathbb{R}^3 \, \middle| \, |x-y| \leqslant \epsilon \, \right\},$$

where $\epsilon > 0$ is suitably small and the ball B is shown in Figure 0.3. Then we can average the orientations of the molecules in this ball and define the director $\mathbf{n}(x) \in \mathbb{S}^2$ at this point to be given by this average orientation. One subtle flaw in this idea is that the head to tail symmetry of the molecules implies that there should not be any distinction between $\mathbf{n}(x)$ and $-\mathbf{n}(x)$. Hence $\mathbf{n}(x)$ should in fact be a line field rather than a vector field. We will return to this issue in due course in Chapters 4 and 5. By using symmetries and other material properties, which we will fully outline in Chapter 2, Oseen and Frank derived the free energy functional

$$I(\mathbf{n}) = \int_\Omega K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n}+t)^2 + K_3|\mathbf{n}\times\nabla\times\mathbf{n}|^2 + (K_2+K_4)\left(\mathrm{tr}\,(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2\right) dx \quad (0.4)$$

where $K_1, K_2, K_3 \geqslant 0$ and $t = \frac{2\pi}{P}$ (P is the pitch of the cholesteric). The final term is often discarded because if $\mathbf{n}$ is sufficiently smooth then

$$\mathrm{tr}\,(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2 = \nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n}), \quad (0.5)$$

so by the divergence theorem this only contributes to the surface energy. We will not be disregarding it though because the realistic problems we consider do not have prescribed boundary conditions on the whole of Ω, so that surface energies will play a role. An important feature of this theory is that if it is assumed that $K_1 = K_2 = K_3 = K$ and $K_4 = 0$ then (0.4) reduces to the very elegant one-constant Oseen-Frank energy

$$I(\mathbf{n}) = K \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \, dx. \tag{0.6}$$

As with each of the macroscopic continuum theories, the Oseen-Frank energy is predicated on the assumption that the elastic strains are appropriate to model the energy. The function space usually applied alongside (0.4) or (0.6) is $W^{1,2}\left(\Omega, \mathbb{S}^2\right)$. However in the later chapters we will investigate whether this assumption is entirely warranted given our initial dismissal of the head to tail symmetry issue. A generalisation of this theory was proposed by Ericksen [33] which includes a scalar order parameter $s(x) \in \left[-\frac{1}{2}, 1\right]$ to represent how well ordered the molecules are at the point x with respect to the director. If $s(x) = 1$ then all of the molecules are perfectly aligned with the director whereas if $s(x) = -\frac{1}{2}$ then all of the molecules are aligned perpendicular to the director but are uniformly distributed in that plane. He proposed a free energy of the form [92]

$$\begin{aligned} &I(s, \mathbf{n}) \\ &= \int_\Omega K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n} + t)^2 + K_3|\mathbf{n} \times \nabla \times \mathbf{n}|^2 + (K_2 + K_4)\left(\mathrm{Tr}\,(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2\right) \\ &\quad + H_1|\nabla s|^2 + H_2(\nabla s \cdot \mathbf{n})^2 + H_3\,(\nabla \cdot \mathbf{n})\,(\nabla s \cdot \mathbf{n}) + H_4 \nabla s \cdot (\nabla \mathbf{n})\mathbf{n} + \sigma(s)\, dx, \end{aligned} \tag{0.7}$$

where $\sigma(s) := \frac{a}{2}s^2 - \frac{b}{3}s^3 + \frac{c}{4}s^4$. The function σ represents the energetic competition between the disordered isotropic phase and the liquid crystal phase. Therefore the coefficients a, b, and c are temperature dependent. For this theory, the set of relations which correspond to the one constant approximation from the Oseen-Frank theory is

$$K_1 = K_2 = K_3 = s^2 K, \;\; K_4 = 0, \;\; H_1 = H, \;\; H_2 = H_3 = H_4 = 0,$$

so that (0.7) reduces to

$$I(s, \mathbf{n}) = \int_\Omega K s^2 \left(|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2\right) + H|\nabla s|^2 + \sigma(s)\, dx.$$

In this form it is clear that this Ericksen free energy is a generalisation of the Oseen-Frank one. A benefit of the extra layer of complexity is that within this structure all orientable defects, whether they be point, line or plane defects, have finite energy. This is because it is possible to model the core of the defects with a region where $s = 0$. This has commonly been referred to as melting in the core of the defects because $s = 0$ represents the disordered isotropic phase which occurs at higher temperatures.

The Landau-de Gennes and Q-tensor theories use different order parameters to encapsulate their data. They both use a symmetric, traceless, matrix order parameter $\mathbf{Q} : \Omega \to \mathbb{R}^{3\times 3}$. The Q-tensor theory also imposes a restriction on the size of the eigenvalues of $\mathbf{Q}$ to ensure their

physicality. Just as in the derivation of the Oseen-Frank free energy, the free energy density should be invariant under rotations and translations so that if ϵ_{ijk} denotes the Levi-Cevita connection then the free energy can be written as [72]

$$I(\mathbf{Q}) = \int_\Omega W(\mathbf{Q}, \nabla\mathbf{Q}) + \psi_B(\mathbf{Q})\, dx \tag{0.8}$$

where

$$W(\mathbf{Q}, \nabla\mathbf{Q}) = L_1\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k} + L_2\mathbf{Q}_{ij,j}\mathbf{Q}_{ik,k} + L_3\mathbf{Q}_{ik,j}\mathbf{Q}_{ij,k} + L_4\epsilon_{lik}\mathbf{Q}_{lj}\mathbf{Q}_{ij,k} + L_6\mathbf{Q}_{lk}\mathbf{Q}_{ij,l}\mathbf{Q}_{ij,k} \tag{0.9}$$

and

$$\psi_B(\mathbf{Q}) = a\text{tr}\left(\mathbf{Q}^2\right) + \frac{2b}{3}\text{tr}\left(\mathbf{Q}^3\right) + c\text{tr}\left(\mathbf{Q}^4\right).$$

The function ψ_B models the bulk energy competition between the isotropic and ordered phases. It corresponds to the function σ from Ericksen's theory. In reality a, b, and c will all be temperature dependent but it is normally assumed for convenience that b and c are independent of temperature, $c > 0$ and $a = \alpha(T - T^*)$, where $\alpha > 0$, T is the temperature and T^* is the temperature at which the isotropic phase becomes unstable. Following the logic of [69] a suitable one-constant approximation for (0.9) is

$$L_1 = \frac{K}{2},\ L_4 = 2tK,\ L_2 = L_3 = L_6 = 0$$

so that (0.8) reduces to

$$I(\mathbf{Q}) = \int_\Omega \frac{K}{2}\left[|\nabla\mathbf{Q}|^2 + 4t\mathbf{Q}\cdot\nabla\times\mathbf{Q}\right] + \psi_B(\mathbf{Q})\, dx,$$

where $(\nabla\times\mathbf{Q})_{ij} = \epsilon_{jab}\mathbf{Q}_{ib,a}$. As the matrix $\mathbf{Q}$ is trace-free, its eigenvalues sum to zero. This gives rise to two distinct categories of Q-tensors. If all the eigenvalues are different then $\mathbf{Q}$ is said to be *biaxial* and can be written as

$$\mathbf{Q} = s_1\left(\mathbf{n}_1\otimes\mathbf{n}_1 - \frac{1}{3}I\right) + s_2\left(\mathbf{n}_2\otimes\mathbf{n}_2 - \frac{1}{3}I\right) \tag{0.10}$$

where $\mathbf{n}_1, \mathbf{n}_2 \in \mathbb{S}^2$, $s_1, s_2 \in \mathbb{R}$ and $\mathbf{n}_1\cdot\mathbf{n}_2 = 0$. If two of the eigenvalues of the matrix are equal then $\mathbf{Q}$ is said to be *uniaxial* and can be written as

$$\mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right) \tag{0.11}$$

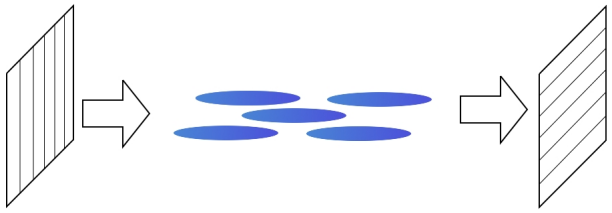
for $\mathbf{n} \in \mathbb{S}^2$ and $s \in \mathbb{R}$. Equations (0.10) and (0.11) highlight an advantage of using a matrix order parameter. They both respect the head to tail symmetry of the molecules so there is no distinction between $\mathbf{n}$ and $-\mathbf{n}$. It is intuitively clear that all of these continuum theories that we have detailed lie in some sort of hierarchy. They have seemingly comparable free energy densities and in Chapter 4 we discuss the relationship between the various theories. It transpires that finding minimisers in the uniaxial Landau-de Gennes framework is equivalent to minimising in the Ericksen framework with the appropriate function spaces. One of the fundamental problems in the mathematical study of liquid crystals is which theory is best

in which situation; is the added complexity of Landau-de Gennes worthwhile because it is capable of predicting more complex behaviour which Oseen-Frank cannot? Is Ericksen's theory merely an intermediate one between Oseen-Frank and the Q-tensor theory? Is Ericksen's theory therefore redundant because it is not as simple as Oseen-Frank without being able to predict the complexities which the Q-tensor theory can explain? While we will not be able to conclusively answer these questions, Chapters 4 and 5 shed some significant light on them. In the final part of the thesis we propose the idea of studying the Oseen-Frank energy functional over SBV functions and see that this brings some of the complex cholesteric structures within reach of the analyst rather than being accessible only through numerical simulations.

Liquid Crystal Devices

The main incentive for the study of liquid crystals, from an industrial point of view, is to create improved liquid crystal displays (LCD). The simplest LCD is the twisted nematic LCD whose basic operation is shown in Figure 0.4. The liquid crystal is held between two parallel plates with boundary conditions that are in the plane of the plates. Two polarisers are then placed on either side of the liquid crystal sample. Then in the absence of any electric field, the molecules align in a planar fashion and twist the polarised light to allow it to pass through the second polariser.

(a) Without electric field



(b) With electric field

Figure 0.4: Twisted nematic device [88]

However when an electric field above a critical threshold is applied, the molecules prefer to align more perpendicular to the plates so that the polarised light is no longer twisted within the cell. This prevents it from passing through the second polariser and forms the off state. An aspect of this design of LCD which is inferior to its competitor OLED (organic light emitting diode) is the pixel response time. Current LCD pixels can operate at around 240Hz, an order of magnitude slower than OLED displays. To design improved pixels would reduce motion blur on the screen as well as indirectly reducing power consumption by allowing the removal

of the colour filters and using a coloured back-light instead. However we will not be looking into this switching process because we focus our attention on static issues instead.

A second drawback of the device in Figure 0.4 is that a current must be applied at least 60 times a second in order that the 'off-state' does not flicker. Therefore the ideal situation which is sought would be a system with two or more distinct minimisers that can be traversed with just a single applied voltage. Some such examples have been constructed using different grating patterns on the surface or by restricting the director to lie in a single plane [18, 90]. However no such example has yet emerged with sufficiently controllable and distinct optical properties for industry to consider replacing the well established LCD design.

Chapter 1

Analysis of Local Minima for Constrained Minimisation Problems

1.1 Introduction

As was outlined in the introduction, the canonical problem in the vectorial calculus of variations is to minimise the integral functional

$$I(\mathbf{n}) = \int_{\Omega} F(x, \mathbf{n}(x), \nabla \mathbf{n}(x))\, dx \tag{1.1}$$

where $\mathbf{n} : \mathbb{R}^d \to \mathbb{R}^k$ lies in an appropriate Sobolev space together with some boundary conditions. Global minimisers for this problem exist provided that the Lagrangian F satisfies certain quasiconvexity and growth conditions (see Dacorogna [26] for a summary). For local minimisers, the conditions heavily depend upon which distance metric is chosen. To formulate necessary and sufficient conditions for strong and weak local minimisers the first and second variations of the functional I are considered, just as for finite-dimensional functions. Such local results were first proved by, for example, Graves [42], van Hove [47], Meyers [65] and Ball & Marsden [11]. A sufficiency result for strong local minimisers has proved to be the trickiest local result to derive, but the recent paper of Grabovsky & Mengesha [41] has shed new light on the subject.

However these classical results do not apply directly for variational problems with pointwise constraints. This is simply because if we take any test function ϕ, $\mathbf{n} + t\phi$ will not satisfy the same constraint in general. This is particularly pertinent in the Oseen-Frank or Ericksen theory where the director satisfies $|\mathbf{n}| = 1$ as it represents an orientation. The focus of this chapter is to address this issue by proving analogues of the unconstrained local minimiser results for a wide variety of constrained problems. These results are then applicable in the study of liquid crystals, micromagnetics and other constrained variational problems, providing the constraint is of sufficient regularity.

In research on liquid crystals, designing multi-stable, power efficient, devices is one of the core aims in the industry, but the relevant stability questions are not usually considered within a precise mathematical framework. Hence local stability is typically approached through a linearisation argument and phase plane analysis [24], or a study of the Euler-Lagrange

equations [27], or simply through experimental data. The results of this chapter supplement such analysis by providing a carefully formulated and rigorous mathematical structure in which to operate. In Chapter 3 we will illustrate how these results can be used, both by analysts and numerical analysts, to deduce stability predictions. For example, in Theorem 3.1 we quantify the stability of the constant state $\mathbf{n} = \mathbf{e}_3$ for the one-constant Oseen-Frank energy for cholesterics

$$I(\mathbf{n}) = K \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \, dx,$$

where $K, t > 0$. The domain Ω will be a cuboid. If its height is d, we show that $t = \frac{\pi}{d}$ is the critical value for the stability of the constant state; it is unstable if $t > \frac{\pi}{d}$ and stable if $t < \frac{\pi}{d}$. This prediction is qualitatively consistent with the experimental data of Gartland et al. [39].

The minimisation problem (1.1) takes on a much greater level of complexity if the unknown $\mathbf{n} : N \to M$ is a mapping between two manifolds $N \subset \mathbb{R}^d$ and $M \subset \mathbb{R}^k$. In this situation the corresponding Sobolev spaces are defined as

$$W^{1,p}(N, M) := \left\{ \mathbf{n} \in W^{1,p}\left(N, \mathbb{R}^k\right) \,\middle|\, \mathbf{n}(x) \in M \text{ a.e.} \right\}.$$

However, in this setting some of the standard notions about Sobolev spaces for mappings between Euclidean spaces do not hold. For example, Bethuel & Zheng [14] proved that depending on the topology of the manifold M, smooth maps are not always dense in $W^{1,p}(N, M)$. As was mentioned in the introduction, these spaces are the natural ones for harmonic maps where the object is to minimise

$$E(\mathbf{n}) = \int_N \|D\mathbf{n}\|^2 \, d\mu_N,$$

for $\mathbf{n} \in W^{1,2}(N, M)$. The second variation of this functional was derived by Smith [86] and has interesting properties. Xin [95] showed that if $k > 1$ then there is no non-constant stable harmonic map from $\mathbb{S}^{k-1}$ to any Riemannian manifold and there are many other related results [58, 82]. Urakawa [91] has a good overview of a number of such instability theorems. These results all emphasise that a constrained variational problem must be carefully considered in its own right, since its properties can be very different to its unconstrained analogue.

In this chapter we will explore some middle ground between the study of harmonic maps and the standard vectorial minimisation problems. We restrict our domains to be bounded Lipschitz domains in $\mathbb{R}^d$, but we consider a much wider class of Lagrangians than in harmonic maps. The motivation for this work came from $\mathbb{S}^2$ valued maps, but we generalise our constraint to $\mathbf{n}(x) \in M$ where $M \subset \mathbb{R}^k$ is a manifold of sufficient regularity. The regularity we impose on M is necessary to ensure that the nearest point projection map $P : \mathbb{R}^k \to M$ has an appropriate differentiability. We need the regularity of P because the first variation we will be using in this chapter is of the form

$$\frac{d}{d\epsilon} I(P(\mathbf{n} + \epsilon\phi))\bigg|_{\epsilon=0}.$$

An advantage of this style of variation is that the test functions themselves are unconstrained. This makes the problem more accessible to numerical and computational methods for investigating stability as we shall see in Chapter 3.

The chapter contains a number of results, each of which either proves necessary or sufficient conditions for a given state to be a local minimiser. In Section 1.3 we begin by establishing necessary conditions for a weak local minimiser. The first result, Theorem 1.6, is the expected condition that a weak local minimiser must have a vanishing first variation and non-negative second variation. The second necessary condition for a weak local minimiser is a Legendre condition which is slightly modified from the standard version due to the curvature of the target manifold.

From there we prove the weak sufficiency theorem, Theorem 1.8, that a vanishing first variation and strictly positive second variation yield a strict weak local minimiser. In Section 1.5 we examine the extra necessary conditions which a strong local minimiser satisfies: quasiconvexity in the interior, at the free boundary, and the Weierstrass condition. Then we establish two strong sufficiency results, Theorems 1.14 and 1.17, with different sets of assumptions. The first uses Taheri's result [89, Theorem 3.3] with a pointwise Weierstrass condition, while the second uses Grabovsky & Mengesha's result [41], which is much more technical, but also more general. We finish the chapter with an application of our results. It illustrates how the study of global minimisers is very different with a pointwise constraint. In the application we study the Dirichlet energy

$$I(\mathbf{n}) = \int_0^1 |\mathbf{n}_x|^2 \, dx$$

for $\mathbf{n} : (0,1) \to \mathbb{S}^1$, and find infinitely many strong local minimisers which are not global minimisers. This cannot be the case without the constraint because in that situation the convexity of the Lagrangian ensures that the Euler-Lagrange equation has a unique solution.

1.2 Preliminaries and Notation

Throughout this chapter, unless stated otherwise, $\Omega \subset \mathbb{R}^d$ denotes a bounded Lipschitz domain with boundary $\partial\Omega$. We suppose that the boundary has two disjoint, relatively open, measurable components $\partial\Omega_1$ and $\partial\Omega_2$ such that $\partial\Omega = \overline{\partial\Omega_1} \cup \overline{\partial\Omega_2}$. We will also be supposing throughout that $M \subset \mathbb{R}^k$ is a closed, bounded manifold of class C^4. The embedding theorems of Whitney and Nash ensure that these regularity assumptions can also apply to a wide array of abstract manifolds when embedded in Euclidean spaces. For $1 \leqslant p \leqslant \infty$ we define the Sobolev space $W^{1,p}(\Omega, M)$ as

$$W^{1,p}(\Omega, M) := \left\{ \mathbf{n} \in W^{1,p}\left(\Omega, \mathbb{R}^k\right) \,\middle|\, \mathbf{n}(x) \in M \text{ a.e.} \right\}.$$

Then we consider the problem of minimising

$$I(\mathbf{n}) = \int_\Omega F(x, \mathbf{n}(x), \nabla\mathbf{n}(x)) \, dx,$$

over the set of admissible mappings

$$\mathcal{A} := \left\{ \mathbf{n} \in W^{1,1}(\Omega, M) \,\middle|\, \mathbf{n} = \mathbf{n}_0 \text{ on } \partial\Omega_1 \right\},$$

where $k, d \in \mathbb{N}$ and $\mathbf{n}_0 \in W^{1,1}(\Omega, M)$. We denote the corresponding set of test functions, or variations, by

$$\mathrm{Var}_{\mathcal{A}} := \left\{ \mathbf{v} \in C^\infty\left(\overline{\Omega}, \mathbb{R}^k\right) \,\middle|\, \mathbf{v} = 0 \text{ on } \partial\Omega_1 \right\}.$$

We assume (unless stated otherwise) that

- $F \in C\left(\overline{\Omega} \times M \times \mathbb{R}^{k\times d}\right)$
- There exists some open neighbourhood O of M such that for every $x \in \Omega$,

$$F(x, \cdot, \cdot) \in C^2\left(O \times \mathbb{R}^{k\times d}\right).$$

These assumptions are sufficient to ensure that the second variation is well defined. In order to prove our results we will study unconstrained functionals which are related to I, so that we can apply standard results to them. However in order to do this we need a result about the regularity of the nearest point projection map. We remind the reader that a manifold $M \subset \mathbb{R}^k$ is a C^r-manifold, of codimension d, around some point $x \in M$, if there exists some open set $V \subset \mathbb{R}^k$ and C^r function $F : V \to \mathbb{R}^d$ such that

$$M \cap V = \{x \in V \,|\, F(x) = 0\}.$$

Lemma 1.1. *[59, Lemma 4] Let $M \subset \mathbb{R}^k$ be a manifold of class C^r (with $r \geqslant 2$) around some $x \in M$. Then there exists a $\delta > 0$ such that the nearest point projection $P : B(x, \delta) \to M$ is unique and of class C^{r-1}.*

It follows from the lemma, using a simple compactness argument, that for any closed and bounded manifold $M \subset \mathbb{R}^k$ of class C^4, there is some open set U, containing M, such that the nearest point projection $P : U \to M$ is unique and is C^3. We assume without loss of generality that $O \subset U$. We also choose $\delta^* > 0$ such that if $d(x, M) < \delta^*$ then $x \in O$ and define a corresponding cut-off function $\psi \in C^\infty\left(\mathbb{R}^k, \mathbb{R}\right)$ such that

$$\psi(x) \equiv 0 \quad \text{if } d(x, M) > \delta^* \quad \text{and} \quad \psi(x) \equiv 1 \quad \text{if } d(x, M) < \frac{\delta^*}{2}. \tag{1.2}$$

Then we can define two associated functionals

$$J(\mathbf{m}) := \int_\Omega G(x, \mathbf{m}, \nabla\mathbf{m})\, dx = \int_\Omega \psi(\mathbf{m})\, F(x, P(\mathbf{m}), \nabla[P(\mathbf{m})])\, dx \tag{1.3}$$

and

$$\begin{aligned} K(\mathbf{m}) :=& \int_\Omega H(x, \mathbf{m}, \nabla\mathbf{m})\, dx \\ =& J(\mathbf{m}) + \int_\Omega \psi(\mathbf{m}) \left[|\mathbf{m} - P(\mathbf{m})|^2 + |\nabla\mathbf{m} - \nabla[P(\mathbf{m})]|^2 \right] dx. \end{aligned} \tag{1.4}$$

These functionals both act on the set

$$\mathcal{B} := \left\{ \mathbf{m} \in W^{1,1}\left(\Omega, \mathbb{R}^k\right) \,\middle|\, \mathbf{m} = \mathbf{n}_0 \text{ on } \partial\Omega_1 \right\}.$$

Then from the definitions (1.2), (1.3) and (1.4), together with the assumptions on the Lagrangian F, we have that

- $G, H \in C\left(\overline{\Omega} \times \mathbb{R}^k \times \mathbb{R}^{k\times d}\right)$
- For every $x \in \Omega$, $G(x,\cdot,\cdot), H(x,\cdot,\cdot) \in C^2\left(\mathbb{R}^k \times \mathbb{R}^{k\times d}\right)$.

It is also worth noting that the set of variations for the functionals J and K are the same as for the original functional I so that

$$\mathrm{Var}_{\mathcal{B}} = \mathrm{Var}_{\mathcal{A}}.$$

We will denote the unit ball in $\mathbb{R}^n$ simply by $\mathbf{B}$. The function space $C_0^\infty\left(U, \mathbb{R}^k\right)$ will denote the space of smooth maps from U to $\mathbb{R}^k$ with compact support in U. For ease of notation if $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$ we will often use the functions $\mathbf{w}_t(x)$ and $g(t)$ defined as

$$\mathbf{w}_t(x) := P(\mathbf{n}(x) + t\mathbf{v}(x)) \quad \text{and} \quad g(t) := I(\mathbf{w}_t). \tag{1.5}$$

So $\mathbf{w}_t$ represents our small perturbation and $g(t)$ is the energy of the perturbed state. We will use the notation that primes denote derivatives with respect to t:

$$\mathbf{w}_t'(x) := \frac{d}{dt}\mathbf{w}_t(x).$$

We also need to introduce some theoretical notions which will arise in this chapter. We recall that strong and weak local minimisers are L^∞ and $W^{1,\infty}$ local minimisers respectively, as defined in Definition 0.2.

Definition 1.2. *The Weierstrass excess function of a Lagrangian F is given by*

$$\mathcal{E}_F(x, z, p, q) := F(x, z, q) - F(x, z, p) - F_p(x, z, p) : (q - p).$$

Definition 1.3 (Quasiconvexity)**.** *A continuous function $f : \mathbb{R}^{k\times d} \to \mathbb{R}$ is quasiconvex at a point $\zeta \in \mathbb{R}^{k\times d}$ if*

$$f(\zeta) \leqslant \frac{1}{|D|}\int_D f\left(\zeta + \nabla\phi(x)\right)\, dx$$

for every set $D \subset \mathbb{R}^d$ which is open and bounded and every $\phi \in W_0^{1,\infty}\left(D, \mathbb{R}^k\right)$.

Definition 1.4 (Rank-One Convexity)**.** *A continuous function $f : \mathbb{R}^{k\times d} \to \mathbb{R}$ is rank-one convex at a point $\zeta \in \mathbb{R}^{k\times d}$ if*

$$f(\zeta) \leqslant tf(A_1) + (1-t)f(A_2)$$

for any $A_1, A_2 \in \mathbb{R}^{k\times d}$, $t \in [0,1]$, such that $\zeta = tA_1 + (1-t)A_2$ and rank $(A_1 - A_2) \leqslant 1$.

In most of the results and proofs given below we will apply a result from the unconstrained theory to either the functional J or K, and then relate the condition back to I. Many of the standard results can be found in Giaquinta and Hildebrandt [40, Ch 4], although where appropriate we will use the simple extension of their results from C^1 minimisers to $W^{1,\infty}$ minimisers. This is straightforward when studying the first and second variations, but we have to be more careful when proving point-wise conditions like quasiconvexity or the Legendre-Hadamard condition for $W^{1,\infty}$ functions. Indeed in Section 1.5 we prove directly the unconstrained result that a Lipschitz function which is a strong local minimiser satisfies the quasiconvexity condition almost everywhere in the interior. There is no explicit result concerning this in the literature that we are aware of.

The Case $M = \mathbb{S}^{k-1}$

In the situation where $M = \mathbb{S}^{k-1}$ it is instructive to note the explicit forms for these abstract concepts as we will return to this case in later chapters. The projection map $P : \mathbb{R}^k \setminus \{0\} \to \mathbb{S}^{k-1}$ is given by $P(x) = \frac{x}{|x|}$, so that if $x \in \mathbb{R}^k$ and $\mathbf{m} \in \mathcal{B}$ then

$$\nabla P(x) = \frac{1}{|x|} I - \frac{x \otimes x}{|x|^3} \quad \text{and} \quad \nabla \left[P(\mathbf{m}) \right] = \frac{\nabla \mathbf{m}}{|\mathbf{m}|} - \frac{\mathbf{m} \otimes \left(\mathbf{m}^T \nabla \mathbf{m} \right)}{|\mathbf{m}|^3}.$$

In this instance we also have explicit forms for the perturbations. Using the definitions in (1.5), if $\mathbf{n} \in \mathcal{A}$ and $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$, then

$$\mathbf{w}_0 = \mathbf{n}, \quad \mathbf{w}_0' = \mathbf{v} - \mathbf{n} \left(\mathbf{n} \cdot \mathbf{v} \right), \quad \mathbf{w}_0'' = -2\mathbf{v} \left(\mathbf{n} \cdot \mathbf{v} \right) - \mathbf{n}|\mathbf{v}|^2 + 3\mathbf{n} \left(\mathbf{n} \cdot \mathbf{v} \right)^2. \tag{1.6}$$

All of the results in Sections 1.3-1.6 can be understood for mappings into spheres by using these relations in the statements rather than the more general forms for mappings into differentiable manifolds.

Remark 1.5. *If $x \in M$ then $\nabla P(x)$ is the matrix representation of the orthogonal projection onto the tangent space of M at x. Similarly $\mathbf{w}_0'(x)$ will always lie in the tangent space to M at $\mathbf{n}(x)$. This can help with the interpretation of a number of the statements below. For example, in Theorem 1.8 we see that the positivity of the second variation we require is in fact positivity in all tangential directions of M at $\mathbf{n}(x)$.*

1.3 Necessary Conditions for a Weak Local Minimiser

Theorem 1.6. *Suppose that $\mathbf{n} \in \mathcal{A} \cap W^{1,\infty}(\Omega, M)$ is a weak local minimiser of I and for $\mathbf{v} \in Var_{\mathcal{A}}$ define (see* (1.5)*)*

$$g(t) = I\left(P(\mathbf{n} + t\mathbf{v})\right) = I(\mathbf{w}_t).$$

Then

$$g'(0) = 0 \quad \textit{and} \quad g''(0) \geqslant 0 \quad \forall \mathbf{v} \in Var_{\mathcal{A}}.$$

Proof

Since $\mathbf{n}$ is a weak local minimiser, we know that there exists some $\alpha > 0$ such that

$$I(\mathbf{m}) \geqslant I(\mathbf{n}) \quad \text{for all} \quad \mathbf{m} \in \mathcal{A} \quad \text{such that} \quad \|\mathbf{n} - \mathbf{m}\|_{1,\infty} < \alpha. \tag{1.7}$$

The main goal of the proof is to show that (1.7) implies $\mathbf{n}$ is a weak local minimiser of J. We take some $\mathbf{m} \in \mathcal{B}$, and without loss of generality we assume that $\|\mathbf{n} - \mathbf{m}\|_\infty \leqslant \frac{\delta^*}{2}$. We first obtain an upper bound for $\|\mathbf{n} - P(\mathbf{m})\|_{1,\infty}$ in terms of $\|\mathbf{n} - \mathbf{m}\|_{1,\infty}$. We do this with two straightforward calculations.

$$\begin{aligned} |\mathbf{n} - P(\mathbf{m})| &\leqslant |\mathbf{n} - \mathbf{m}| + |\mathbf{m} - P(\mathbf{m})| \\ &\leqslant 2|\mathbf{n} - \mathbf{m}| \end{aligned} \tag{1.8}$$

since $P(\mathbf{m})$ is the closest point projection onto M. As for the derivatives we first note the relation

$$\nabla \left[P(\mathbf{m}(x))\right] = \nabla P(\mathbf{m}(x))\, \nabla \mathbf{m}(x), \tag{1.9}$$

with the right-hand side of (1.9) being understood as two matrices multiplied together. As P is C^3 in a neighbourhood of M, and $\|\mathbf{n} - \mathbf{m}\|_\infty < \frac{\delta^*}{2}$, we infer $\nabla \left[P(\mathbf{m})\right] \in L^1$. Hence $P(\mathbf{m}) \in \mathcal{A}$. Furthermore

$$\begin{aligned} |\nabla \mathbf{n} - \nabla \left[P(\mathbf{m})\right]| &= |\nabla P(\mathbf{m}) \nabla \mathbf{m} - \nabla P(\mathbf{m}) \nabla \mathbf{n} + \nabla P(\mathbf{m}) \nabla \mathbf{n} - \nabla \mathbf{n}| \\ &\leqslant |\nabla P(\mathbf{m})|\, |\nabla \mathbf{m} - \nabla \mathbf{n}| + |\nabla \mathbf{n}|\, |\nabla P(\mathbf{m}) - \nabla P(\mathbf{n})|. \end{aligned}$$

In order to bound these terms we use the fact that the projection map P is twice differentiable and the mean value theorem to see that

$$|\nabla \mathbf{n} - \nabla \left[P(\mathbf{m})\right]| \leqslant C_1 \left(|\nabla \mathbf{m} - \nabla \mathbf{n}| + |\mathbf{m} - \mathbf{n}|\right). \tag{1.10}$$

Combining (1.8) and (1.10) tells us that $\|\mathbf{n} - P(\mathbf{m})\|_{1,\infty} \leqslant D\, \|\mathbf{n} - \mathbf{m}\|_{1,\infty}$, where D is independent of $\mathbf{m}$. Therefore if $\|\mathbf{n} - \mathbf{m}\|_{1,\infty}$ is sufficiently small

$$J(\mathbf{m}) = I\left(P(\mathbf{m})\right) \geqslant I(\mathbf{n}) = J(\mathbf{n}). \tag{1.11}$$

In other words $\mathbf{n}$ is a weak local minimiser of J. Equation (1.11) holds because $\|\mathbf{m} - \mathbf{n}\|_\infty \leqslant \frac{\delta^*}{2}$ implies $\psi(\mathbf{m}) \equiv 1$. Now we can apply the standard result (see for example [40, Ch 4,1.1]) to say that

$$\delta J(\mathbf{n})(\mathbf{v}) := \left.\frac{d}{dt} J(\mathbf{n} + t\mathbf{v})\right|_{t=0} = 0$$

and

$$\delta^2 J(\mathbf{n})(\mathbf{v}, \mathbf{v}) := \left.\frac{d^2}{dt^2} J(\mathbf{n} + t\mathbf{v})\right|_{t=0} \geqslant 0,$$

for all $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$. In order to relate these conditions to I, it can simply be calculated that for all $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$

$$\left.\frac{d}{dt} \psi(\mathbf{n} + t\mathbf{v})\right|_{t=0} = \left.\frac{d^2}{dt^2} \psi(\mathbf{n} + t\mathbf{v})\right|_{t=0} = 0,$$

so that the construction of the functional J implies, as required, that

$$g'(0) = \frac{d}{dt} I\left(P(\mathbf{n} + t\mathbf{v})\right)\Big|_{t=0} = \frac{d}{dt} J(\mathbf{n} + t\mathbf{v})\Big|_{t=0} = 0$$

and

$$g''(0) = \frac{d^2}{dt^2} I\left(P(\mathbf{n} + t\mathbf{v})\right)\Big|_{t=0} = \frac{d^2}{dt^2} J(\mathbf{n} + t\mathbf{v})\Big|_{t=0} \geqslant 0.$$

□

Theorem 1.7 (Legendre's Condition)**.** *Suppose that* $\mathbf{n} \in \mathcal{A} \cap W^{1,\infty}(\Omega, M)$ *is a weak local minimiser of* I *and denote* $F(x, \mathbf{n}(x), \nabla\mathbf{n}(x))$ *by* F*, then*

$$\sum_{i,j,k,l} \frac{\partial^2 F}{\partial \mathbf{n}_{i,j} \partial \mathbf{n}_{k,l}} \eta_j \eta_l \left[\nabla P(\mathbf{n})\zeta\right]_i \left[\nabla P(\mathbf{n})\zeta\right]_k \geqslant 0,$$

for all $\eta \in \mathbb{R}^d$*,* $\zeta \in \mathbb{R}^k$ *and almost every* $x \in \Omega$*.*

Proof

We take an arbitrary $\phi \in C_0^\infty\left(\Omega, \mathbb{R}^k\right)$ and let $\mathbf{w}_t = \mathbf{n} + t\phi$. As part of this proof we need an explicit form for the second variation. Therefore with a brief calculation we find

$$\begin{aligned} L(\phi) :&= \int_\Omega W(x, \phi, \nabla\phi)\, dx \\ &= \frac{d^2}{dt^2} I\left(\mathbf{w}_t\right)\Big|_{t=0} \\ &= \int_\Omega \mathbf{w}_0'^T F_{\mathbf{nn}}(x)\mathbf{w}_0' + 2\left[F_{\mathbf{n}\nabla\mathbf{n}}(x)\nabla\mathbf{w}_0'\right]\cdot\mathbf{w}_0' + \nabla\mathbf{w}_0'^T F_{\nabla\mathbf{n}\nabla\mathbf{n}}(x)\nabla\mathbf{w}_0' \\ &\qquad + F_{\mathbf{n}}(x)\cdot\mathbf{w}_0'' + F_{\nabla\mathbf{n}}(x) : \nabla\mathbf{w}_0''\, dx \end{aligned} \tag{1.12}$$

where

$$F(x) := F(x, \mathbf{n}(x), \nabla\mathbf{n}(x)),$$

$$\mathbf{w}_0'(x)_i = \textstyle\sum_j P_{i,j}(\mathbf{n}(x))\phi_j(x),$$

$$\mathbf{w}_0{}''(x)_i = \textstyle\sum_{j,k} P_{i,jk}(\mathbf{n}(x))\phi_j(x)\phi_k(x).$$

The summation notations we are using in (1.12) are

$$(F_{\mathbf{n}})\cdot\mathbf{b} = \frac{\partial F}{\partial \mathbf{n}_i}\mathbf{b}_i, \quad (F_{\nabla\mathbf{n}}) : \mathbf{A} = \frac{\partial F}{\partial \mathbf{n}_{i,j}}\mathbf{A}_{i,j}, \quad \mathbf{b}^T(F_{\mathbf{nn}})\,\mathbf{b} = \frac{\partial^2 F}{\partial \mathbf{n}_i \partial \mathbf{n}_j}\mathbf{b}_i\mathbf{b}_j,$$

and

$$\left[(F_{\mathbf{n}\nabla\mathbf{n}})\,\mathbf{A}\right]\cdot\mathbf{b} = \frac{\partial^2 F}{\partial \mathbf{n}_i \partial \mathbf{n}_{j,k}}\mathbf{A}_{j,k}\mathbf{b}_i, \quad \mathbf{A}^T(F_{\nabla\mathbf{n}\nabla\mathbf{n}})\,\mathbf{A} = \frac{\partial^2 F}{\partial \mathbf{n}_{i,j} \partial \mathbf{n}_{k,l}}\mathbf{A}_{i,j}\mathbf{A}_{k,l}.$$

We know from Theorem 1.6 that since $\mathbf{n} \in \mathcal{A} \cap W^{1,\infty}(\Omega, M)$ is a weak local minimiser of I, its second variation is non-negative. Therefore

$$L(\phi) \geqslant 0 \quad \forall\phi \in C_0^\infty\left(\Omega, \mathbb{R}^k\right). \tag{1.13}$$

By using a simple density argument we can expand upon (1.13) and say

$$L(\phi) \geqslant 0 \quad \forall \phi \in W_0^{1,2}\left(\Omega, \mathbb{R}^k\right).$$

So certainly, $\phi = 0$ is a strong local minimiser of the functional L. Now we can apply Corollary 1.13 (which will be proved in Section 1.5) to deduce that for almost every $x \in \Omega$

$$\mathcal{E}_W(x, 0, 0, \zeta \otimes \eta) \geqslant 0 \quad \forall\, \zeta \in \mathbb{R}^k,\ \eta \in \mathbb{R}^d. \tag{1.14}$$

Since W is a quadratic function in ϕ we know that $W_{\nabla\phi}(x, 0, 0) = 0$. Therefore we simplify (1.14) to find

$$\begin{aligned} 0 &\leqslant \mathcal{E}_W(x, 0, 0, \zeta \otimes \eta) \\ &= W(x, 0, \zeta \otimes \eta) \\ &= \sum_{i,j,k,l} \frac{\partial^2 F}{\partial \mathbf{n}_{i,j} \partial \mathbf{n}_{k,l}} \eta_j \eta_l \left[\nabla P(\mathbf{n})\zeta\right]_i \left[\nabla P(\mathbf{n})\zeta\right]_k . \end{aligned}$$

□

1.4 Sufficient Conditions for a Weak Local Minimiser

Theorem 1.8. *Let* $\mathbf{n} \in \mathcal{A} \cap W^{1,\infty}(\Omega, M)$ *and for* $\mathbf{v} \in Var_{\mathcal{A}}$ *define (see* (1.5)*)*

$$g(t) = I\left(P(\mathbf{n} + t\mathbf{v})\right) = I(\mathbf{w}_t).$$

Suppose there exists some $\gamma > 0$ *such that*

$$g'(0) = 0 \quad \textit{and} \quad g''(0) \geqslant \gamma \|\mathbf{w}_0'\|_{1,2}^2 \quad \forall \mathbf{v} \in Var_{\mathcal{A}}.$$

Then $\mathbf{n}$ *is a strict weak local minimiser of* I.

Proof

For the sufficiency results we will use the functional K as the unconstrained counterpart to I. The reason that we cannot use J as we did in the necessity proofs, is that the inherent structure of J means it cannot have a strict local minimiser. This is because if we take any two functions $\mathbf{m}_1, \mathbf{m}_2 \in \mathcal{B}$ such that $P(\mathbf{m}_1) = P(\mathbf{m}_2)$, then $J(\mathbf{m}_1) = J(\mathbf{m}_2)$. We will use our assumptions to show that at $\mathbf{n}$, the first variation of K is zero and its second variation is strictly positive. We take a test function $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$ and recall that the function $\mathbf{w}_t$ is defined by $\mathbf{w}_t = P(\mathbf{n} + t\mathbf{v})$ so that

$$\mathbf{w}_0(x) = \mathbf{n}(x).$$

Then

$$\begin{aligned}
\delta K(\mathbf{n})(\mathbf{v}) :=& \left.\frac{d}{dt}K(\mathbf{n}+t\mathbf{v})\right|_{t=0} \\
=& \left.\frac{d}{dt}\int_\Omega \psi\left(\mathbf{n}+t\mathbf{v}\right)\left[F\left(x,\mathbf{w}_t,\nabla\mathbf{w}_t\right)+|\mathbf{n}+t\mathbf{v}-\mathbf{w}_t|^2+|\nabla(\mathbf{n}+t\mathbf{v})-\nabla\mathbf{w}_t|^2\right]dx\right|_{t=0} \\
=& g'(0)+\int_\Omega \left.\frac{d}{dt}\psi(\mathbf{n}+t\mathbf{v})\right|_{t=0}(*)\,dx \\
&+\left.\frac{d}{dt}\int_\Omega \psi\left(\mathbf{n}+t\mathbf{v}\right)\left[|\mathbf{n}+t\mathbf{v}-\mathbf{w}_t|^2+|\nabla(\mathbf{n}+t\mathbf{v})-\nabla\mathbf{w}_t|^2\right]dx\right|_{t=0} \\
=& g'(0)+\int_\Omega \left.\frac{d}{dt}\psi(\mathbf{n}+t\mathbf{v})\right|_{t=0}(**)+2\,\psi(\mathbf{n}+t\mathbf{v})(\mathbf{n}+t\mathbf{v}-\mathbf{w}_t)\cdot(\mathbf{v}-\mathbf{w}_t')\big|_{t=0} \\
&+2\psi(\mathbf{n}+t\mathbf{v})\left(\nabla(\mathbf{n}+t\mathbf{v})-\nabla\mathbf{w}_t\right):\left(\nabla\mathbf{v}-\nabla\mathbf{w}_t'\right)\big|_{t=0}\,dx \\
=& g'(0) \\
=& 0,
\end{aligned} \tag{1.15}$$

where $(*)$ and $(**)$ denote other terms. When it comes to the second variation, we simply take one more derivative than (1.15) and find

$$\begin{aligned}
&\delta^2 K(\mathbf{n})(\mathbf{v},\mathbf{v}) \\
=& \left.\frac{d^2}{dt^2}K(\mathbf{n}+t\mathbf{v})\right|_{t=0} \\
=& \left.\frac{d^2}{dt^2}\int_\Omega \psi\left(\mathbf{n}+t\mathbf{v}\right)\left[F\left(x,\mathbf{w}_t,\nabla\mathbf{w}_t\right)+|\mathbf{n}+t\mathbf{v}-\mathbf{w}_t|^2+|\nabla(\mathbf{n}+t\mathbf{v})-\nabla\mathbf{w}_t|^2\right]dx\right|_{t=0} \\
=& g''(0)+\int_\Omega \left.\frac{d^2}{dt^2}\psi(\mathbf{n}+t\mathbf{v})\right|_{t=0}(*)+\left.\frac{d}{dt}\psi(\mathbf{n}+t\mathbf{v})\right|_{t=0}(**) \\
&+2\left[|\mathbf{v}-\mathbf{w}_t'|^2-\mathbf{w}_t''\cdot(\mathbf{n}+t\mathbf{v}-\mathbf{w}_t)+|\nabla\mathbf{v}-\nabla\mathbf{w}_t'|^2-\left(\nabla(\mathbf{n}+t\mathbf{v})-\nabla\mathbf{w}_t\right):\nabla\mathbf{w}_t''\right]\Big|_{t=0}dx \\
=& g''(0)+2\int_\Omega |\mathbf{v}-\mathbf{w}_0'|^2+|\nabla\mathbf{v}-\nabla\mathbf{w}_0'|^2\,dx.
\end{aligned} \tag{1.16}$$

In both (1.15) and (1.16) we have been implicitly using the definition of ψ to know that for any given t small enough $\psi(\mathbf{n}+t\mathbf{v})\equiv 1$. Now we use our assumption on the second variation of I to show that the above expression is strictly positive.

$$\begin{aligned}
\delta^2 K(\mathbf{n})(\mathbf{v},\mathbf{v}) \geqslant& \int_\Omega \gamma|\mathbf{w}_0'|^2+\gamma|\nabla\mathbf{w}_0'|^2+2|\mathbf{v}-\mathbf{w}_0'|^2+2|\nabla\mathbf{v}-\nabla\mathbf{w}_0'|^2\,dx. \\
=& \frac{4}{2+\gamma}\int_\Omega \left|\mathbf{v}-\left(1+\frac{\gamma}{2}\right)\mathbf{w}_0'\right|^2+\left|\nabla\mathbf{v}-\left(1+\frac{\gamma}{2}\right)\nabla\mathbf{w}_0'\right|^2\,dx \\
&+\frac{2\gamma}{2+\gamma}\|\mathbf{v}\|_{1,2}^2 \\
\geqslant& \frac{2\gamma}{2+\gamma}\|\mathbf{v}\|_2^{1,2}
\end{aligned}$$

This proves the positivity of the second variation of K. Therefore the unconstrained result (see [40, Ch 4,1.1]) is applicable and implies that $\mathbf{n}$ is a strict weak local minimiser of K.

Thus there exists some $\epsilon > 0$ such that

$$K(\mathbf{m}) > K(\mathbf{n}) \quad \text{if} \quad \mathbf{m} \in \mathcal{B} \quad \text{and} \quad 0 < \|\mathbf{n} - \mathbf{m}\|_{1,\infty} < \epsilon.$$

This implies that if $\mathbf{m} \in \mathcal{A} \subset \mathcal{B}$ and $0 < \|\mathbf{m} - \mathbf{n}\|_{1,\infty} < \epsilon$, then

$$I(\mathbf{m}) = K(\mathbf{m}) > K(\mathbf{n}) = I(\mathbf{n}).$$

Therefore $\mathbf{n}$ is a strict weak local minimiser of I.

□

1.5 Necessary Conditions for a Strong Local Minimiser

Now we examine the extra conditions that a strong local minimiser must satisfy in addition to the conditions proved in Section 1.3. However in order to prove our constrained quasiconvexity in the interior result, we need an unconstrained result which we can apply to our functional J. Husseinov [49, Th. 1.8] has proved such a result but its technicalities mean that it requires a degree of manipulation to be applicable in our situation. Hence we will present our own self-contained proof (following an unpublished argument of John Ball), which we can readily apply. Solely for the purposes of our next theorem the set of admissible functions will be

$$\mathcal{B} = \left\{ \mathbf{n} \in W^{1,1}\left(\Omega, \mathbb{R}^k\right) \,\middle|\, \mathbf{n} = \mathbf{n}_0 \text{ on } \partial\Omega_1 \right\},$$

with the slight alteration that $\mathbf{n}_0 \in W^{1,1}\left(\Omega, \mathbb{R}^k\right)$. We also do not require any differentiability of the Lagrangian in order to prove the quasiconvexity results. Hence just for the duration of the next three quasiconvexity proofs, we will only assume the Lagrangian is continuous in its arguments. So for Theorem 1.9 we assume that

$$F \in C\left(\overline{\Omega} \times \mathbb{R}^d \times \mathbb{R}^{k\times d}\right)$$

and for Theorems 1.10 and 1.11 we assume that

$$F \in C\left(\overline{\Omega} \times M \times \mathbb{R}^{k\times d}\right).$$

Theorem 1.9 (Quasiconvexity in the interior - Unconstrained)**.** *Suppose that the admissible function* $\mathbf{n} \in \mathcal{B} \cap W^{1,\infty}\left(\Omega, \mathbb{R}^k\right)$ *is a strong local minimiser of I. Then for almost every* $x \in \Omega$

$$F(x, \mathbf{n}(x), \nabla\mathbf{n}(x)) \leqslant \frac{1}{|D|}\int_D F(x, \mathbf{n}(x), \nabla\mathbf{n}(x) + \nabla_y\boldsymbol{\psi}(y))\, dy,$$

for every open and bounded $D \subset \mathbb{R}^d$ *and* $\boldsymbol{\psi} \in W_0^{1,\infty}\left(D, \mathbb{R}^k\right)$.

Proof

We take an open and bounded $D \subset \mathbb{R}^d$, $\psi \in W_0^{1,\infty}\left(D, \mathbb{R}^k\right)$, and pick some $x \in \Omega$. We choose a $\delta > 0$ such that $B(x, 2\delta) \subset \Omega$ and define

$$\phi_\epsilon^z(x) := \epsilon\psi\left(\frac{x-z}{\epsilon}\right),$$

for some $z \in B(x, \delta)$. Then we can say that since $\mathbf{n}$ is a strong local minimiser of I, if ϵ is sufficiently small, $\phi_\epsilon^z \in C_0^\infty\left(\Omega, \mathbb{R}^k\right)$ and

$$I(\mathbf{n} + \phi_\epsilon^z) - I(\mathbf{n}) \geqslant 0.$$

Since this applies for each $z \in B(x, \delta)$, we can take some $f \in C_0^\infty\left(B(x, \delta)\right)$, which is non-negative, to deduce

$$0 \leqslant \int_{B(x,\delta)} f(z)\left[I(\mathbf{n} + \phi_\epsilon^z) - I(\mathbf{n})\right] dz. \tag{1.17}$$

Now we can change variables using the coordinate transformation

$$y = \frac{x-z}{\epsilon},$$

so that when we multiply through by ϵ^{-d}, (1.17) becomes

$$\begin{aligned} 0 \leqslant &\int_{B(x,\delta)} \int_D f(z) F(z + \epsilon y, \mathbf{n}(z + \epsilon y) + \epsilon\psi(y), \nabla\mathbf{n}(z + \epsilon y) + \nabla_y\psi(y))\, dy\, dz \\ &- \int_{B(x,\delta)} \int_D f(z) F(z + \epsilon y, \mathbf{n}(z + \epsilon y), \nabla\mathbf{n}(z + \epsilon y))\, dy\, dz. \end{aligned}$$

From here we swap the integrals and perform another change of variables $z' = z + \epsilon y$ to find

$$\begin{aligned} 0 \leqslant &\int_D \int_{B(x,\delta)+\epsilon y} f(z' - \epsilon y) F(z', \mathbf{n}(z') + \epsilon\psi(y), \nabla\mathbf{n}(z') + \nabla_y\psi(y))\, dz'\, dy \\ &- \int_D \int_{B(x,\delta)+\epsilon y} f(z' - \epsilon y) F(z', \mathbf{n}(z'), \nabla\mathbf{n}(z'))\, dz'\, dy. \end{aligned} \tag{1.18}$$

It is clear that we would like to use the Dominated Convergence Theorem on the integral in (1.18). We see that this is possible by rewriting the integral as (we define the indicator function $\mathbb{1}_\epsilon(z')$ to be $\mathbb{1}_{B(x,\delta)+\epsilon y}(z')$)

$$\begin{aligned} &\int_D \int_{B(x,\delta)+\epsilon y} f(z' - \epsilon y) F(z', \mathbf{n}(z') + \epsilon\psi(y), \nabla\mathbf{n}(z') + \nabla_y\psi(y))\, dz' dy \\ &- \int_D \int_{B(x,\delta)+\epsilon y} f(z' - \epsilon y) F(z', \mathbf{n}(z'), \nabla\mathbf{n}(z'))\, dz'\, dy \\ = &\int_D \int_{B(x,2\delta)} f(z' - \epsilon y) F(z', \mathbf{n}(z') + \epsilon\psi(y), \nabla\mathbf{n}(z') + \nabla_y\psi(y)) \mathbb{1}_\epsilon(z')\, dz'\, dy \\ &- \int_D \int_{B(x,2\delta)} f(z' - \epsilon y) F(z', \mathbf{n}(z'), \nabla\mathbf{n}(z')) \mathbb{1}_\epsilon(z')\, dz'\, dy. \end{aligned}$$

Since f is smooth, F is continuous and $\mathbf{n} \in W^{1,\infty}(\Omega, M)$, we can easily take the limit of this as $\epsilon \to 0$ to see that it converges to

$$\int_D \int_{B(x,\delta)} f(z)\left[F(z, \mathbf{n}(z), \nabla\mathbf{n}(z) + \nabla_y\psi(y)) - F(z, \mathbf{n}(z), \nabla\mathbf{n}(z))\right] dz\, dy.$$

Writing this in an alternative fashion we find

$$\begin{aligned}&\int_{B(x,\delta)} f(z) \int_D F(z, \mathbf{n}(z), \nabla \mathbf{n}(z) + \nabla_y \psi(y)) - F(z, \mathbf{n}(z), \nabla \mathbf{n}(z))\, dy dz \\ &= \int_{B(x,\delta)} f(z) g(z)\, dz \geqslant 0.\end{aligned}$$

However since this is true for every non-negative $f \in C_0^\infty(B(x,\delta))$, we conclude, using a standard mollification argument, that $g(z) \geqslant 0$ almost everywhere in $B(x,\delta)$. Since x was arbitrary, this gives us the result.

□

Now we can use Theorem 1.9 to prove the more general constrained quasiconvexity result. We return to our original set of admissible functions $\mathcal{A}$ with the boundary condition $\mathbf{n}_0 \in W^{1,1}(\Omega, M)$ once more.

Theorem 1.10 (Quasiconvexity in the interior)**.** *Suppose that* $\mathbf{n} \in \mathcal{A} \cap W^{1,\infty}(\Omega, M)$ *is a strong local minimiser of* I*. Then for almost every* $x \in \Omega$

$$F(x, \mathbf{n}(x), \nabla \mathbf{n}(x)) \leqslant \frac{1}{|D|} \int_D F(x, \mathbf{n}(x), \nabla \mathbf{n}(x) + \nabla P(\mathbf{n}(x)) \nabla \phi(y))\, dy, \tag{1.19}$$

for any open and bounded $D \subset \mathbb{R}^d$ *and* $\phi \in W_0^{1,\infty}\left(D, \mathbb{R}^k\right)$.

Proof

We take D and ϕ as given in the statement. We know $\mathbf{n}$ is a strong local minimiser of I and returning to the logic in (1.8), we showed that if we take some $\mathbf{m} \in \mathcal{B}$, then

$$\|\mathbf{n} - \mathbf{m}\|_\infty < \frac{\delta^*}{2} \quad \Rightarrow \quad P(\mathbf{m}) \in \mathcal{A} \quad \text{and} \quad \|\mathbf{n} - P(\mathbf{m})\|_\infty < 2 \|\mathbf{n} - \mathbf{m}\|_\infty .$$

Therefore if $\|\mathbf{n} - \mathbf{m}\|_\infty$ is small enough

$$J(\mathbf{m}) = I(P(\mathbf{m})) \geqslant I(\mathbf{n}) = J(\mathbf{n}),$$

so $\mathbf{n}$ is a strong local minimiser of J. Therefore we can apply Theorem 1.9 to deduce that for almost every $x \in \Omega$

$$G(x, \mathbf{n}(x), \nabla \mathbf{n}(x)) \leqslant \frac{1}{|D|} \int_D G(x, \mathbf{n}(x), \nabla \mathbf{n}(x) + \nabla \phi(y))\, dy. \tag{1.20}$$

To relate this back to F we note that from the definition of J we have

$$G(x, \mathbf{n}, \mathbf{Q}) = \psi(\mathbf{n}) F(x, P(\mathbf{n}), \nabla P(\mathbf{n}) \mathbf{Q}). \tag{1.21}$$

By substituting this back into we (1.20) we obtain

$$\begin{aligned}F(x, \mathbf{n}(x), \nabla \mathbf{n}(x)) &\leqslant \frac{1}{|D|} \int_\Omega \psi(\mathbf{n}(x)) F(x, \mathbf{n}(x), \nabla P(\mathbf{n}(x))(\nabla \mathbf{n}(x) + \nabla \phi(y)) \\ &= \frac{1}{|D|} \int_D F(x, \mathbf{n}(x), \nabla \mathbf{n}(x) + \nabla P(\mathbf{n}(x)) \nabla \phi(y))\, dy.\end{aligned} \tag{1.22}$$

□

Theorem 1.11 (Quasiconvexity at the boundary)**.** *Suppose that* $\mathbf{n} \in \mathcal{A} \cap C^1\left(\overline{\Omega}, M\right)$ *is a strong local minimiser of I. The exterior unit normal to* Ω *at a point x is given by* $\boldsymbol{\nu}(x)$*. Then*

$$F\left(x, \mathbf{n}(x), \nabla \mathbf{n}(x)\right) \leqslant \frac{1}{|\mathbf{B}^-_{\boldsymbol{\nu}(x)}|} \int_{\mathbf{B}^-_{\boldsymbol{\nu}(x)}} F\left(x, \mathbf{n}(x), \nabla \mathbf{n}(x) + \nabla P(\mathbf{n}(x)) \nabla \phi(y)\right) \, dy,$$

for all $\phi \in \left\{ \phi \in W^{1,\infty}\left(\mathbf{B}^-_{\boldsymbol{\nu}(x)}, \mathbb{R}^k\right) \,\middle|\, \phi = 0 \text{ on } \partial \mathbf{B} \cap \partial \mathbf{B}^-_{\boldsymbol{\nu}(x)} \right\}$ *where*

$$\mathbf{B}^-_{\boldsymbol{\nu}(x)} = \{ y \in \mathbf{B} \,|\, y \cdot \boldsymbol{\nu}(x) < 0 \}. \tag{1.23}$$

This holds for $\mathcal{H}^{d-1}$ *almost every* $x \in \partial\Omega_2$ *where* $\partial\Omega_2$ *is locally* C^1*.*

Remark 1.12. *Note that this condition only holds on the free boundary,* $\partial\Omega_2$*, of our problem and not on the entirety of* $\partial\Omega$*.*

Proof

In this instance we will apply the unconstrained result of Ball and Marsden [11] to J. From the proof of Theorem 1.10 we know that since $\mathbf{n}$ is a strong local minimiser of I it is also a strong local minimiser of J. Hence [11] implies

$$G\left(x, \mathbf{n}(x), \nabla \mathbf{n}(x)\right) \leqslant \frac{1}{|\mathbf{B}^-_{\boldsymbol{\nu}}|} \int_{\mathbf{B}^-_{\boldsymbol{\nu}}} G\left(x, \mathbf{n}(x), \nabla \mathbf{n}(x) + \nabla \phi(y)\right) \, dy,$$

for $\mathcal{H}^{d-1}$ almost every $x \in \partial\Omega_2$ and ϕ as given in the statement. Now we can proceed with exactly the same logic as in the previous proof, using (1.21) and (1.22) to obtain the assertion.

□

With our necessary quasiconvexity conditions in place we return to assuming that our Lagrangian is twice continuously differentiable in its second two arguments. The following corollary shows that quasiconvexity in the interior implies the more classical result of Weierstrass. This is intuitively understood from the fact that the Weierstrass condition is in reality a rank-one convexity condition in the interior which is weaker than quasiconvexity. This corollary motivates why in the next section we only need to strengthen the quasiconvexity conditions in order to prove the fundamental strong local minimum sufficiency result.

Corollary 1.13 (Weierstrass Condition)**.** *Suppose that* $\mathbf{n} \in \mathcal{A} \cap W^{1,\infty}(\Omega, M)$ *is a strong local minimiser of I. Then for almost every* $x \in \Omega$

$$\mathcal{E}_F\left(x, \mathbf{n}, \nabla \mathbf{n}, \nabla \mathbf{n} + [\nabla P(\mathbf{n})\zeta] \otimes \eta\right) \geqslant 0$$

for any $\zeta \in \mathbb{R}^k$ *and* $\eta \in \mathbb{R}^d$*.*

Proof

By appealing to Theorem 1.10 we know that (1.19) holds for almost every $x \in \Omega$. Now for $\mathbf{Q} \in \mathbb{R}^{k \times d}$ we define

$$\tilde{F}(\mathbf{Q}) := F\left(x, \mathbf{n}(x), \nabla P(\mathbf{n}(x))\mathbf{Q}\right).$$

Then using this new entity $\tilde{F}$, (1.19) simply says that

$$\frac{1}{|D|}\int_D \tilde{F}(\nabla \mathbf{n} + \nabla\phi(y))\,dy \geqslant \tilde{F}(\nabla \mathbf{n}),$$

for all $\phi \in W_0^{1,\infty}\left(D, \mathbb{R}^k\right)$. Therefore $\tilde{F}$ is quasiconvex at $\nabla\mathbf{n}(x)$ (for almost every x). We take some $\zeta \otimes \eta \in \mathbb{R}^{k\times d}$, then for $t \in [0,1)$, define

$$A_1^t := \nabla \mathbf{n} + (1-t)\zeta\otimes\eta, \quad A_2^t := \nabla\mathbf{n} - t\zeta\otimes\eta.$$

Then $tA_1^t + (1-t)A_2^t = \nabla\mathbf{n}$ and $A_1^t - A_2^t = \zeta\otimes\eta$. We also know that quasiconvexity implies rank-one convexity [26] so that from Definition 1.4

$$\tilde{F}(\nabla\mathbf{n}) \leqslant t\tilde{F}(A_1^t) + (1-t)\tilde{F}(A_2^t). \tag{1.24}$$

Hence by rewriting (1.24) and scaling ζ, we find

$$\tilde{F}(\nabla\mathbf{n}) \leqslant t\tilde{F}(\nabla\mathbf{n} + \zeta\otimes\eta) + (1-t)\tilde{F}\left(\nabla\mathbf{n} - \frac{t}{1-t}\zeta\otimes\eta\right). \tag{1.25}$$

To finish we notice that the right side of (1.25) is a continuously differentiable function in $t \in [0,1)$ which achieves its lower bound at $t = 0$. Thus it has non-negative derivative at zero and we differentiate to find

$$\begin{aligned}
0 &\leqslant \tilde{F}(\nabla\mathbf{n} + \zeta\otimes\eta) - \tilde{F}(\nabla\mathbf{n}) - \sum_{i,j}\tilde{F}_{\mathbf{Q}_{i,j}}(\nabla\mathbf{n})\zeta_i\eta_j \\
&= \tilde{F}(\nabla\mathbf{n} + \zeta\otimes\eta) - \tilde{F}(\nabla\mathbf{n}) - \sum_{i,j}\left[\sum_{\alpha,\beta} F_{\mathbf{n}_{\alpha,\beta}}(x,\mathbf{n},\nabla\mathbf{n})P_{\alpha,i}(\mathbf{n})\delta_{\beta\,j}\right]\zeta_i\eta_j \\
&= F(x,\mathbf{n},\nabla\mathbf{n} + [\nabla P(\mathbf{n})\zeta]\otimes\eta) - F(x,\mathbf{n},\nabla\mathbf{n}) - F_{\nabla\mathbf{n}}(x,\mathbf{n},\nabla\mathbf{n}) : [\nabla P(\mathbf{n})\zeta]\otimes\eta,
\end{aligned}$$

which is what we set out to prove.

□

1.6 Sufficient Conditions for a Strong Local Minimiser

Before we prove our strong sufficiency theorem using the result of Grabovsky & Mengesha we prove a preliminary theorem based on a result by Taheri [89]. It shows that if we assume a very strong Weierstrass condition then there is almost no distinction between weak local minimisers and strong local minimisers. For these sufficiency results we need to assume some extra regularity conditions for our Lagrangian F, the first of which is a differentiability condition.

(L1) $F \in C^2\left(U\times O\times\mathbb{R}^{k\times d}\right)$ where U and O are open neighbourhoods of $\overline{\Omega}$ and M respectively.

Theorem 1.14. *Let* $\mathbf{n} \in \mathcal{A}\cap C^1\left(\overline{\Omega}, M\right)$ *and for* $\mathbf{v} \in Var_{\mathcal{A}}$ *define (see* (1.5)*)*

$$g(t) = I\left(P(\mathbf{n} + t\mathbf{v})\right) = I(\mathbf{w}_t).$$

Suppose that the Lagrangian F satisfies (L1) and there exists some $\gamma > 0$ such that

$$g'(0) = 0 \quad \textit{and} \quad g''(0) \geqslant \gamma \|\mathbf{w}_0'\|_{1,2}^2 \quad \forall \mathbf{v} \in \mathit{Var}_{\mathcal{A}}.$$

In addition, suppose that

$$\mathcal{E}_F(x, \mathbf{m}, \mathbf{Q}_1, \mathbf{Q}_2) \geqslant \gamma |\mathbf{Q}_1 - \mathbf{Q}_2|^2 \tag{1.26}$$

for any $x \in \overline{\Omega}$, $\mathbf{m} \in M$, and $\mathbf{Q}_1, \mathbf{Q}_2 \in \mathbb{R}^{k\times d}$. Then $\mathbf{n}$ is a strict strong local minimiser of I.

Remark 1.15. *This theorem shows that any C^1 weak local minimiser is in fact a strong local minimiser if the Lagrangian is convex with respect to the gradient term.*

Proof

As this is a sufficiency proof we will be using the functional K as the unconstrained problem which is related to I. We will show that K satisfies all of the required conditions to apply Taheri's sufficiency result [89, Theorem 3.3]. Recall from the proof of Theorem 1.8 that our assumptions immediately imply that

$$\delta K(\mathbf{n})(\mathbf{v}) = 0 \quad \text{and} \quad \delta^2 K(\mathbf{n})(\mathbf{v}, \mathbf{v}) \geqslant \frac{2\gamma}{2+\gamma} \|\mathbf{v}\|_{1,2}^2,$$

for every test function $\mathbf{v} \in \mathrm{Var}_{\mathcal{B}}$. To be able to apply Taheri's result we now need to show what strengthened Weierstrass condition is satisfied by H. We choose $0 < \epsilon < \frac{\delta^*}{2}$ so that if $|\mathbf{m} - \mathbf{n}(x)| < \epsilon$ then $\psi(\mathbf{m}) = 1$. Then for any $x \in \overline{\Omega}$, $|\mathbf{m} - \mathbf{n}(x)| < \epsilon$ and $\mathbf{Q} \in \mathbb{R}^{k\times d}$ we have

$$\begin{aligned}
& \mathcal{E}_H\left(x, \mathbf{m}, \nabla\mathbf{n}(x), \mathbf{Q}\right) \\
= \;& H(x, \mathbf{m}, \mathbf{Q}) - H(x, \mathbf{m}, \nabla\mathbf{n}) - H_{\nabla\mathbf{m}}(x, \mathbf{m}, \nabla\mathbf{n}) : (\mathbf{Q} - \nabla\mathbf{n}) \\
= \;& F(x, P(\mathbf{m}), \nabla P(\mathbf{m})\mathbf{Q}) + |(I - \nabla P(\mathbf{m}))\mathbf{Q}|^2 \\
& - F(x, P(\mathbf{m}), \nabla P(\mathbf{m})\nabla\mathbf{n}) - |(I - \nabla P(\mathbf{m}))\nabla\mathbf{n}|^2 \\
& - F_{\nabla\mathbf{n}}(x, P(\mathbf{m}), \nabla P(\mathbf{m})\nabla\mathbf{n}) : (\nabla P(\mathbf{m})\mathbf{Q} - \nabla P(\mathbf{m})\nabla\mathbf{n}) \\
& - 2((I - \nabla P(\mathbf{m}))^T (I - \nabla P(\mathbf{m}))\nabla\mathbf{n}) : (\mathbf{Q} - \nabla\mathbf{n}) \\
= \;& \mathcal{E}_F(x, \mathbf{m}, \nabla P(\mathbf{m})\nabla\mathbf{n}, \nabla P(\mathbf{m})\mathbf{Q}) + |(I - \nabla P(\mathbf{m}))(\mathbf{Q} - \nabla\mathbf{n})|^2 \\
\geqslant \;& \gamma |\nabla P(\mathbf{m})(\mathbf{Q} - \nabla\mathbf{n})|^2 + |(I - \nabla P(\mathbf{m}))(\mathbf{Q} - \nabla\mathbf{n})|^2 \\
= \;& \frac{\gamma}{\gamma+1} |\mathbf{Q} - \nabla\mathbf{n}|^2 + \frac{1}{\gamma+1} |(I - (\gamma+1)\nabla P(\mathbf{m}))(\mathbf{Q} - \nabla\mathbf{n})|^2 \\
\geqslant \;& \frac{\gamma}{\gamma+1} |\mathbf{Q} - \nabla\mathbf{n}|^2.
\end{aligned}$$

This means that we can apply [89, Theorem 3.3] to deduce that there exist two constants, $\sigma_1, \sigma_2 > 0$ such that if $\mathbf{m} \in \mathcal{B}$ with $\|\mathbf{m} - \mathbf{n}\|_\infty < \sigma_1$ then

$$K(\mathbf{m}) - K(\mathbf{n}) \geqslant \sigma_2 \|\mathbf{m} - \mathbf{n}\|_{1,2}^2.$$

Therefore $\mathbf{n}$ is a strict strong local minimiser of K. As $\mathcal{A} \subset \mathcal{B}$ this means that $\mathbf{n}$ is also a strict strong local minimiser of I.

□

While Theorem 1.14 is very useful, we do not want to restrict ourselves to just considering Lagrangians satisfying (1.26). So to finish this section we will be applying the recently proved sufficiency result of Grabovsky & Mengesha [41] which requires much weaker quasiconvexity assumptions. However in order to use their result we need to set up our problem in a slightly different way and we refer the reader to their paper for full details. We have four conditions that we will assume our Lagrangian satisfies: the differentiability condition (L1), a growth condition, a coercivity condition and a uniform continuity condition.

(L2) There exists constants $C > 0$ and $p \geqslant 2$ such that for all $\mathbf{Q} \in \mathbb{R}^{k\times d}$ and $|\mathbf{n}| = 1$

$$|F(x, \mathbf{n}, \mathbf{Q})| \leqslant C\left(1 + |\mathbf{Q}|^p\right),$$

$$|F_{\mathbf{Q}}(x, \mathbf{n}, \mathbf{Q})| \leqslant C\left(1 + |\mathbf{Q}|^{p-1}\right) \quad \text{and} \quad |F_{\mathbf{n}}(x, \mathbf{n}, \mathbf{Q})| \leqslant C\left(1 + |\mathbf{Q}|^p\right).$$

(L3) We assume that F is bounded below, and that we have $C_1 > 0$ and $C_2 > 0$ such that

$$\int_\Omega F(x, \mathbf{m}(x), \nabla\mathbf{m}(x))\, dx \geqslant C_1\|\mathbf{m}\|^p_{1,p} - C_2, \tag{1.27}$$

for all $\mathbf{m} \in \mathcal{A}$. If $p > 2$, we assume in addition that there exists some $D_1 > 0$ and $D_2 > 0$, such that for every $\mathbf{m} \in \mathcal{A}$ with $\|\mathbf{m} - \mathbf{n}\|_\infty \leqslant \frac{\delta^*}{2}$ we have

$$\int_\Omega F\left(x, \mathbf{m}, \nabla\mathbf{m}\right) - F(x, \mathbf{n}, \nabla\mathbf{n})\, dx \geqslant D_1\|\mathbf{m} - \mathbf{n}\|^p_{1,p} - D_2\|\mathbf{m} - \mathbf{n}\|^2_{1,2}. \tag{1.28}$$

(L4) For every $\epsilon > 0$ there exists a $\delta > 0$ such that for every $\mathbf{Q} \in \mathbb{R}^{k\times d}$, $|\mathbf{n}| = 1$, and $x_1, x_2 \in \overline{\Omega}$ with $|x_1 - x_2| \leqslant \delta$

$$\frac{|F(x_1, \mathbf{n}, \mathbf{Q}) - F(x_2, \mathbf{n}, \mathbf{Q})|}{1 + |\mathbf{Q}|^p} < \epsilon.$$

Remark 1.16. *These assumptions are slightly different to those in [41] but when we relate them to another functional they do come into line with those used in their result. In (L3) to avoid any issues with the projection map we assumed that $\|\mathbf{m} - \mathbf{n}\|_\infty < \frac{\delta^*}{2}$ but since we are investigating L^∞ local behaviour this does not lose us any generality.*

Theorem 1.17. *Suppose that Ω is a C^1 bounded domain and the Lagrangian F satisfies (L1)-(L4). Assume that $\mathbf{n} \in \mathcal{A} \cap C^1\left(\overline{\Omega}, M\right)$ satisfies the following set of assumptions.*

- *There exists some $\gamma > 0$ such that for all $\mathbf{v} \in Var_{\mathcal{A}}$*

$$g'(0) = 0 \quad \textit{and} \quad g''(0) \geqslant \gamma\|\mathbf{w}_0'\|^2_{1,2}.$$

- *For every open, bounded set $D \subset \mathbb{R}^d$, $\phi \in W^{1,\infty}_0\left(D, \mathbb{R}^k\right)$ and $x \in \Omega$*

$$\begin{aligned}\int_D \mathcal{E}_F\left(x, \mathbf{n}(x), \nabla\mathbf{n}(x), \nabla\mathbf{n}(x) + \nabla P(\mathbf{n}(x))\nabla\phi(y)\right)\, dy \\ \geqslant \gamma\int_D |\nabla P(\mathbf{n})\nabla\phi(y)|^2\, dy.\end{aligned} \tag{1.29}$$

- *For every* $\phi \in \left\{ \phi \in W^{1,\infty}\left(\mathbf{B}^-_{\nu(x)}, \mathbb{R}^k\right) \,\middle|\, \phi = 0 \text{ on } \partial\mathbf{B} \cap \partial\mathbf{B}^-_{\nu(x)} \right\}$ *and* $x \in \partial\Omega_2$ *(where* $\mathbf{B}^-_{\nu(x)}$ *is given in* (1.23)*)*

$$\begin{aligned} \int_{\mathbf{B}^-_\nu} \mathcal{E}_F\left(x, \mathbf{n}(x), \nabla\mathbf{n}(x), \nabla\mathbf{n}(x) + \nabla P(\mathbf{n}(x))\nabla\phi(y)\right)\, dy \\ \geqslant \gamma \int_{\mathbf{B}^-_\nu} |\nabla P(\mathbf{n})\nabla\phi(y)|^2 \, dy. \end{aligned} \tag{1.30}$$

Then $\mathbf{n}$ *is a strong local minimiser of* I*.*

Proof

Unfortunately in this proof we cannot simply use the functional K to apply [41, Theorem 5.1] and then relate the condition back to I. This is because K does not satisfy the required coercivity conditions unless $p = 2$. Therefore we introduce and study a related functional $\tilde{K}$. If $p = 2$ we let $\tilde{K} = K$, otherwise we define

$$\begin{aligned} \tilde{K}(\mathbf{m}) &:= \int_\Omega \tilde{H}(x, \mathbf{m}, \nabla\mathbf{m})\, dx \\ &= K(\mathbf{m}) + \int_\Omega \psi(\mathbf{m})\left(|\mathbf{m} - P(\mathbf{m})|^p + |\nabla\mathbf{m} - \nabla\left[P(\mathbf{m})\right]|^p\right) dx. \end{aligned}$$

In other words this functional has been given a form of stability with respect to the $W^{1,p}$ norm as well as the $W^{1,2}$ norm. The first thing to note about this functional $\tilde{K}$ is that

$$\delta\tilde{K}(\mathbf{n})(\mathbf{v}) = \delta K(\mathbf{n})(\mathbf{v}) \quad \text{and} \quad \delta^2\tilde{K}(\mathbf{n})(\mathbf{v}, \mathbf{v}) = \delta^2 K(\mathbf{n})(\mathbf{v}, \mathbf{v}) \quad \forall\ \mathbf{v} \in \mathrm{Var}_{\mathcal{B}}.$$

Therefore when we take an arbitrary $\mathbf{v} \in \mathrm{Var}_{\mathcal{B}}$, using the same logic as from the proof of the weak sufficiency theorem, we deduce

$$\delta\tilde{K}(\mathbf{n})(\mathbf{v}) = 0 \quad \text{and} \quad \delta^2\tilde{K}(\mathbf{n})(\mathbf{v}, \mathbf{v}) \geqslant \frac{2\gamma}{2+\gamma}\|\mathbf{v}\|^2_{1,2}.$$

We also need to show that the strengthened quasiconvexity conditions used in [41, Theorem 5.1] hold for $\tilde{K}$, given that F satisfies (1.29) and (1.30). This is achieved with a careful calculation, if $p > 2$ then

$$\begin{aligned} & \mathcal{E}_{\tilde{H}}\left(x, \mathbf{n}, \nabla\mathbf{n}, \nabla\mathbf{n} + \nabla\phi(y)\right) \\ = \;& \tilde{H}(x, \mathbf{n}, \nabla\mathbf{n} + \nabla\phi(y)) - \tilde{H}(x, \mathbf{n}, \nabla\mathbf{n}) - \nabla\phi(y) : \tilde{H}_{\nabla\mathbf{n}}(x, \mathbf{n}, \nabla\mathbf{n}) \\ = \;& F\left(x, \mathbf{n}, \nabla\mathbf{n} + \nabla P(\mathbf{n})\nabla\phi(y)\right) + |\nabla\phi(y) - \nabla P(\mathbf{n})\nabla\phi(y)|^2 - F(x, \mathbf{n}, \nabla\mathbf{n}) \\ & + |\nabla\phi(y) - \nabla P(\mathbf{n})\nabla\phi(y)|^p - \nabla P(\mathbf{n})\nabla\phi(y) : F_{\nabla\mathbf{n}}\left(x, \mathbf{n}, \nabla\mathbf{n}\right) \\ \geqslant \;& \mathcal{E}_F\left(x, \mathbf{n}, \nabla\mathbf{n}, \nabla\mathbf{n} + \nabla P(\mathbf{n})\nabla\phi(y)\right) + |\nabla\phi(y) - \nabla P(\mathbf{n})\nabla\phi(y)|^2, \end{aligned} \tag{1.31}$$

and the $p = 2$ case is the same but without the term with the p^{th} power. Now we can apply

our strengthened quasiconvexity condition to (1.31) to find

$$\begin{aligned}
&\int_D \mathcal{E}_{\tilde{H}}\left(x, \mathbf{n}(x), \nabla \mathbf{n}(x), \nabla \mathbf{n}(x) + \nabla \phi(y)\right)\, dy \\
\geqslant &\int_D \gamma |\nabla P(\mathbf{n}) \nabla \phi(y)|^2 + |(I - \nabla P(\mathbf{n}))\, \nabla \phi(y)|^2 \, dy \\
= &\int_D \gamma |\nabla P(\mathbf{n}) \nabla \phi(y)|^2 + |\nabla \phi(y)|^2 dy \\
&- \int_D 2 \nabla P(\mathbf{n}) \nabla \phi(y) : \nabla \phi(y) + |\nabla P(\mathbf{n}) \nabla \phi(y)|^2 \, dy \\
= &\int_D \frac{\gamma}{1+\gamma} |\nabla \phi(y)|^2 + \frac{1}{1+\gamma} |\nabla \phi(y) - (1+\gamma) \nabla P(\mathbf{n}) \nabla \phi(y)|^2 \, dy \\
\geqslant &\frac{\gamma}{1+\gamma} \int_D |\nabla \phi(y)|^2 \, dy
\end{aligned} \tag{1.32}$$

for any open, bounded D and $\phi \in W_0^{1,\infty}\left(D, \mathbb{R}^k\right)$. The same is also true of the quasiconvexity at the boundary. Therefore the final thing to consider before we can apply [41, Theorem 5.1] are the conditions which $\tilde{H}$ must satisfy as the counterparts to (L1)-(L4). From the definition of K, the regularity assumption (L1) implies that

$$H \in C^2\left(U \times \mathbb{R}^k \times \mathbb{R}^{k \times d}\right), \tag{1.33}$$

and the additional terms for $\tilde{H}$ are clearly twice differentiable so that $\tilde{H}$ also satisfies (1.33). Equally it is clear to see that the growth condition (L2) must also hold for $\tilde{H}$. For the uniform continuity condition we can show that $\tilde{H}$ satisfies a slightly different condition to (L4).

(L4*) For every $R > 0$ and $\epsilon > 0$ there exists a $\delta > 0$ such that for every $\mathbf{Q} \in \mathbb{R}^{k \times d}$, $|\mathbf{n}| < R$, and $x_1, x_2 \in \overline{\Omega}$ with $|x_1 - x_2| \leqslant \delta$

$$\frac{|\tilde{H}(x_1, \mathbf{n}, \mathbf{Q}) - \tilde{H}(x_2, \mathbf{n}, \mathbf{Q})|}{1 + |\mathbf{Q}|^p} < \epsilon.$$

In the language of Grabovsky & Mengesha's paper this means that $\tilde{H}$ satisfies conditions (H1), (H2) and (H4) so that we only need to deal with the coercivity condition in order to apply their result. They use the coercivity condition to show that the problem of strong local minimisers can effectively be reduced to $W^{1,p}$ local minimisers. We will prove this directly with our (L3) assumption mimicking the reasoning in [41, Section 7]. On a technical note we choose $\epsilon > 0$ to be a fixed constant, sufficiently small, such that if $\mathbf{m} \in \mathcal{B}$ and $\|\mathbf{m} - \mathbf{n}\|_\infty < \epsilon$ then

$$\max\left\{\epsilon, \|\mathbf{n} - P(\mathbf{m})\|_\infty\right\} \leqslant \frac{\delta^*}{2}.$$

When we rewrite (1.27) and (1.28) as conditions on $\tilde{K}$ we see that if we take an $\mathbf{m} \in \mathcal{B}$ with $\|\mathbf{m} - \mathbf{n}\|_\infty < \epsilon$

$$\tilde{K}(\mathbf{m}) \geqslant C_1 \|P(\mathbf{m})\|_{1,p}^p - C_2 + \|\mathbf{m} - P(\mathbf{m})\|_{1,2}^2 + \|\mathbf{m} - P(\mathbf{m})\|_{1,p}^p, \tag{1.34}$$

and if $p = 2$ we do not have the final term in the equation above. As for the additional assumption (1.28), if we take $\mathbf{m} \in \mathcal{B}$ with $\|\mathbf{n} - \mathbf{m}\|_\infty < \epsilon$, then

$$\begin{aligned}
\tilde{K}(\mathbf{m}) - \tilde{K}(\mathbf{n}) \geqslant &D_1 \|\mathbf{n} - P(\mathbf{m})\|_{1,p}^p - D_2 \|\mathbf{n} - P(\mathbf{m})\|_{1,2}^2 \\
&+ \|\mathbf{m} - P(\mathbf{m})\|_{1,2}^2 + \|\mathbf{m} - P(\mathbf{m})\|_{1,p}^p.
\end{aligned} \tag{1.35}$$

Here we need to introduce a little notation from [41] to follow their reasoning.

Definition 1.18. *We say that a sequence* $\left(\mathbf{m}_j\right) \subset \mathcal{B}$ *is a strong variation if* $\|\mathbf{m}_j - \mathbf{n}\|_\infty \to 0$ *as* $j \to \infty$.

To avoid any technical difficulties we will always assume that $\|\mathbf{m}_j - \mathbf{n}\|_\infty < \epsilon$ for all j for any strong variation. With this definition Grabovsky & Mengesha look to prove that the normalized increment

$$\liminf_{j\to\infty} \frac{\tilde{K}(\mathbf{m}_j) - \tilde{K}(\mathbf{n})}{\|\mathbf{m}_j - \mathbf{n}\|_{1,2}^2} \geqslant 0 \tag{1.36}$$

for any strong variation $\left(\mathbf{m}_j\right)$. The estimate (1.34) means that if we take a strong variation $\left(\mathbf{m}_j\right)$ such that $\|\nabla \mathbf{m}_j\|_p \to \infty$, we automatically have

$$\tilde{K}(\mathbf{m}_j) \geqslant \tilde{K}(\mathbf{n}) \quad \forall\, j \geqslant N,$$

for some $N > 0$, which means that the normalized increment condition (1.36) is satisfied. Therefore we only need to consider strong variations $\left(\mathbf{m}_j\right)$ such that $\mathbf{m}_j \rightharpoonup \mathbf{n}$ in $W^{1,p}$. Let

$$\alpha_j = \|\mathbf{m}_j - \mathbf{n}\|_{1,2} \leqslant D\|\mathbf{m}_j - \mathbf{n}\|_{1,p} = \beta_j,$$

and we will show that (1.36) holds unless

$$\lim_{j\to\infty} \alpha_j = \lim_{j\to\infty} \beta_j = 0 \quad \text{and} \quad \lim_{j\to\infty} \frac{\beta_j^p}{\alpha_j^2} < \infty.$$

Since $\mathbf{m} \rightharpoonup \mathbf{n}$ in $W^{1,p}$ we know that $\left(\alpha_j\right)$ and $\left(\beta_j\right)$ are bounded sequences and without loss of generality we assume that $\alpha_j \to \alpha_0 > 0$. Let $Q\tilde{H}(x, \mathbf{n}, \mathbf{Q})$ be the quasiconvexification of $\tilde{H}(x, \mathbf{n}, \mathbf{Q})$ with respect to $\mathbf{Q}$, and we exploit the fact that the quasiconvexified functional is $W^{1,p}$ sequentially weakly lower semicontinuous [26, Theorem 8.11] with (1.32) to obtain

$$\begin{aligned}
\liminf_{j\to\infty} \frac{\tilde{K}(\mathbf{m}_j) - \tilde{K}(\mathbf{n})}{\alpha_j^2} &= \frac{1}{\alpha_0^2} \liminf_{j\to\infty} \int_\Omega \tilde{H}(x, \mathbf{m}_j, \nabla \mathbf{m}_j) - \tilde{H}(x, \mathbf{n}, \nabla \mathbf{n})\, dx \\
&\geqslant \frac{1}{\alpha_0^2} \liminf_{j\to\infty} \int_\Omega Q\tilde{H}(x, \mathbf{m}_j, \nabla \mathbf{m}_j) - \tilde{H}(x, \mathbf{n}, \nabla \mathbf{n})\, dx \\
&\geqslant \frac{1}{\alpha_0^2} \int_\Omega Q\tilde{H}(x, \mathbf{n}, \nabla \mathbf{n}) - \tilde{H}(x, \mathbf{n}, \nabla \mathbf{n})\, dx \\
&= 0.
\end{aligned}$$

Therefore we need only look at the cases where $\alpha_j \to 0$ which is all we require if $p = 2$. A corollary of the fact that $\alpha_j \to 0$ for a strong variation $\left(\mathbf{m}_j\right)$ is that

$$P\left(\mathbf{m}_j\right) \to \mathbf{n} \quad \text{in} \quad W^{1,2}\left(\Omega, \mathbb{R}^k\right).$$

If $p > 2$, this corollary, together with (1.35), shows us that if $\alpha_j \to 0$, the normalized increment from (1.36) is automatically non-negative unless

$$\mathbf{n} - P\left(\mathbf{m}_j\right) \to 0 \quad \text{and} \quad \mathbf{m}_j - P\left(\mathbf{m}_j\right) \to 0 \quad \text{in} \quad W^{1,p} \;\Rightarrow\; \mathbf{m}_j \to \mathbf{n} \quad \text{in} \quad W^{1,p}.$$

This means that we have reduced the problem to $W^{1,p}$ local minimisers for $\tilde{K}$, exactly as in [41, Section 7]. Now we have amassed all of these conditions and dealt with the (L3) assumption, we are in a position to apply [41, Theorem 5.2] and its direct corollary [41, Theorem 5.1]. This tells us that $\mathbf{n}$ is a strong local minimiser of $\tilde{K}$ which implies that there exists some $\delta > 0$ such that if $\mathbf{m} \in \mathcal{A} \subset \mathcal{B}$ such that $\|\mathbf{m} - \mathbf{n}\|_\infty < \delta$ then

$$I(\mathbf{m}) = \tilde{K}(\mathbf{m}) \geqslant \tilde{K}(\mathbf{n}) = I(\mathbf{n}).$$

Thus $\mathbf{n}$ is a strong local minimiser of I.

□

1.7 Illustrative Application

In this final section we will apply our results to an example problem. This application will show the strength of the results of this section as well as illustrating how the study of global minimisers is a very different prospect with a constraint. The constrained results presented in Sections 1.3-1.6 roughly mimic those of the classical problems. However not all ideas from the classical study of the calculus of variations translate to their constrained counterparts. In our example we will use the circle $\mathbb{S}^1$ as our target space. Then we will discover that having a Lagrangian which is convex in the gradient does not guarantee a weak local minimiser is actually a global minimiser. In fact we will go further and show that the problem has countably many strong local minimisers which are not global minima. Results and ideas of this kind are already known but have not been approached from this angle to the best of our knowledge. Consider the simplest one dimensional functional

$$I(\mathbf{n}) = \int_0^1 |\mathbf{n}_x|^2 \, dx,$$

over the set of admissible functions

$$\mathcal{A} := \left\{ \mathbf{n} \in W^{1,2}\left((0,1), \mathbb{S}^1\right) \,\middle|\, \mathbf{n}(0) = \mathbf{n}(1) = \mathbf{e}_1 \right\}.$$

It is a simple exercise (see [34, p. 496]) to show that the weak form of the Euler-Lagrange equation for this one variable problem is

$$\int_0^1 \mathbf{v}_x \cdot \mathbf{n}_x - (\mathbf{n} \cdot \mathbf{v}) |\mathbf{n}_x|^2 \, dx = 0, \tag{1.37}$$

for all $\mathbf{v} \in C_0^\infty\left((0,1), \mathbb{R}^2\right)$. It is also easy enough to realise that we have an infinite number of solutions to this differential equation by noting that

$$\mathbf{n}_k(x) := \begin{pmatrix} \cos(2k\pi x) \\ \sin(2k\pi x) \end{pmatrix}$$

satisfies (1.37) for every $k \in \mathbb{Z}$. In order to show that these are strong local minimisers, we just need to show that we satisfy all of the conditions which are required in Theorem 1.14.

Proposition 1.19. *For each $k \in \mathbb{Z}$ the function $\mathbf{n}_k$ is a strict strong local minimiser of I.*

Proof

We begin by noting that we could apply either Theorem 1.17 or Theorem 1.14 to this problem as our domain Ω is of class C^1. We will use Theorem 1.14 because it is a little simpler and has a slightly stronger conclusion. Our Lagrangian is smooth and convex with respect to the gradient so we know that (1.26) is satisfied. Hence in order to apply Theorem 1.14 we just need to show the positivity of the second variation. We take some $\mathbf{v} \in C_0^\infty\left((0,1), \mathbb{R}^2\right)$ and for ease of notation, during this proof we will denote $\mathbf{w}_0'$ simply by $\mathbf{w}'$ and similarly $\mathbf{w}_0''$ by $\mathbf{w}''$. We remind the reader that they have the explicit form as given in (1.6).

We fix an index k. Since $\mathbf{w}'' \in W_0^{1,1}(0,1)$ and $\mathbf{n}_k \in W^{1,\infty}(0,1)$, they are an admissible pair of functions in (1.37) using a basic density argument. Using this fact, together with the easily verifiable identity $|\mathbf{w}'|^2 = -\mathbf{n}_k \cdot \mathbf{w}''$, the second variation simplifies as follows

$$\begin{aligned}
\frac{d^2}{dt^2} I\left(\frac{\mathbf{n}_k + t\mathbf{v}}{|\mathbf{n}_k + t\mathbf{v}|}\right)\bigg|_{t=0} &= 2\int_0^1 |\nabla \mathbf{w}'|^2 + \nabla \mathbf{w}'' : \nabla \mathbf{n}_k \, dx \\
&= 2\int_0^1 |\nabla \mathbf{w}'|^2 + |\nabla \mathbf{n}_k|^2 \left(\mathbf{w}'' \cdot \mathbf{n}_k\right) \, dx \\
&= 2\int_0^1 |\nabla \mathbf{w}'|^2 - |\nabla \mathbf{n}_k|^2 |\mathbf{w}'|^2 \, dx \\
&= 2\int_0^1 |\nabla \mathbf{w}'|^2 - 4k^2\pi^2 |\mathbf{w}'|^2 \, dx.
\end{aligned} \tag{1.38}$$

To show this is positive we note that $\mathbf{w}' \cdot \mathbf{n}_k = 0$, therefore we can denote $\mathbf{w}'$ by

$$\mathbf{w}' := f(x) \begin{pmatrix} \sin(2k\pi x) \\ -\cos(2k\pi x) \end{pmatrix},$$

for some $f \in W_0^{1,2}(0,1)$. Substituting this into (1.38) simplifies the expression to

$$\begin{aligned}
\frac{d^2}{dt^2} I\left(\frac{\mathbf{n}_k + t\mathbf{v}}{|\mathbf{n}_k + t\mathbf{v}|}\right)\bigg|_{t=0} &= 2\int_0^1 f'(x)^2 \, dx \\
&\geqslant 2\pi^2 \int_0^1 f(x)^2 \, dx \\
&= 2\pi^2 \int_0^1 |\mathbf{w}'|^2 \, dx.
\end{aligned} \tag{1.39}$$

The inequality above is simply a Poincaré inequality with the optimal constant for $W_0^{1,2}(0,1)$ (See [30] or Lemma 2.15). Now we know that (1.39) holds we proceed to prove that for some $\gamma > 0$

$$\frac{d^2}{dt^2} I\left(\frac{\mathbf{n}_k + t\mathbf{v}}{|\mathbf{n}_k + t\mathbf{v}|}\right)\bigg|_{t=0} \geqslant \gamma \|\mathbf{w}'\|_{1,2}^2, \tag{1.40}$$

for all test functions $\mathbf{v}$. For a contradiction we suppose (1.40) does not hold, Then for $j = 1, 2 \ldots$ there exist $\mathbf{v}_j \in W_0^{1,2}(0,1)$, such that

$$\|\mathbf{w}_j'\|_{1,2} = 1 \quad \forall\, j \quad \text{and} \quad \frac{d^2}{dt^2} I\left(\frac{\mathbf{n}_k + t\mathbf{v}_j}{|\mathbf{n}_k + t\mathbf{v}_j|}\right)\bigg|_{t=0} \to 0 \quad \text{as} \quad j \to \infty.$$

The estimate (1.39) tells us that

$$\int_0^1 |\mathbf{w}_j'|^2 \, dx \to 0. \tag{1.41}$$

However since the second variation converges to zero it is clear from (1.38) that we must also have

$$\int_0^1 |\nabla \mathbf{w}_j'|^2 \, dx \to 0. \tag{1.42}$$

Equations (1.41) and (1.42) clearly contradict the fact that $\|\mathbf{w}_j'\|_{1,2} = 1$ for all j. So the second variation is strictly positive around each $\mathbf{n}_k$. Thus Theorem 1.14 gives us the assertion.

□

This result can be intuitively grasped from the perspective of the topology of $\mathbb{S}^1$. This is the only sphere which is not simply connected so that each of these maps $\mathbf{n}_k$ are not homotopic to each other. Thus there is no way of moving between these states without traversing a potential well of infinite energy. However similar results exist even if the domain is simply connected; Brezis & Coron [17] and Jost [50] both proved related results for maps into $\mathbb{S}^2$. These results all reinforce the idea that global minimisers for constrained problems is a difficult issue. Proving a global minimiser sufficiency result may not be possible for a general constrained problem without additional topological constraints on the manifold. We were able to circumvent this issue when examining local behaviour because the topology of the manifold is negated at an L^∞ local level.

In terms of the methods we have used, relating the constrained functional to an unconstrained one via a projection cannot be used straightforwardly to study global properties, or indeed L^p local minimisers for $1 \leqslant p < \infty$. This is because if we take an arbitrary $\mathbf{m} \in \mathcal{B}$ we cannot perform our analysis unless $\mathbf{m}$ is L^∞ close to the manifold, so that $P(\mathbf{m})$ is uniquely defined. One final remark about this chapter is that although we considered the case of closed, bounded C^4 manifolds in $\mathbb{R}^k$, one could potentially go further. The condition we really required was a locally unique projection onto the manifold which was itself C^3. Therefore the analysis should all hold if the constraint is $\mathbf{n}(x) \in M$ almost everywhere, and M satisfies this condition.

Chapter 2

Global minimisers for Liquid Crystal Problems

2.1 Introduction

2.1.1 Cholesteric Patterns

In this chapter we begin studying liquid crystals in earnest. As was discussed in Section 0.1, for the problems that we will consider in the next two chapters, the main goal is to better understand cholesteric liquid crystals. More specifically, an improved understanding of cholesterics could potentially aid the design of improved liquid crystals displays. Nematic liquid crystals are generally better understood from an analytical viewpoint as the molecular preference to point in a single direction is simpler than the cholesteric preference to form a helix.

The particular energy minimisation problem that we will consider in this chapter, was motivated by a curious pattern observed in the chirally doped nematic liquid crystal, described in Section 0.1, which occurs above a certain concentration of dopant. The pattern is shown in Figure 2.2, and these sort of patterns are generally seen when the pitch of the cholesteric is sufficiently small, usually of the order of the height of the cell. The two different patterns in Figure 2.2 correspond to two different surface geometries on the bottom of the cell.

The top half of the figure is where the liquid crystal is held between two parallel and flat plates with homeotropic anchoring on both faces. The outcome is what are called cholesteric

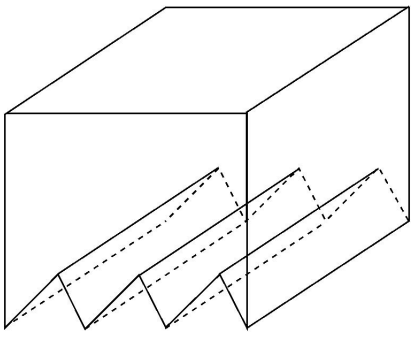


Figure 2.1: Grating pattern

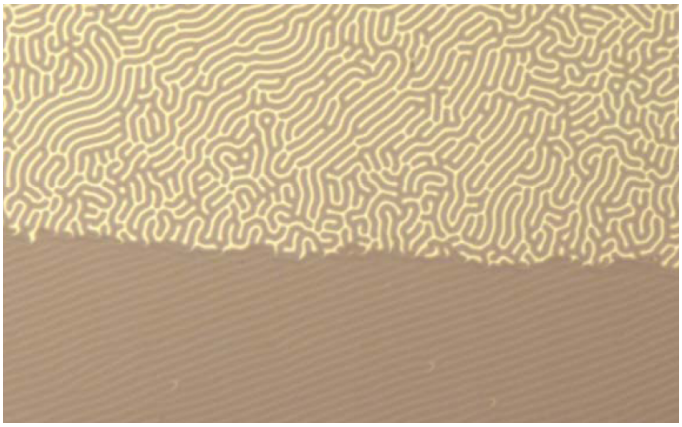


Figure 2.2: Varying cholesteric patterns

fingers, a seemingly random quasi-periodic pattern. The bottom half of the figure however is a different situation. Both the top and bottom faces have homeotropic anchoring as before, but the bottom surface is now a grating as is depicted in Figure 2.1. What is interesting is that this grating pattern seems to have "smoothed out" the cholesteric fingers into a more regular rolling pattern.

Analytically, the geometry in Figure 2.1 represents a significant challenge to finding any explicit energy minimisers. Therefore as an initial modelling step we shall make an approximation about the liquid crystal in and around the grating. The data from HP labs suggests that in the area of the grating, the director approximately aligns horizontally between the peaks and troughs which necessarily creates line defects along them. Thus we will model this tilted state (compare with Figure 0.1(b)) by using a rectangular domain with the conditions that $\mathbf{n} = \mathbf{e}_1$ on the bottom face and $\mathbf{n} = \mathbf{e}_3$ on the top face (where $\mathbf{e}_i$ are the usual basis vectors in $\mathbb{R}^3$).

The pattern observed in Figure 2.2 is far from being an anomalous situation. In fact one of the main reasons for the analytical interest in cholesteric liquid crystals is that they can form a number of defect structures, none of which are fully understood analytically. The patterns from Figure 2.2 are part of a larger group of structures called cholesteric fingers, of which there are at least four distinct types [77, 85]. These fingers can easily be created in a sample of liquid crystal between two parallel plates with homeotropic anchoring ($\mathbf{n} = \mathbf{e}_3$), so long as the height of the cell is sufficiently small. It is generally thought that the fingers arise from the competition of two local energy minimisers; the constant state and a more helical state. Near the isotropic transition temperature, some cholesteric liquid crystals consist of cubic lattices of cylinders called blue phases [51, 94] which posses interesting optical properties. They are called blue phases because the periodicity of the lattice is the same length as the wavelength of visible light, so it reflects a certain visible colour. The first such studied liquid crystals reflected blue light, hence their name. We will return to the blue phase in Chapter 3. Even more recently, local structures called torons which comprise a small volume of tightly twisted molecules have been induced by a high power laser and shown to be stable [84]. These torons

appear to be formed when the building block of the blue phase, the double twist cylinder, is twisted upon itself to create a torus. This structure necessarily results in two defects.

Recent technological advances have made it possible to unambiguously reconstruct the director field within any of the above cholesteric structures [85]. An experimental technique called fluoresence confocal polarizing microscopy (FCPM) is used to perform this reconstruction. As a result, the molecular makeup of all of these structures has been found either experimentally or through simulations. However there has been little analytical progress using them to find local or global energy minimisers of an entire system. Much of the work which follows in the rest of this thesis is aimed at being able to predict the existence of these patterns analytically by using and adapting the various continuum models of liquid crystal energies.

2.1.2 Oseen-Frank Energy

For the next two chapters we will be using the director theory of Oseen and Frank to study nematic and cholesteric behaviour. It is the oldest and simplest of the continuum theories but it does accurately predict the behaviour of many systems and so is a very logical theory to study initially. The other continuum theories of Landau-de Gennes and Ericksen both have their advantages but we put them to one side for now as their extra complexity makes it more difficult to find explicit minimisers. We will however return to this issue of the suitability of each model. Discussing the relative strengths of the theories is one of the principal aims of Chapters 4 and 5.

The Oseen-Frank model was briefly outlined in the introduction but now we revisit it in more detail. In order to form the Oseen-Frank free energy, a number of modelling assumptions and material symmetries are used. Firstly it is assumed that the liquid crystal is at a constant temperature and is incompressible. Secondly it is assumed that the elastic free energy density of the system is of the form

$$w = w(\mathbf{n}, \nabla\mathbf{n}), \quad |\mathbf{n}(\mathbf{x})| = 1,$$

with the total elastic energy in a given volume Ω given by

$$I(\mathbf{n}) = \int_\Omega w(\mathbf{n}, \nabla\mathbf{n})\, dx.$$

Physical considerations and material symmetry imply that the free energy density $w(\mathbf{n}, \nabla\mathbf{n})$ must satisfy the following three conditions.

- The head to tail symmetry of the molecules implies

$$w(\mathbf{n}, \nabla\mathbf{n}) = w(-\mathbf{n}, -\nabla\mathbf{n}). \tag{2.1}$$

- Additionally the free energy density should be invariant under rotations and so we have the frame indifference condition

$$w(\mathbf{n}, \nabla\mathbf{n}) = w(R\mathbf{n}, R\nabla\mathbf{n}R^T) \quad \forall R \in \mathrm{SO}(3).$$

- The free energy density must be bounded below so that we have existence of a minimiser; thus by addition of an arbitrary constant it is assumed that

$$w(\mathbf{n}, \nabla\mathbf{n}) \geqslant 0, \tag{2.2}$$

and furthermore that $w(\mathbf{n}, \nabla\mathbf{n}) = 0$ if and only if the liquid crystal is in its "natural orientation".

The methodology employed by Frank was to expand the free energy density as a quadratic function of curvature strains. Applying the frame indifference and symmetry conditions from above then allowed him to conclude his general form of the elastic free energy density for nematics and cholesterics:

$$w(\mathbf{n}, \nabla\mathbf{n}) = \frac{K_1}{2}(\nabla\cdot\mathbf{n})^2 + \frac{K_2}{2}(\mathbf{n}\cdot\nabla\times\mathbf{n} + t)^2 + \frac{K_3}{2}|\mathbf{n}\times\nabla\times\mathbf{n}|^2 + \frac{(K_2+K_4)}{2}(\mathrm{tr}(\nabla\mathbf{n}^2) - (\nabla\cdot\mathbf{n})^2). \tag{2.3}$$

The four constants K_1, K_2, K_3, and K_4 are referred to as the splay, twist, bend, and saddle-splay constants respectively. The constant t is non-zero for cholesterics and is a result of the enantiomorphic nature of cholesteric liquid crystals. Cholesteric liquid crystal molecules are not invariant under reflections since it reverses the handedness of its preferred helical structure. Nematics on the other hand are assumed to consist of straight rod-like molecules which are invariant under reflections and so correspond to $t = 0$. We note again that with a simple calculation, the final term can be written as a null Lagrangian (see (0.5)). In addition, for notational ease we will be dropping the factor of $\frac{1}{2}$ from all subsequent uses of the Oseen-Frank free energy.

Elastic Constants and Ericksen's inequalities

The final deductions which can be made about the free energy density concern the material constants K_i. Using the assumption (2.2) with the form of the free energy density given in (2.3) leads to the following two sets of inequalities.

Theorem 2.1 (Virga [92])**.** *If $t \neq 0$, then*

$$w(\mathbf{n}, \nabla\mathbf{n}) \geqslant 0 \quad \forall\mathbf{n} \in \mathbb{S}^2 \iff K_1 \geqslant 0,\ K_2 \geqslant 0,\ K_3 \geqslant 0,\ K_2 + K_4 = 0.$$

Theorem 2.2 (Ericksen [32])**.** *If $t = 0$, then*

$$w(\mathbf{n}, \nabla\mathbf{n}) \geqslant 0 \quad \forall\mathbf{n} \in \mathbb{S}^2 \iff 2K_1 \geqslant K_2 + K_4,\ K_2 \geqslant |K_4|,\ K_3 \geqslant 0.$$

There is some debate however about whether the assumption that $w(\mathbf{n}, \nabla\mathbf{n})$ is bounded below by zero is suitable. This is because an assumption has been made a-priori about the minimum energy state of the sample. As was discussed in the introduction, this assumption is also not borne out by all the experimental evidence of interesting cholesteric structures. As a result, our one departure from the classical Oseen-Frank theory will be to not assume that $K_2 + K_4 = 0$. A particularly convenient form of the Oseen-Frank free energy density which

is often employed, especially by theoreticians for analytical purposes, is the one constant approximation

$$K_1 = K_2 = K_3 = K \quad K_4 = 0.$$

This simplifies (2.3) considerably. Rewriting the equation in component form, with this approximation we find that

$$\begin{aligned} w(\mathbf{n}, \nabla\mathbf{n}) &= K\left[(\nabla\cdot\mathbf{n})^2 + (\mathbf{n}\cdot\nabla\times\mathbf{n} + t)^2 + |\mathbf{n}\times\nabla\times\mathbf{n}|^2 + \nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n})\right] \\ &= K\left[|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2\right]. \end{aligned} \tag{2.4}$$

This form is such a useful one that we will use it through much of this thesis; however we have to justify its usage. Using specially designed liquid crystal cells it has been possible to measure the first three elastic constants. For example Zwetkoff [29] and Haller [43] measured the elastic constants of two different liquid crystals, PAA at 125°C and MBBA at 25°C. They obtained the following two sets of values

$$K_1 = 4.5\times10^{-12}N, \quad K_2 = 2.9\times10^{-12}N, \quad K_3 = 9.5\times10^{-12}N,$$

$$K_1 = 6\times10^{-12}N, \quad K_2 = 3.8\times10^{-12}N, \quad K_3 = 7.5\times10^{-12}N.$$

Certainly what is clear is that the constants are of the same order of magnitude as each other. For theoretical purposes it is often convenient to reduce the number of elastic constants to one by estimating their ratios. In such a case $K_1 = 2K_2 = K_3 = K$ is widely considered to be a reasonable approximation, but this results in a much less elegant free energy density.

2.2 Boundary Conditions

A very important aspect of the study of liquid crystal variational problems is that of boundary conditions. This is true whether we are using the director order parameter, a matrix order parameter, or indeed any other situation. To set the problem in a rigorous mathematical framework we require certain boundary conditions to be applied. These should, where possible, accurately reflect the surface energy generated between the liquid crystal and the boundary. There are a number of different types of boundary conditions or anchoring which can be applied, but in this section we will proceed to show how the choice of plausible boundary conditions depends extremely heavily on the topology and regularity of the domain. Throughout this chapter we will be working with the director model and so will study anchoring properties from that perspective.

2.2.1 Types of Anchoring

No Anchoring

The simplest boundary condition to apply to a domain Ω is that there is no condition. This may seem convenient but in this situation any minimiser will satisfy a natural boundary condition instead. It is also difficult for this to be realised as manufactured surfaces will invariably interact with the liquid crystal molecules in some way.

Strong Anchoring

The most commonly applied boundary condition is that of strong anchoring. This type of anchoring simply specifies that $\mathbf{n} = \mathbf{v}$ on $\partial\Omega$. On a more practical level it is important to know what sort of strong anchoring conditions are actually viable, and two particular forms of strong anchoring are readily reproducible: homeotropic and planar.

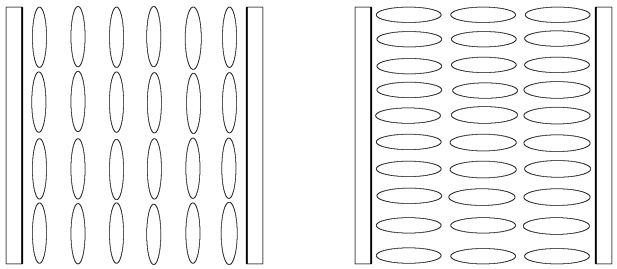


Figure 2.3: Planar and homeotropic alignments

Figure 2.3 shows examples of these two states. Homeotropic anchoring is when the director lies perpendicular to the surface, planar anchoring is when the director lies parallel to the surface. It is important to note that there are two distinct types of planar anchoring.

1. Planar degenerate anchoring is when the director is constrained to lie parallel to the surface but with no fixed direction on the surface.

2. Planar non-degenerate anchoring is when the director lies parallel to the surface but with a fixed direction. Thus its position is fixed uniquely. This type of anchoring is sometimes referred to as rubber anchoring.

Homeotropic alignments can be generated by chemically treating the surface [29], whereas planar non-degenerate anchoring can simply be achieved by rubbing the surface with material, although why this mechanism works is not fully understood. One possible explanation is that it creates small grooves in the substrate along a given direction. Planar degenerate anchoring is usually a property of the surface itself, or can be achieved through chemical treatment. In reality true planar alignment is difficult to obtain. Experiments performed at HP Labs and elsewhere have shown that with the rubbed surface, the director and surface actually form an angle between 2° to 6°. However we will always approximate this by a true planar alignment.

Weak Anchoring

Weak anchoring is a generalisation of strong anchoring in that it doesn't require the director $\mathbf{n}$ to satisfy any specific requirements. However a preferred orientation $\mathbf{v} \in L^\infty\left(\Omega, \mathbb{S}^2\right)$, is chosen on the boundary and the surface energy is modelled with an energy density. For example the following form could be used

$$W \int_{\partial\Omega} |\mathbf{n} - \mathbf{v}|^2 \, dS,$$

where W is a constant to represent the strength of the anchoring. In order to minimise this term clearly it is energetically favourable to have $\mathbf{n} = \mathbf{v}$ on $\partial\Omega$, but this energy competes with the bulk energy to determine the minimiser in this case. Strong anchoring in some sense is simply the limit as $W \to \infty$ to rigidly apply that $\mathbf{n} = \mathbf{v}$ on $\partial\Omega$.

To illustrate the importance of the choice of boundary conditions we look at three example domains and examine whether we can mathematically apply homeotropic or planar boundary conditions. In theoretical literature on liquid crystals the variational problems are often subjected to an abstract strong anchoring: $\mathbf{n}$ is given on $\partial\Omega$. However there is little to be gained by focusing on boundary conditions which cannot be experimentally realised. Therefore in each of the three cases we ask the question of whether there exists a director field of sufficient regularity which satisfies the planar or homeotropic boundary conditions. Effectively, is the problem a non-empty one? If the problem is empty then this could indicate a potential flaw in our mathematical model of the problem. Given the form of the free energy density, the natural function space to study the Oseen-Frank energy is $W^{1,2}\left(\Omega, \mathbb{S}^2\right)$. Therefore in the following examples we work within this Sobolev space.

2.2.2 Three Examples

Unit Ball

For our first example we define

$$\Omega := \left\{ \mathbf{x} \in \mathbb{R}^3 \,\middle|\, |\mathbf{x}| < 1 \right\}.$$

For this domain it is far from obvious whether a suitable director field exists with planar anchoring because of the hairy ball theorem [31]. Other researchers have studied tangential unit vector fields on a sphere with respect to liquid crystals [48, 56]. However we are not aware of any which prove the existence of such a field with Sobolev regularity as we do in the proposition below.

Theorem (Hairy Ball Theorem,[31])**.** *There does not exist a non-vanishing continuous tangent vector field on $2d$-dimensional spheres, $\mathbb{S}^{2d}$, for $d \in \mathbb{N}$.*

Remark 2.3. *In particular this theorem implies that there is no continuous, tangential, unit vector field on $\mathbb{S}^2$. That means that if we are to find a director field $\mathbf{n}$ with planar anchoring, then its trace on $\partial\Omega = \mathbb{S}^2$ cannot be continuous.*

Proposition 2.4. *There exist director fields*

$$\mathbf{n}_h,\, \mathbf{n}_p \in W^{1,2}\left(\Omega, \mathbb{S}^2\right), \tag{2.5}$$

such that

$$\mathbf{n}_h = \boldsymbol{\nu} \quad \mathbf{n}_p \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega,$$

where $\boldsymbol{\nu}$ is the unit normal to the sphere.

Proof

The first part of the proof is relatively simple; to find the homeotropic alignment we just note

$$\mathbf{n}_h(\mathbf{x}) := \frac{\mathbf{x}}{|\mathbf{x}|} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right).$$

It is a well known result that this function is indeed in $W^{1,2}\left(\Omega, \mathbb{S}^2\right)$ in 3 dimensions [12], and it is clearly homeotropic on the surface of the sphere. Determining $\mathbf{n}_p$ explicitly however is trickier. Omitting its derivation, we define the function

$$\mathbf{n}_p(\mathbf{x}) := \frac{1}{\sqrt{r^2 + \frac{\left(1-|\mathbf{x}|^2\right)^2}{4}}}\left(-z(\mathbf{x} - z\mathbf{e}_3) + \left(r^2 + \frac{1-|\mathbf{x}|^2}{2}\right)\mathbf{e}_3\right), \tag{2.6}$$

where $r = \sqrt{x^2 + y^2}$. It is clearly perpendicular to the radial vector $(x, y, z)^T$ on the boundary of the ball. To show that it has the suitable regularity, we note that the function is smooth except at $(0, 0, \pm 1)$. Therefore we change variables to examine the behaviour around these points. Let

$$\mathbf{x}' = \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} := \mathbf{x} - \mathbf{e}_3.$$

Then rewriting equation (2.6) in these coordinates yields

$$\mathbf{n}_p(\mathbf{x}') = \frac{f(\mathbf{x}')}{|\mathbf{x}'|}\left(-(x_3' + 1)\left(\mathbf{x}' - x_3'\mathbf{e}_3\right) + \left({x_1'}^2 + {x_2'}^2 + \frac{|\mathbf{x}'|^2}{2} + x_3'\right)\mathbf{e}_3\right),$$

where

$$f(\mathbf{x}') = \frac{1}{\sqrt{1 + x_3' + \frac{|\mathbf{x}'|^2}{4}}}.$$

Around the point $\mathbf{x}' = 0$, f is a smooth function satisfying $0 < C_1 < f < C_2 < \infty$. From this particular form it is easy to see that by comparison with $\frac{\mathbf{x}}{|\mathbf{x}|}$ that we do indeed have that $\mathbf{n}_p$ is in $W^{1,2}$ about the point $\mathbf{x}' = 0$. We can use an identical argument in a neighbourhood of $-\mathbf{e}_3$. Hence $\mathbf{n}_p \in W^{1,2}(\Omega, \mathbb{S}^2)$.

□

Right Circular Cone

For our second example, we define

$$\Omega := \left\{ \mathbf{x} \in \mathbb{R}^3 \,\middle|\, x^2 + y^2 < z^2,\ z \in (0, 1) \right\}.$$

This is the right circular cone with its vertex at the origin and height 1. What is instructive about this example is that the domain boundary does not need to be differentiable to find these director fields.

Proposition 2.5. *There exist director fields*

$$\mathbf{n}_h,\ \mathbf{n}_p \in W^{1,2}\left(\Omega, \mathbb{S}^2\right),$$

such that

$$\mathbf{n}_h = \boldsymbol{\nu} \quad \mathbf{n}_p \cdot \boldsymbol{\nu} = 0 \quad \textit{on } \partial\Omega',$$

where $\partial\Omega'$ is the curved portion of the boundary, and $\boldsymbol{\nu}$ is the normal to this portion of the boundary.

Proof

The details of this proof are much simpler: we can instantly find $\mathbf{n}_p$ by setting

$$\mathbf{n}_p(\mathbf{x}) := \frac{\mathbf{x}}{|\mathbf{x}|} \in W^{1,2}(\Omega, \mathbb{S}^2). \tag{2.7}$$

It is also a relatively easy task to find a function which is normal to the curved portion of the boundary. For example the function

$$\mathbf{n}_h(\mathbf{x}) := \frac{1}{|\mathbf{x}|} \begin{pmatrix} x \\ y \\ -z \end{pmatrix},$$

satisfies the conditions required: it is a unit vector and is normal to the curved portion of the boundary. It is also in $W^{1,2}(\Omega, \mathbb{S}^2)$ using the same logic as is used to show that (2.7) holds.

□

Cube

Our final example is the least regular domain of the three in that a cube has non-differentiable boundary along a line rather than just a single point. We define

$$\Omega := \left\{ \mathbf{x} \in \mathbb{R}^3 \,\middle|\, x, y, z \in (0, 1) \right\}.$$

In this case the question of planar boundary conditions is an extremely involved one, which was the main topic of the doctoral thesis by Majumdar [62]. Hence we will not cover it here. Its complication arises from the fact that planar boundary conditions give a degree of freedom to the director at each point of the boundary. We will focus on the uniquely determined ($\mathcal{H}^2$ almost everywhere) homeotropic boundary conditions case.

Proposition 2.6. *There is no function $\mathbf{n}_h \in W^{1,2}(\Omega, \mathbb{S}^2)$ such that*

$$\mathbf{n}_h = \boldsymbol{\nu} \quad \textit{on} \quad \partial\Omega,$$

where, as usual, $\boldsymbol{\nu}$ is the normal to the domain Ω.

Proof

Simply put, this proposition holds because Sobolev functions still retain some regularity up to the boundary of suitable domains, and the normal to a cube does not have this regularity across its edges. The Sobolev Trace theorem [57] states that if $\mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2)$ then

$$\operatorname{Tr} \mathbf{n} \in W^{\frac{1}{2},2}\left(\partial\Omega, \mathbb{S}^2\right).$$

Thankfully we have a characterisation of this fractional Sobolev space given by the following condition [57]. If $U \subset \mathbb{R}^d$ is an open set then

$$\mathbf{f} \in W^{\frac{1}{2},2}\left(\partial U, \mathbb{R}^k\right) \quad \Longleftrightarrow \quad \int_{\partial U}\int_{\partial U} \frac{|\mathbf{f}(x_1)-\mathbf{f}(x_2)|^2}{|x_1-x_2|^d}\, dx_1\, dx_2 < \infty,$$

provided that ∂U is uniformly Lipschitz. This means that a necessary criterion for the existence of a director field $\mathbf{n}_h$ with our desired properties is that

$$\boldsymbol{\nu} \in W^{\frac{1}{2},2}\left(\partial\Omega, \mathbb{S}^2\right).$$

We will proceed to show that

$$I := \int_{\partial\Omega}\int_{\partial\Omega} \frac{|\boldsymbol{\nu}(x_1)-\boldsymbol{\nu}(x_2)|^2}{|x_1-x_2|^3}\, dx_1\, dx_2 = \infty. \tag{2.8}$$

Firstly we use the fact that the integrand is non-negative to bound (2.8) from below. We restrict the domain so that we only integrate x_1 over the face $y = 0$ and x_2 over the face $z = 1$. Then we have the estimate that

$$\begin{aligned} I &\geqslant \int_{z=1}\int_{y=0} \frac{|\boldsymbol{\nu}(x_1)-\boldsymbol{\nu}(x_2)|^2}{|x_1-x_2|^3}\, dx_1\, dx_2 \\ &= \int_{z=1}\int_{y=0} \frac{2}{|x_1-x_2|^3}\, dx_1\, dx_2 \\ &= \int_0^1\int_0^1\int_0^1\int_0^1 \frac{2}{\left((a_1-b_1)^2+a_2^2+(1-b_3)^2\right)^{\frac{3}{2}}}\, da_1\, da_2\, db_1\, db_3 \\ &:= J. \end{aligned}$$

We can perform the integration over a_2 exactly to find that

$$J = \int_0^1\int_0^1\int_0^1 \frac{1}{\sqrt{(a_1-b_1)^2+1+(b_3-1)^2}}\left(\frac{2}{(a_1-b_1)^2+(b_3-1)^2}\right) da_1\, db_1\, db_3. \tag{2.9}$$

The left hand term in the integrand of (2.9) is actually bounded below since

$$\frac{1}{\sqrt{(a_1-b_1)^2+1+(b_3-1)^2}} \geqslant \frac{1}{\sqrt{3}},$$

so we can deduce that

$$J \geqslant \frac{1}{\sqrt{3}}\int_0^1\int_0^1\int_0^1 \left(\frac{2}{(a_1-b_1)^2+(b_3-1)^2}\right) da_1\, db_1\, db_3. \tag{2.10}$$

In (2.10) we can easily perform the b_3 integration to leave us with

$$J \geqslant \frac{1}{\sqrt{3}}\int_0^1\int_0^1 \frac{2\arctan\left(\frac{1}{a_1-b_1}\right)}{a_1-b_1}\, da_1\, db_1. \tag{2.11}$$

We now make one final estimate to simplify the integral. For every $a_1, b_1 \in [0,1]$ we can readily see that

$$\frac{\arctan\left(\frac{1}{a_1-b_1}\right)}{a_1-b_1} \geqslant \begin{cases} \frac{\arctan(1)}{a_1-b_1} & \text{if} \quad a_1 > b_1 \\ -\frac{\arctan(1)}{a_1-b_1} & \text{if} \quad a_1 < b_1 \end{cases} = \frac{\arctan(1)}{|a_1-b_1|}. \tag{2.12}$$

So substituting (2.12) into (2.11) gives

$$J \geqslant \frac{\pi}{2\sqrt{3}} \int_0^1 \int_0^1 \frac{1}{|a_1 - b_1|}\, da_1\, db_1.$$

Now we know that for any fixed $b_1 \in [0,1]$

$$\int_0^1 \frac{1}{|a_1 - b_1|}\, da_1 = \infty,$$

and since this is true for all $b_1 \in [0,1]$, we can conclude that $I \geqslant J = \infty$ and so $\boldsymbol{\nu} \notin W^{\frac{1}{2},2}\left(\partial\Omega, \mathbb{S}^2\right)$.

□

What these three examples are meant to illustrate, with respect to the further chapters in particular, is that the choice of boundary conditions very heavily influences the structure of any minimiser, and even whether it exists. Of greatest interest to industry are usually liquid crystal problems set in a cuboid domain since these are much easier to produce reliably. However Proposition 2.6 demonstrates that with such a domain, we cannot simply choose homeotropic boundary conditions on every face. Indeed, we cannot choose any boundary condition with a jump discontinuity over the edges of the cuboid, as no $W^{1,2}$ function could satisfy these anchoring conditions. Interestingly though, an experiment with just such a set of boundary conditions has been conducted [90] and multiple stable states were found. This shows us a possible limitation of our mathematical approach, either the Oseen-Frank theory, using Sobolev functions , or applying strong anchoring could be limiting the model. We will perform a more thorough examination of these issues in Chapters 4 and 5.

Certainly there is plenty of opportunity to delve further into these ideas, which we do not do here, by considering large classes of domains. Hardt and Lin [44] showed that in a bounded domain with smooth boundary there exists a director field $\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right)$ with homeotropic boundary conditions. For another example, Proposition 2.6 could clearly be generalised to any domain which has an edge but is C^1 locally around the edge, such as any polygonal domain. Our core aim in this thesis however is to investigate concrete minimisation problems, and so we turn our attentions to that end.

2.3 Framing the Problem

For the remainder of this chapter and the next, our domain $\Omega \subset \mathbb{R}^3$ will be a general cuboid,

$$\Omega := (-L_1, L_1) \times (-L_2, L_2) \times (0, L_3).$$

We are interested in finding energy minimisers of the functional

$$I(\mathbf{n}) = \int_\Omega w(\mathbf{n}, \nabla\mathbf{n})\, dx,$$

where $w(\mathbf{n}, \nabla\mathbf{n})$ is given in (2.3) and the set of admissible functions is given by

$$\mathcal{A} := \left\{ \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right) \,\middle|\, \mathbf{n}|_{z=0} = \mathbf{e}_1,\ \mathbf{n}|_{z=L_3} = \mathbf{e}_3,\ \mathbf{n}|_{x=-L_1} = \mathbf{n}|_{x=L_1},\ \mathbf{n}|_{y=-L_2} = \mathbf{n}|_{y=L_2} \right\}. \tag{2.13}$$

We have included periodicity in the lateral directions for two reasons. Firstly we are looking to describe a periodic pattern. Secondly we wish to avoid the issue of the interaction of the liquid crystal with the side walls of the domain because standard liquid crystal cells are much wider than they are tall. However we can simplify the domain slightly by performing a change of variables: $(x, y, z) \to \frac{1}{L_3}(x, y, z)$. Under this transformation

$$I(\mathbf{n}) = \int_\Omega w(\mathbf{n}, \nabla\mathbf{n})\, dx = L_3 \int_{\Omega'} w'(\mathbf{n}, \nabla\mathbf{n})\, dx',$$

where $\Omega' := \left(-\frac{L_1}{L_3}, \frac{L_1}{L_3}\right) \times \left(-\frac{L_2}{L_3}, \frac{L_2}{L_3}\right) \times (0, 1)$, and w' is given by

$$w'(\mathbf{n}, \nabla\mathbf{n}) = K_1(\nabla\cdot\mathbf{n})^2 + K_2\left(\mathbf{n}\cdot\nabla\times\mathbf{n} + tL_3\right)^2 + K_3\left|\mathbf{n}\times\nabla\times\mathbf{n}\right|^2 + (K_2+K_4)\nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n}). \tag{2.14}$$

Equation (2.14) shows us that this change of variables simply corresponds to changing the cholesteric twist by a factor of L_3. We are looking to investigate the existence and uniqueness of global or local minima as t varies, therefore without loss of generality we can assume that $L_3 = 1$. So from here on we will refer to Ω as the set

$$\Omega := (-L_1, L_1) \times (-L_2, L_2) \times (0, 1). \tag{2.15}$$

Remark 2.7. *The head to tail symmetry of nematic and cholesteric molecules should actually lead us to consider the boundary conditions* $\mathbf{n}|_{z=0} = \pm\mathbf{e}_1$ *and* $\mathbf{n}|_{z=1} = \pm\mathbf{e}_3$. *However, without loss of generality we can choose* $\mathbf{n}|_{z=0} = \mathbf{e}_1$. *Then if we had a director field* $\mathbf{n}$ *such that* $\mathbf{n}|_{z=0} = \mathbf{e}_1$ *and* $\mathbf{n}|_{z=1} = -\mathbf{e}_3$ *we could use the rotational invariance* (2.5) *to perform a rotation in* (x, y) *using the matrix*

$$R := \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \in SO(3),$$

which does not change the energy of the state. This new state $\mathbf{n}'$ *would satisfy* $\mathbf{n}'|_{z=0} = -\mathbf{e}_1$ *and* $\mathbf{n}'|_{z=1} = -\mathbf{e}_3$ *so we can use the head to tail symmetry of the molecules* (2.1) *to deduce that this is directly equivalent to* $\mathbf{n}'|_{z=0} = \mathbf{e}_1$ *and* $\mathbf{n}'|_{z=1} = \mathbf{e}_3$. *Thus we are not losing any generality by using the boundary conditions given in* (2.13)

Now the problem has been fully laid out we can begin to explore its various properties and prove results. In the literature, the case where $t = 0$, a nematic liquid crystal, has been extensively studied and is well understood in the situation without external electromagnetic fields. Our focus however will be largely on cholesteric liquid crystals. These are of interest in particular to industry as it is not currently known whether the structures that cholesterics can form could be harnessed for a new design of LCD. Initially we will find the global minimisers of the problem for functions which just depend on the height z. Then we investigate the question of whether these states are minimisers of the full problem. We will show the answer is affirmative for nematic liquid crystals and very much more complex in the cholesteric setting.

2.4 One-dimensional Results

From here on we will be assuming that $t \geqslant 0$ and the reason we can do this is that the sign of t simply determines the direction of the helix that the molecules prefer to form. Thus if $t < 0$ we can perform the change of variables $\mathbf{x}' = (x', y', z') = -\mathbf{x} = (x, y, z)$ to derive a situation where $t \geqslant 0$. Hence we consider the problem of minimising

$$I(\mathbf{n}) = \int_\Omega K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n} + t)^2 + K_3|\mathbf{n}\times\nabla\times\mathbf{n}|^2 + (K_2+K_4)\nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n})\,dx, \quad (2.16)$$

over the set of admissible functions

$$\mathcal{A} := \left\{ \mathbf{v} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right) \,\middle|\, \mathbf{v}|_{z=0} = \mathbf{e}_1,\ \mathbf{v}|_{z=1} = \mathbf{e}_3,\ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \right\}.$$

As described above we will assume initially that $\mathbf{n}$ is a function of z only, which will simplify the free energy significantly. To avoid degeneracy we also assume that $K_1, K_2, K_3 > 0$. We will tackle the problem by considering it in terms of the Euler angles $\theta(z)$ and $\phi(z)$ associated with the director field $\mathbf{n}$. By substituting

$$\mathbf{n} = \begin{pmatrix} \cos\phi\cos\theta \\ \sin\phi\cos\theta \\ \sin\theta \end{pmatrix},$$

into (2.16), we lose any contribution from the saddle-splay term since it vanishes for functions which depend on only one variable. Then we simplify to find

$$I(\mathbf{n}) = 4L_1L_2 \int_0^1 \left(K_1\cos^2\theta + K_3\sin^2\theta\right)\theta'^2 + \cos^2\theta\left[\left(K_2\cos^2\theta + K_3\sin^2\theta\right)\phi'^2 - 2tK_2\phi'\right] + t^2K_2\,dz. \quad (2.17)$$

Converting the problem into one involving the Euler angles is convenient from a computational standpoint as the unit vector constraint is automatically satisfied. However regularity issues come into play because we need to find the appropriate function spaces for θ and ϕ and ϕ is undefined when $\theta = \pm\frac{\pi}{2}$. Intuitively it seems sensible that θ and ϕ should have a comparable regularity to the entire function. However by simple calculations we can see that

$$\int_\Omega |\nabla\mathbf{n}|^2\,dx = \int_\Omega |\nabla\theta|^2 + \cos^2\theta\,|\nabla\phi|^2\,dx < \infty \ \forall\ \mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2).$$

This means that formally we might only expect $\nabla\theta, \cos\theta\,\nabla\phi \in L^2(\Omega, \mathbb{R}^3)$ so that $\theta \in W^{1,2}$ but we need not have that $\nabla\phi \in L^2$. The following proposition proves this regularity for θ and fortunately the precise form of the Lagrangian in (2.17) will then allow us to deal with the terms involving ϕ relatively simply.

Proposition 2.8. *Let $d \in \mathbb{N}$ and suppose that $\Omega \subset \mathbb{R}^d$ is an open set. If $\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right)$ then*

$$\theta \in W^{1,2}\left(\Omega, \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]\right)$$

where θ is the Euler angle out of the (x, y)-plane associated with $\mathbf{n}$.

Proof

The first element of the proof is to show the following pointwise inequality for any $\mathbf{n}_1, \mathbf{n}_2 \in \mathbb{S}^2$:

$$|\mathbf{n}_1 - \mathbf{n}_2|^2 \geqslant C\,|\theta_1 - \theta_2|^2\,. \tag{2.18}$$

We take $\mathbf{n}_1, \mathbf{n}_2 \in \mathbb{S}^2$. Then in terms of their Euler angles

$$\mathbf{n}_1 = \begin{pmatrix} \cos\theta_1 \cos\phi_1 \\ \cos\theta_1 \sin\phi_1 \\ \sin\theta_1 \end{pmatrix} \quad \mathbf{n}_2 = \begin{pmatrix} \cos\theta_2 \cos\phi_2 \\ \cos\theta_2 \sin\phi_2 \\ \sin\theta_2 \end{pmatrix}, \tag{2.19}$$

where $\theta_1, \theta_2 \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ and $\phi_1, \phi_2 \in [0, 2\pi)$. We substitute (2.19) into the left-hand side of (2.18) to find

$$\begin{aligned} |\mathbf{n}_1 - \mathbf{n}_2|^2 &= 2 - 2\mathbf{n}_1 \cdot \mathbf{n}_2 \\ &= 2 - 2\sin\theta_1 \sin\theta_2 - 2\cos\theta_1 \cos\theta_2 \cos(\phi_1 - \phi_2) \\ &\geqslant 2 - 2\sin\theta_1 \sin\theta_2 - 2\cos\theta_1 \cos\theta_2 \\ &= 2\,(1 - \cos(\theta_1 - \theta_2))\,. \end{aligned} \tag{2.20}$$

A simple exercise in L'Hôpital's rule gives us that

$$\lim_{x\to 0} \frac{1 - \cos(x)}{x^2} = \frac{1}{2}.$$

Therefore

$$\inf_{x\in[-\pi,\pi]} \frac{1 - \cos(x)}{x^2} := C > 0. \tag{2.21}$$

Then by combining (2.21) and (2.20) we see that $|\mathbf{n}_1 - \mathbf{n}_2|^2 \geqslant C|\theta_1 - \theta_2|^2$. We can now conclude by using the difference quotient characterisation of $W^{1,2}$ (see [57, Thm 10.55] or Proposition 4.2). We take our $\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right)$. Then for almost every $x_0 \in \Omega$

$$\int_\Omega |\mathbf{n}(x) - \mathbf{n}(x_0)|^2\,dx \geqslant C \int_\Omega |\theta(x) - \theta(x_0)|^2\,dx < \infty,$$

so that $\theta \in L^2\,(\Omega, \mathbb{R})$. The form of the inequality (2.18) allows us to go further and say that

$$\|\mathbf{n}(\cdot + h\mathbf{e}_j) - \mathbf{n}(\cdot)\|_{2,\Omega'} \geqslant C^{\frac{1}{2}} \|\theta(\cdot + h\mathbf{e}_j) - \theta(\cdot)\|_{2,\Omega'}$$

for every $\Omega' \subset\subset \Omega$, $|h| < d(\Omega', \partial\Omega)$ and $j \in \{1, \ldots, n\}$. Therefore as $\mathbf{n}$ satisfies the difference quotient characterisation, so must θ, which gives the result.

□

Now that we know the precise regularity of θ we can return to (2.17). Clearly with regards to minimisation, the final constant term in (2.17) is unimportant as its energy contribution is the same for all states. We apply a very direct approach to minimising the contributions from ϕ. If we look simply at the central term involving ϕ we can minimise it formally. To do this we note that

$$f(x) := ax^2 - bx \geqslant f\left(\frac{b}{2a}\right) = -\frac{b^2}{4a}.$$

Thus if we simply set

$$\phi' = \frac{K_2 t}{\left(K_2 \cos^2\theta + K_3 \sin^2\theta\right)} \quad \phi(0) = 0, \tag{2.22}$$

then we have minimised the contribution with regards to ϕ' and have the following inequality

$$\begin{aligned} I(\mathbf{n}) &\geqslant 4L_1L_2 \int_0^1 \left(K_1 \cos^2\theta + K_3 \sin^2\theta\right)\theta'^2 - \frac{K_2^2 t^2 \cos^2\theta}{\left(K_2 \cos^2\theta + K_3 \sin^2\theta\right)} + K_2 t^2 \, dz \\ &=: 4L_1L_2 \int_0^1 f(\theta)\theta'^2 - g(\theta) + K_2 t^2 \, dz. \end{aligned}$$

This reduces the problem to a one-dimensional functional of one variable which is easier to investigate. In order to find its minimum we first prove a preliminary lemma whereby we will show that it is not energetically favourable for θ to reach either of the poles of the sphere, $\pm(0,0,1)$, except at $z = 1$. For the lemma we introduce the following notation:

$$\begin{aligned} F_\alpha(v) &:= \int_0^\alpha f(v)v'^2 - g(v) + K_2 t^2 \, dz, \\ \mathcal{A}_\alpha &:= \left\{ \, v \in W^{1,2}(0,\alpha) \,\middle|\, v(0) = 0, \;\; v(\alpha) = \frac{\pi}{2} \, \right\}. \end{aligned}$$

Lemma 2.9. *If* $0 < \alpha < \beta < \infty$ *then*

$$\inf_{v \in \mathcal{A}_\alpha} F_\alpha(v) > \inf_{w \in \mathcal{A}_\beta} F_\beta(w).$$

Proof

We know that $\inf_{v\in\mathbb{R}} f(v) = \min\{K_1, K_3\} > 0$ so the Lagrangian is convex with respect to the gradient. Therefore the 1-dimensional theory of the calculus of variations tells us that for each α, the problem of minimising F_α over $\mathcal{A}_\alpha$ has a smooth minimiser [26, Ch.4.2] which satisfies the following Euler-Lagrange equation

$$(2f(v)v')' = -g'(v).$$

This equation has the first integral

$$f(v)v'^2 + g(v) = C_\alpha,$$

where C_α is a constant. For the consistency of this equation $C_\alpha \geqslant K_2 t^2$ because

$$f(v(z)) > 0 \quad \text{and} \quad g(v(0)) = K_2 t^2.$$

Importantly we need to eliminate the possibility that $C_\alpha = K_2 t^2$ so that we can deduce v' has a fixed sign. If $C_\alpha = K_2 t^2$, then we would be looking to solve

$$v'^2 = \frac{K_2 t^2 - g(v)}{f(v)}, \quad v(0) = 0. \tag{2.23}$$

We know that the minimiser we are searching for is smooth. Then we can use simple argument looking at intervals where v' has fixed sign. If $v \neq 0$ then without loss of generality there exists some interval (a, b) such that $v' \geqslant 0$ on (a, b) and $v(a) = 0$. By taking the square root of (2.23) and using the Picard-Lindelöf theorem [45, p.8] we find that the unique solution to the resulting ODE on (a, b) is simply $v = 0$. The repeated application of this logic proves that the unique solution to (2.23) is $v = 0$ and this clearly fails to match our boundary conditions. Hence $C_\alpha > K_2 t^2$ and v' has a fixed sign, so taking the square-root of (2.23) gives

$$v' = \frac{\left(C_\alpha - \frac{K_2^2 t^2 \cos^2 v}{(K_2 \cos^2 v + K_3 \sin^2 v)}\right)^{\frac{1}{2}}}{\left(K_1 \cos^2 v + K_3 \sin^2 v\right)^{\frac{1}{2}}} := k(z, v), \quad v(0) = 0.$$

We can use the Picard-Lindelöf Theorem again here to deduce existence and uniqueness of this ODE [45, p.8]. It is applicable since the function $k(z, v)$ is smooth in its arguments, hence Lipschitz on any bounded set. This means that we have a unique solution of this ODE, v_α, given implicitly by

$$\int_0^{v_\alpha(z)} \frac{\left(K_1 \cos^2 u + K_3 \sin^2 u\right)^{\frac{1}{2}}}{\left(C_\alpha - \frac{K_2^2 t^2 \cos^2 u}{(K_2 \cos^2 u + K_3 \sin^2 u)}\right)^{\frac{1}{2}}} \, du = z.$$

We finalise the definition of v_α by applying the top boundary condition of $v_\alpha(\alpha) = \frac{\pi}{2}$. This is possible because the functional

$$\eta(C) := \int_0^{\frac{\pi}{2}} \frac{\left(K_1 \cos^2 u + K_3 \sin^2 u\right)^{\frac{1}{2}}}{\left(C - \frac{K_2^2 t^2 \cos^2 u}{(K_2 \cos^2 u + K_3 \sin^2 u)}\right)^{\frac{1}{2}}} \, du,$$

is a strictly monotone decreasing function satisfying

$$\eta(K_2 t^2) = \infty \quad \text{and} \quad \eta(C) \to 0 \quad \text{as} \quad C \to \infty.$$

This means that there is a unique solution to the equation $\eta(C_\alpha) = \alpha$. Therefore we have established that for all $\alpha > 0$ we have a unique smooth v_α satisfying

$$F_\alpha(v_\alpha) = \inf_{v \in \mathcal{A}_\alpha} F_\alpha(v).$$

Now we note that for $\beta > \alpha > 0$

$$v(z) := \begin{cases} 0 & \text{if} \quad z \in (0, \beta - \alpha) \\ \\ v_\alpha(z - (\beta - \alpha)) & \text{if} \quad z \in (\beta - \alpha, \beta) \end{cases} \in \mathcal{A}_\beta, \tag{2.24}$$

with the property that

$$F_\beta(v) = F_\alpha(v_\alpha) = \inf_{w \in \mathcal{A}_\alpha} F_\alpha(w). \tag{2.25}$$

An immediate consequence of (2.25) is that

$$F_\beta(v_\beta) = \inf_{u \in \mathcal{A}_\beta} F_\beta(u) \leqslant F_\beta(v) = \inf_{w \in \mathcal{A}_\alpha} F_\alpha(w). \tag{2.26}$$

To conclude that this inequality is strict we need to show that $v \neq v_\beta$. However we know this to be true because $C_\beta > K_2 t^2$ tells us that $v'_\beta(z) \neq 0$ for any $z \in [0,1]$ whereas $v'(z) = 0$ for $z \in (0, \beta - \alpha)$ in (2.24). Hence the inequality in (2.26) is strict.

□

We can now prove the main result of this section by finding the one variable global minimisers.

Theorem 2.10. *The function $\theta^* = \theta^*(z)$ given implicitly by the equation*

$$\int_0^{\theta^*} \frac{\left(K_1 \cos^2 u + K_3 \sin^2 u\right)^{\frac{1}{2}}}{\left(C - \frac{K_2^2 t^2 \cos^2 u}{(K_2 \cos^2 u + K_3 \sin^2 u)}\right)^{\frac{1}{2}}}\, du = z, \quad \theta^*(1) = \frac{\pi}{2}, \tag{2.27}$$

with ϕ^* as defined by (2.22)*, determines a director field $\mathbf{n}^*$ which is the global minimum of* (2.16) *over admissible functions which depend only on z. Moreover the constant C in* (2.27) *is determined by the unique solution to*

$$\int_0^{\frac{\pi}{2}} \frac{\left(K_1 \cos^2 u + K_3 \sin^2 u\right)^{\frac{1}{2}}}{\left(C - \frac{K_2^2 t^2 \cos^2 u}{(K_2 \cos^2 u + K_3 \sin^2 u)}\right)^{\frac{1}{2}}}\, du = 1. \tag{2.28}$$

Proof

For an arbitrary $\mathbf{n} \in \mathcal{A}$ which depends only on z, we know that

$$\begin{aligned} I(\mathbf{n}) &\geqslant 4L_1L_2 \int_0^1 \left(K_1 \cos^2\theta + K_3 \sin^2\theta\right)\theta'^2 - \frac{K_2^2 t^2 \cos^2\theta}{(K_2 \cos^2\theta + K_3 \sin^2\theta)} + K_2 t^2\, dz \\ &= 4L_1L_2 \int_0^1 f(\theta)\theta'^2 - g(\theta) + K_2 t^2\, dz. \end{aligned} \tag{2.29}$$

We also know that $\theta \in W^{1,2}(0,1) \subset\subset C[0,1]$, so θ is a continuous function. Lemma 2.9 tells us that if $\theta(\alpha) = \pm\frac{\pi}{2}$ for some $0 < \alpha < 1$ then we cannot have the minimum energy of (2.29)(ii). In short

$$\int_0^1 f(\theta)\theta'^2 - g(\theta) + K_2 t^2\, dz \geqslant \int_0^1 f(\theta^*)\theta^{*\prime 2} - g(\theta^*) + K_2 t^2\, dz. \tag{2.30}$$

where $\theta^* = v_1$ in the notation of Lemma 2.9. Additionally the uniqueness of the minimiser from Lemma 2.9 for each positive α means that we have equality in (2.30) if and only if $\theta = \theta^*$. For completeness we need to note that given a smooth θ^*, the equation involving ϕ, (2.22), defines a unique smooth function $\phi^*(z)$ by Picard-Lindelöf. So now we can say that

$$I(\mathbf{n}) \geqslant 4L_1L_2 \int_0^1 f(\theta^*)\theta^{*\prime 2} - g(\theta^*) + K_2 t^2\, dz = I(\mathbf{n}^*),$$

with equality if and only if $\theta = \theta^*$ and also

$$\phi' = \frac{K_2 t}{\left(K_2 \cos^2\theta + K_3 \sin^2\theta\right)} \quad \text{and} \quad \phi(0) = 0.$$

Hence $I(\mathbf{n}) \geqslant I(\mathbf{n}^*)$ with equality if and only if $\theta = \theta^*$ and $\phi = \phi^*$, or equivalently $\mathbf{n} = \mathbf{n}^*$.

□

Remark 2.11. *Theorem 2.10 completes our work on the minimisers of functions of z alone. However not having a closed form for these minimisers is a significant problem since we want to find explicit minimisers in order to compare with experimental observations. In order to achieve this we need to assign a relationship between the elastic constants. We will use the one constant approximation because it makes the analysis more tractable which allows us to prove the strongest results.*

2.5 Multi-dimensional Results - Nematic One Constant Approximation

Throughout this section we consider the case $t = 0$. We will show that under the one constant approximation, the one variable function constructed above is in fact the unique global minimiser of the problem. We look to minimise

$$I(\mathbf{n}) = \int_\Omega |\nabla \mathbf{n}|^2 \, dx, \tag{2.31}$$

where Ω is the rectangular domain (2.15), over the set of admissible functions

$$\mathcal{A} := \left\{ \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right) \,\middle|\, \mathbf{n}|_{z=0} = \mathbf{e}_1,\ \mathbf{n}|_{z=1} = \mathbf{e}_3,\ \mathbf{n}|_{x=-L_1} = \mathbf{n}|_{x=L_1},\ \mathbf{n}|_{y=-L_2} = \mathbf{n}|_{y=L_2} \right\}. \tag{2.32}$$

Since this Lagrangian is much simpler, we can directly calculate the Euler-Lagrange equation associated with it. As we showed in Chapter 1, we must take care in doing this because of the unit vector constraint. We derive the Euler-Lagrange equation here in a similar way to Evans [34, Ch.8.4].

Lemma 2.12. *Suppose* $\mathbf{n} \in \mathcal{A}$ *is a* $W^{1,\infty}$ *local minimiser of* (2.31). *Then*

$$\int_\Omega \nabla \mathbf{v} : \nabla \mathbf{n} - |\nabla \mathbf{n}|^2 \mathbf{n} \cdot \mathbf{v} \, dx = 0 \tag{2.33}$$

for all $\mathbf{v} \in Var_{\mathcal{A}}$ *where*

$$Var_{\mathcal{A}} := \left\{ \mathbf{v} \in C^\infty\left(\overline{\Omega}, \mathbb{R}^3\right) \,\middle|\, \mathbf{v}|_{z=0} = 0,\ \mathbf{v}|_{z=1} = 0,\ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \right\}.$$

Proof

Assume that $\mathbf{n} \in \mathcal{A}$ is a $W^{1,\infty}$ local minimiser of the problem. Let $\mathbf{v} \in \text{Var}_{\mathcal{A}}$ and recall from Chapter 1 that

$$\mathbf{w}_\tau := \frac{\mathbf{n} + \tau \mathbf{v}}{|\mathbf{n} + \tau \mathbf{v}|}.$$

Also recall from the proof of Theorem 1.6 that $\|\mathbf{n} - \mathbf{w}_\tau\|_{1,\infty} \leqslant D\|\mathbf{n} - (\mathbf{n} + \tau \mathbf{v})\|_{1,\infty}$. Hence the fact that $\mathbf{n}$ is a weak local minimiser implies

$$\frac{d}{d\tau} I\left(\frac{\mathbf{n} + \tau \mathbf{v}}{|\mathbf{n} + \tau \mathbf{v}|}\right)\Bigg|_{\tau=0} = 0.$$

When we rewrite this equation in integral form we find that

$$\int_\Omega \nabla \mathbf{w}_0 : \nabla \mathbf{w'}_0 \, dx = 0. \tag{2.34}$$

It is a simple matter to show $\mathbf{w}_0 = \mathbf{n}$ and $\mathbf{w'}_0 = \mathbf{v} - (\mathbf{v} \cdot \mathbf{n})\mathbf{n}$ and substituting these equations into (2.34) immediately gives us our result.

□

Remark 2.13. *The strong form of* (2.33) *is precisely*

$$\Delta \mathbf{n} + |\nabla \mathbf{n}|^2 \mathbf{n} = 0,$$

together with the natural boundary conditions

$$\nabla \mathbf{n} \cdot \boldsymbol{\nu}|_{x=-L_1} = \nabla \mathbf{n} \cdot \boldsymbol{\nu}|_{x=L_1} \quad \textit{and} \quad \nabla \mathbf{n} \cdot \boldsymbol{\nu}|_{y=-L_2} = \nabla \mathbf{n} \cdot \boldsymbol{\nu}|_{y=L_2} .$$

Theorem 2.14. *The minimisation problem as set out in* (2.31) *and* (2.32)*, has a unique global minimiser* $\mathbf{n}^*$ *given by*

$$\mathbf{n}^*(z) = \begin{pmatrix} \cos\left(\frac{\pi z}{2}\right) \\ 0 \\ \sin\left(\frac{\pi z}{2}\right) \end{pmatrix}.$$

Proof

Firstly we note that $\mathbf{n}^*$ satisfies the Euler-Lagrange equation and the natural boundary conditions, so it is a candidate minimiser. Its energy is

$$I(\mathbf{n}^*) = \int_\Omega \frac{\pi^2}{4} \cos^2\left(\frac{\pi z}{2}\right) + \frac{\pi^2}{4} \sin^2\left(\frac{\pi z}{2}\right) dx = \frac{\pi^2 |\Omega|}{4} = \pi^2 L_1 L_2.$$

Now we take an arbitrary element $\mathbf{n} \in \mathcal{A}$. Then

$$\begin{aligned} 0 &\leqslant \int_\Omega |\nabla(\mathbf{n} - \mathbf{n}^*)|^2 \, dx \\ &= \int_\Omega |\nabla \mathbf{n}|^2 + |\nabla \mathbf{n}^*|^2 - 2\nabla \mathbf{n} : \nabla \mathbf{n}^* \, dx \\ &= \int_\Omega |\nabla \mathbf{n}|^2 + \frac{\pi^2}{4} - 2\nabla \mathbf{n} : \nabla \mathbf{n}^* \, dx. \end{aligned} \tag{2.35}$$

We look to rewrite the final term of this equation and utilise the Euler-Lagrange equation:

$$\begin{aligned} \int_\Omega \nabla \mathbf{n} : \nabla \mathbf{n}^* \, dx &= \int_\Omega \mathbf{n}_{i,\alpha} \mathbf{n}^*_{i,\alpha} \, dx \\ &= \int_{\partial\Omega} \mathbf{n}_i \mathbf{n}^*_{i,\alpha} \boldsymbol{\nu}_\alpha \, dS - \int_\Omega \mathbf{n}_i \mathbf{n}^*_{i,\alpha\alpha} \, dx \\ &= - \int_\Omega \mathbf{n}_i \mathbf{n}^*_{i,\alpha\alpha} \, dx. \end{aligned} \tag{2.36}$$

The first equality in (2.36) is simply using the divergence theorem [19, p.10] with $\boldsymbol{\nu}$ the outward pointing normal. The second equality is more involved. We note that $\mathbf{n}^*$ is a function of z only and so the integration over the vertical faces of $\partial\Omega$ are automatically zero. On $z = 0$ we have

$$\mathbf{n}_i \mathbf{n}^*_{i,\alpha} \boldsymbol{\nu}_\alpha = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\pi}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} = 0,$$

and similarly on the face $z = 1$ we find that

$$\mathbf{n}_i \mathbf{n}^*_{i,\alpha} \boldsymbol{\nu}_\alpha = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & -\frac{\pi}{2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0.$$

Now we apply the Euler-Lagrange equation $\mathbf{n}^*_{i,\alpha\alpha} = -\mathbf{n}^*_{j,k}\mathbf{n}^*_{j,k}\mathbf{n}^*_i$ and substitute these results back into (2.35) to obtain

$$\begin{aligned} \int_\Omega |\nabla(\mathbf{n} - \mathbf{n}^*)|^2 \, dx &= \int_\Omega |\nabla \mathbf{n}|^2 + \frac{\pi^2}{4} - 2(\mathbf{n}^*_{j,k}\mathbf{n}^*_{j,k})\mathbf{n}_i\mathbf{n}^*_i \, dx \\ &= I(\mathbf{n}) + \int_\Omega \frac{\pi^2}{4} - \frac{\pi^2}{2}\mathbf{n}\cdot\mathbf{n}^* \, dx \\ &= I(\mathbf{n}) - \pi^2 L_1 L_2 + \frac{\pi^2}{4}\int_\Omega 2(1 - \mathbf{n}\cdot\mathbf{n}^*) \, dx \\ &= I(\mathbf{n}) - \pi^2 L_1 L_2 + \frac{\pi^2}{4}\int_\Omega |\mathbf{n} - \mathbf{n}^*|^2 \, dx. \end{aligned} \tag{2.37}$$

The final equality uses the fact that $|\mathbf{a} - \mathbf{b}|^2 = 2(1 - \mathbf{a}\cdot\mathbf{b})$ for unit vectors $\mathbf{a}$ and $\mathbf{b}$. In order to conclude the proof we now need to show a Poincaré type inequality with an explicit constant.

Lemma 2.15. *Any function*

$$\mathbf{v} \in \left\{ \mathbf{w} \in W^{1,2}\left(\Omega, \mathbb{R}^3\right) \,\middle|\, \mathbf{w}|_{z=0} = 0,\ \mathbf{w}|_{z=1} = 0,\ \mathbf{w}|_{x=-L_1} = \mathbf{w}|_{x=L_1},\ \mathbf{w}|_{y=-L_2} = \mathbf{w}|_{y=L_2} \right\},$$

satisfies

$$\int_\Omega |\mathbf{v}|^2 \, dx \leqslant \frac{1}{\pi^2}\int_\Omega |\nabla \mathbf{v}|^2 \, dx. \tag{2.38}$$

Proof

We wish to attach a specific value to the Poincaré constant for these test functions. To that end we use Wirtinger's inequality, this version of which is from Dym and McKean [30].

$$\int_0^a |f|^2 \, dx \leqslant \frac{a^2}{\pi^2}\int_0^a |f'|^2 \, dx \ \forall\, f \in C^1(0,a) \text{ with } f(0) = f(a) = 0. \tag{2.39}$$

By density arguments we can easily extend the space of test functions to $W^{1,2}_0(0,a)$. Then by taking an arbitrary element $\mathbf{v}$ from our admissible set, we note that for almost every fixed x, y, $\mathbf{v}(x,y,z) \in W^{1,2}_0((0,1),\mathbb{R}^3)$. Therefore we apply (2.39) separately to $\mathbf{v}_1$, $\mathbf{v}_2$, and $\mathbf{v}_3$ to obtain

$$\int_0^1 |\mathbf{v}|^2 \, dz \leqslant \frac{1}{\pi^2}\int_0^1 \left|\frac{\partial \mathbf{v}}{\partial z}\right|^2 \, dz \leqslant \frac{1}{\pi^2}\int_0^1 |\nabla \mathbf{v}|^2 \, dz.$$

Since this is true for almost every x, y we can then integrate this inequality over x and y to deduce (2.38)

□

Now we can finally conclude the proof of Theorem 2.14. Using Lemma 2.15 in (2.37) we obtain

$$I(\mathbf{n}) - \pi^2 L_1 L_2 \geqslant \int_\Omega |\nabla(\mathbf{n} - \mathbf{n}^*)|^2 - \frac{\pi^2}{4}|\mathbf{n} - \mathbf{n}^*|^2 \, dx \geqslant \frac{3\pi^2}{4} \int_\Omega |\mathbf{n} - \mathbf{n}^*|^2 \, dx,$$

and so this proves the existence and uniqueness of our global minimiser:

$$I(\mathbf{n}) - I(\mathbf{n}^*) \geqslant \frac{3\pi^2}{4} \int_\Omega |\mathbf{n} - \mathbf{n}^*|^2 \, dx \quad \forall \mathbf{n} \in \mathcal{A}.$$

□

Thus with the one constant approximation, an explicit and unique global minimiser exists for the problem. This marks the end of our analysis of nematic liquid crystals within the traditional Oseen-Frank framework. The simple form of the Lagrangian leaves no possibility that a function which depends on more than one variable is energetically favourable. We will now turn to the cholesteric one constant approximation and see that there are not such clear cut deductions.

2.6 Multi-dimensional Results - Cholesteric One Constant Approximation

When we apply the one constant approximation to (2.3), the general cholesteric energy reduces to

$$I(\mathbf{n}) = K \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \, dx, \tag{2.40}$$

with the usual set of admissible functions

$$\mathcal{A} := \left\{ \mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2) \,\middle|\, \mathbf{n}|_{z=0} = \mathbf{e}_1, \ \mathbf{n}|_{z=1} = \mathbf{e}_3, \ \mathbf{n}|_{x=-L_1} = \mathbf{n}|_{x=L_1}, \ \mathbf{n}|_{y=-L_2} = \mathbf{n}|_{y=L_2} \right\}. \tag{2.41}$$

We already know the form of the one variable minimiser of this functional from Theorem 2.10, and so we begin this section with a simple corollary which is just a specific case of Theorem 2.10.

Corollary 2.16. *The function, $\theta(z)$, given implicitly by the equation*

$$\int_0^{\theta(z)} \frac{1}{(D - t^2 \cos^2 u)^{\frac{1}{2}}} \, du = z, \tag{2.42}$$

where the constant D is defined by

$$\int_0^{\frac{\pi}{2}} \frac{1}{(D - t^2 \cos^2 u)^{\frac{1}{2}}} \, du = 1, \tag{2.43}$$

and

$$\phi = tz, \tag{2.44}$$

determines a director field $\mathbf{n}^*$ *which is the unique global minimum of* (2.40) *over* $\mathbf{n} \in \mathcal{A}$ *which depend only on* z*.*

Proof

By substituting $K_1 = K_2 = K_3 = K$ into (2.27) and (2.28), and by setting

$$D = \frac{C}{K},$$

we immediately obtain the result

□

Before we proceed further, to better understand our one variable minimiser it is instructive to compute the explicit solutions of (2.42) and (2.43) for various values of t. For all of the numerical calculations the standard ODE solver in Matlab was used, a fourth order Runge-Kutta method. The four figures below: Figures 2.4a, 2.4b, 2.4c, and 2.4d, each show a plot of θ against the height of the cell, each for a different value of the cholesteric twist strength, t.

The trend is clear to see. Small values of t correspond to a slight bending of the case $t = 0$ ($\Rightarrow \theta = \frac{\pi z}{2}$). Larger values of t have much more curvature towards the top of the cell. The reason for this can be seen by looking at (2.40) and substituting $\phi' = t$. We obtain that the energy purely in terms of θ is given by

$$\int_0^1 \theta'^2 + t^2 \sin^2\theta \, dz.$$

Hence it is no surprise that as t increases the second term becomes more dominant, meaning that θ remains small so as to minimise $\sin^2\theta$. These graphs also show agreement with the phenomenon observed in our motivational problem from HP Labs that adding more chiral dopant to the cholesteric (which decreases the pitch), flattens the tilted profile which increases light absorption in the 'dark' state of the pixel.

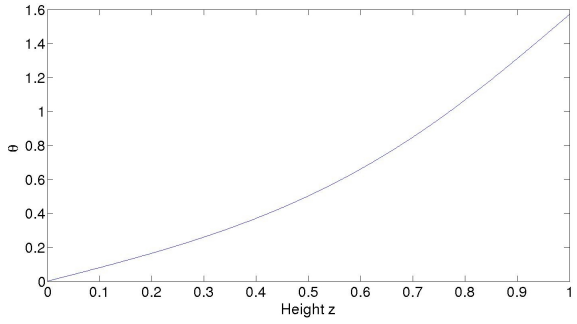
Alternate Boundary Conditions

At this juncture it is also of interest to briefly consider problems with slightly different boundary conditions. During our modelling discussion we made the informed decision to approximate the grating area of the tilted state (see Figure 0.1(b)) by a bottom substrate which is flat and the boundary condition $\mathbf{n}(x, y, 0) = \mathbf{e}_1$. But how stable is this problem to perturbations of this boundary condition? Suppose that we alter our problem in the sense that on the bottom face $z = 0$ we set

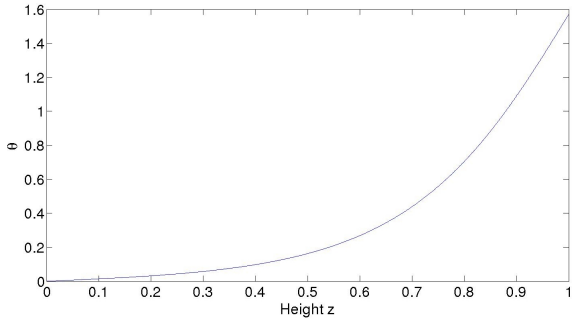
$$\mathbf{n} = \begin{pmatrix} \cos\alpha \\ 0 \\ \sin\alpha \end{pmatrix}.$$

This merely corresponds to setting $\theta(0) = \alpha \in \left[0, \frac{\pi}{2}\right)$. If we do so then much of the analysis in this chapter still applies and we can simply use the ODE solver from Matlab to calculate the global minimiser amongst functions of z only by finding its corresponding $\theta(z)$. The results of this are shown in the figures below. Figures 2.5a, 2.5b, and 2.5c correspond to tilt angles on the bottom face of the liquid crystal of $\frac{\pi}{16}$, $\frac{\pi}{4}$, and $\frac{7\pi}{16}$ radians respectively. To reduce

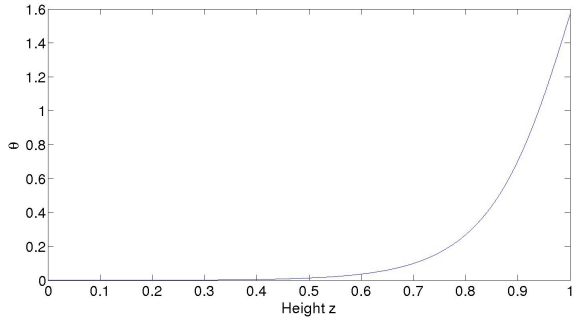
the number of graphs, for each tilt angle, four values of the cholesteric twist t have been plotted, the same four that were used in Figure 2.4. What is encouraging about these figures is that we are seeing the same sort of behaviour of the minimisers amongst all tilted boundary conditions. This means that $\alpha = 0$ seems to be, qualitatively, stable under a perturbation of the lower boundary condition. The case when $\alpha = \frac{\pi}{2}$, so that we have homeotropic anchoring



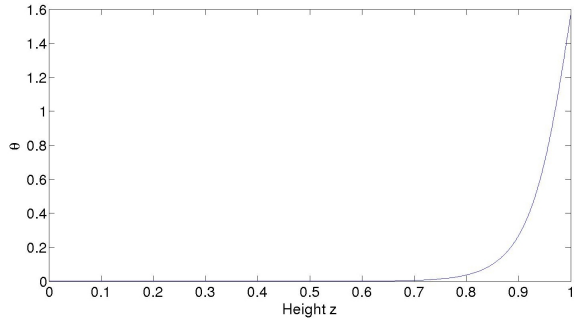
(a) $t = 2.5$



(b) $t = 5$



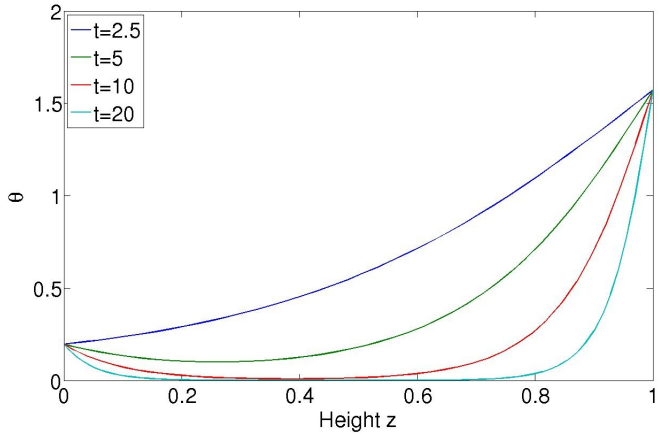
(c) $t = 10$



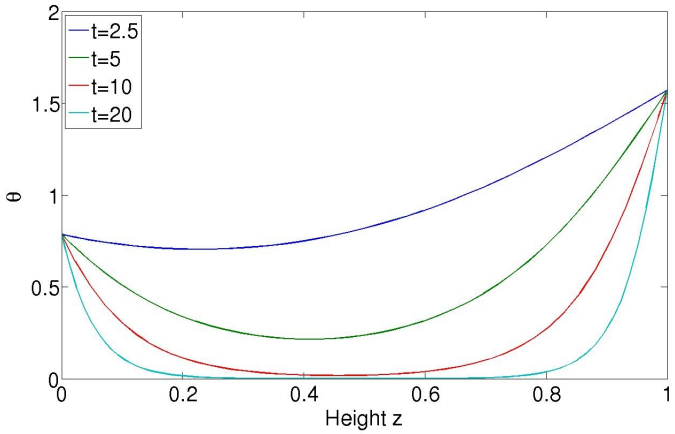
(d) $t = 20$

Figure 2.4: θ plots for various values of t

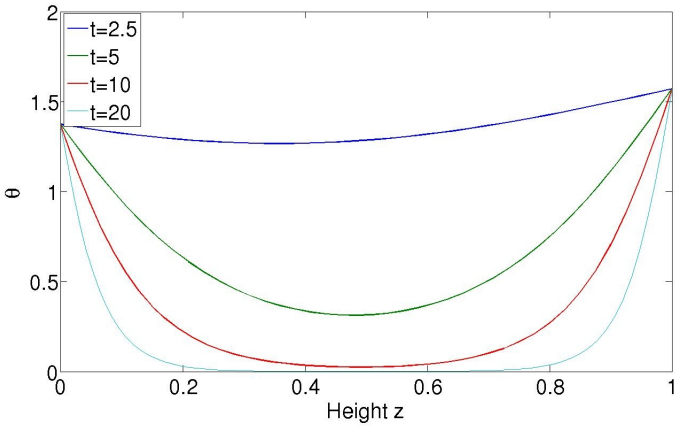
on both faces, is however a special case. This is because $\mathbf{n} = \mathbf{e}_3$ is always a solution of the Euler-Lagrange equation. We will study that problem in the next chapter.



(a) Tilt angle $\frac{\pi}{16}$



(b) Tilt angle $\frac{\pi}{4}$



(c) Tilt angle $\frac{7\pi}{16}$

Figure 2.5: Alternate boundary bonditions

2.6.1 Global Minimum for Long Cholesteric Pitch

Let us now return to the problem set out in (2.40) and (2.41). We now know that we have found the global minimiser of this problem over functions of z alone. The very natural question from that point is to ask whether these functions, pictorially represented in Figure 2.4, are the global minimisers of the entire problem. The question will be partly answered using Theorem 2.18 below. The theorem will utilise the fact that our candidate minimiser satisfies the full Euler-Lagrange equations for the problem. The equations themselves are given below in Lemma 2.17 but the proof is omitted since it is essentially identical to the derivation in the nematic case: Lemma 2.12.

Lemma 2.17. *If* $\mathbf{n} \in \mathcal{A}$ *is a weak local minimum of* (2.40) *then it satisfies the following Euler-Lagrange equations (in the sense of distributions)*

$$\Delta \mathbf{n} - 2t\nabla \times \mathbf{n} + \left(|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n}\right)\mathbf{n} = 0.$$

Theorem 2.18. *There exists some* $t^* > 0$ *such that whenever* $t \leqslant t^*$*, the function defined by* (2.42)*,* (2.43)*, and* (2.44) *is in fact the unique global minimiser of*

$$I(\mathbf{n}) = \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \, dx,$$

over all *admissible functions* $\mathbf{n} \in \mathcal{A}$*.*

Proof

We have our candidate minimiser of this functional $\mathbf{n}^*$ which is given by the equation

$$\mathbf{n}^* = \begin{pmatrix} \cos\theta\cos(tz) \\ \cos\theta\sin(tz) \\ \sin\theta \end{pmatrix}, \tag{2.45}$$

where θ is a solution of

$$\theta'' = t^2 \cos\theta \sin\theta, \quad \theta(0) = 0, \quad \theta(1) = \frac{\pi}{2}. \tag{2.46}$$

However we can find the first integral of (2.46) by multiplying by θ' and integrating to deduce that (for $\delta_t > 0$)

$$\theta'^2 + t^2 \cos^2\theta = \delta_t + t^2, \quad \theta(0) = 0, \quad \theta(1) = \frac{\pi}{2}. \tag{2.47}$$

The proof that this is indeed the global minimum uses two main calculations.

- Firstly we will show the following relation for an arbitrary $\mathbf{n} \in \mathcal{A}$

  $$H(\mathbf{n} - \mathbf{n}^*) = I(\mathbf{n}) - I(\mathbf{n}^*),$$

  where the functional H is given by

  $$H(\mathbf{v}) := \int_\Omega |\nabla \mathbf{v}|^2 + 2t\mathbf{v} \cdot \nabla \times \mathbf{v} - \left(|\nabla \mathbf{n}^*|^2 + 2t\mathbf{n}^* \cdot \nabla \times \mathbf{n}^*\right)|\mathbf{v}|^2 \, dx.$$

H takes functions from $\mathcal{B}$ which is the set given by

$$\mathcal{B} := \left\{ \mathbf{v} \in W^{1,2}\left(\Omega, \mathbb{R}^3\right) \,\middle|\, \mathbf{v}|_{z=0} = 0,\ \mathbf{v}|_{z=1} = 0,\ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \right\}.$$

- Secondly we will show that if t is small enough then for all $\mathbf{v} \in \mathcal{B}$

$$H(\mathbf{v}) \geqslant \gamma_t \int_\Omega |\nabla \mathbf{v}|^2 \, dx,$$

for some $\gamma_t > 0$.

$I(\mathbf{n}) - I(\mathbf{n}^*)$ Calculation

Take an arbitrary $\mathbf{n} \in \mathcal{A}$. Then

$$\int_\Omega |\nabla \mathbf{n} - \nabla \mathbf{n}^*|^2 \, dx = \int_\Omega |\nabla \mathbf{n}|^2 + |\nabla \mathbf{n}^*|^2 - 2\nabla \mathbf{n} : \nabla \mathbf{n}^* \, dx. \tag{2.48}$$

Now we can use the Euler-Lagrange equation to rewrite the final term in the relation above. The strong form of the Euler-Lagrange equation which is satisfied by our function $\mathbf{n}^*$ is

$$\Delta \mathbf{n}^* - 2t\nabla \times \mathbf{n}^* + \left(|\nabla \mathbf{n}^*|^2 + 2t\mathbf{n}^* \cdot \nabla \times \mathbf{n}^*\right)\mathbf{n}^* = 0.$$

We multiply this equation by $\mathbf{n}$ and then we can use integration by parts to rewrite the equation as follows

$$\begin{aligned}
0 &= \int_\Omega \mathbf{n} \cdot \Delta \mathbf{n}^* - 2t\mathbf{n} \cdot \nabla \times \mathbf{n}^* + \lambda(\mathbf{n} \cdot \mathbf{n}^*) \, dx \\
&= \int_\Omega \mathbf{n}_i \mathbf{n}^*_{i,33} - 2t\mathbf{n} \cdot \nabla \times \mathbf{n}^* + \lambda(\mathbf{n} \cdot \mathbf{n}^*) \, dx \\
&= \int_\Omega -\mathbf{n}_{i,3} \mathbf{n}^*_{i,3} - 2t\mathbf{n} \cdot \nabla \times \mathbf{n}^* + \lambda(\mathbf{n} \cdot \mathbf{n}^*) \, dx \\
&= \int_\Omega -\nabla \mathbf{n} : \nabla \mathbf{n}^* - 2t\mathbf{n} \cdot \nabla \times \mathbf{n}^* + \lambda(\mathbf{n} \cdot \mathbf{n}^*) \, dx,
\end{aligned}$$

where $\lambda := |\nabla \mathbf{n}^*|^2 + 2t\mathbf{n}^* \cdot \nabla \times \mathbf{n}^*$. We know that the integration by parts holds in the above calculation due to the definitions of $\mathbf{n}$ and $\mathbf{n}^*$. The boundary integrals are zero because

$$\mathbf{n}_i \mathbf{n}^*_{i,3}(0) = \mathbf{n}^*_{1,3}(0) = \left. -t \sin(tz) \cos\theta - \theta' \cos(tz) \sin\theta \right|_{z=0} = 0,$$

and similarly

$$\mathbf{n}_i \mathbf{n}^*_{i,3}(1) = \mathbf{n}^*_{3,3}(1) = \left. \theta' \cos\theta \right|_{z=1} = 0.$$

Thus (2.48) can be written as

$$\int_\Omega |\nabla \mathbf{n} - \nabla \mathbf{n}^*|^2 \, dx = \int_\Omega |\nabla \mathbf{n}|^2 + |\nabla \mathbf{n}^*|^2 + 4t\mathbf{n} \cdot \nabla \times \mathbf{n}^* - 2\lambda(\mathbf{n} \cdot \mathbf{n}^*) \, dx.$$

Using the facts that $2(1-\mathbf{n}\cdot\mathbf{n}^*) = |\mathbf{n}-\mathbf{n}^*|^2$ and $I(\mathbf{n}^*) = \int_\Omega \lambda + t^2\,dx$, we perform the following calculation

$$\begin{aligned}
\int_\Omega |\nabla\mathbf{n} - \nabla\mathbf{n}^*|^2\,dx &= \int_\Omega |\nabla\mathbf{n}|^2 + |\nabla\mathbf{n}^*|^2 + 4t\mathbf{n}\cdot\nabla\times\mathbf{n}^* - 2\lambda\mathbf{n}\cdot\mathbf{n}^*\,dx \\
&= \int_\Omega |\nabla\mathbf{n}|^2 + |\nabla\mathbf{n}^*|^2 + 4t\mathbf{n}\cdot\nabla\times\mathbf{n}^* + 2\lambda(1-\mathbf{n}\cdot\mathbf{n}^*) - 2\lambda\,dx \\
&= \int_\Omega |\nabla\mathbf{n}|^2 + |\nabla\mathbf{n}^*|^2 + 4t\mathbf{n}\cdot\nabla\times\mathbf{n}^* + \lambda|\mathbf{n}-\mathbf{n}^*|^2 + 2t^2\,dx - 2I(\mathbf{n}^*) \\
&= I(\mathbf{n}) + I(\mathbf{n}^*) + 2t\int_\Omega 2(\mathbf{n}\cdot\nabla\times\mathbf{n}^*) - (\mathbf{n}\cdot\nabla\times\mathbf{n}) - (\mathbf{n}^*\cdot\nabla\times\mathbf{n}^*) \\
&\quad + \lambda|\mathbf{n}-\mathbf{n}^*|^2\,dx - 2I(\mathbf{n}^*) \\
&= I(\mathbf{n}) - I(\mathbf{n}^*) + 2t\int_\Omega 2(\mathbf{n}\cdot\nabla\times\mathbf{n}^*) - (\mathbf{n}\cdot\nabla\times\mathbf{n}) - (\mathbf{n}^*\cdot\nabla\times\mathbf{n}^*)\,dx \\
&\quad + \int_\Omega \lambda|\mathbf{n}-\mathbf{n}^*|^2\,dx.
\end{aligned} \tag{2.49}$$

Looking at the central integral in the equation above, we can rearrange the expression to get

$$\begin{aligned}
&\int_\Omega 2(\mathbf{n}\cdot\nabla\times\mathbf{n}^*) - (\mathbf{n}\cdot\nabla\times\mathbf{n}) - (\mathbf{n}^*\cdot\nabla\times\mathbf{n}^*)\,dx \\
&= \int_\Omega \left[(\mathbf{n}-\mathbf{n}^*)\cdot\nabla\times(\mathbf{n}^*-\mathbf{n})\right] + (\mathbf{n}\cdot\nabla\times\mathbf{n}^*) - (\mathbf{n}^*\cdot\nabla\times\mathbf{n})\,dx.
\end{aligned} \tag{2.50}$$

Then using integration by parts we find that

$$\int_\Omega \mathbf{n}\cdot\nabla\times\mathbf{n}^*\,dx = \int_\Omega \mathbf{n}_i\epsilon_{ijk}\mathbf{n}^*_{k,j} = \int_{\partial\Omega}\mathbf{n}_i\mathbf{n}^*_k\epsilon_{ijk}\boldsymbol{\nu}^j\,dS - \int_\Omega \mathbf{n}^*_k\epsilon_{ijk}\mathbf{n}_{i,j}\,dx = \int_\Omega \mathbf{n}^*\cdot\nabla\times\mathbf{n}\,dx. \tag{2.51}$$

The surface integral is easily seen to be zero by applying the boundary conditions from the set $\mathcal{A}$. We are now in a position to conclude the calculation by combining the final line of (2.49), (2.50) and (2.51):

$$\int_\Omega |\nabla\mathbf{n} - \nabla\mathbf{n}^*|^2 + 2t\left[(\mathbf{n}-\mathbf{n}^*)\cdot\nabla\times(\mathbf{n}-\mathbf{n}^*)\right] - \lambda|\mathbf{n}-\mathbf{n}^*|^2\,dx = H(\mathbf{n}-\mathbf{n}^*) = I(\mathbf{n}) - I(\mathbf{n}^*).$$

Integral estimate

Now we look to find a lower bound for the integral functional H and we begin by noting the following relation obtained just by simple algebra (using (2.45) and (2.47))

$$|\nabla\mathbf{n}^*|^2 + 2t\mathbf{n}^*\cdot\nabla\times\mathbf{n}^* = \delta_t - t^2 + 2t^2\sin^2\theta. \tag{2.52}$$

Thus we can rewrite H in the following, more concrete, form

$$H(\mathbf{v}) = \int_\Omega |\nabla\mathbf{v}|^2 + 2t\mathbf{v}\cdot\nabla\times\mathbf{v} - (\delta_t - t^2 + 2t^2\sin^2\theta)|\mathbf{v}|^2\,dx.$$

Firstly we infer that $0 < \delta_t \leqslant \frac{\pi^2}{4}$. This is clearly true because looking at (2.47) simply shows that $\theta'^2 > \delta_t$. Hence if $\delta_t > \frac{\pi^2}{4}$ then necessarily $\theta(1) > \frac{\pi}{2}$. It is also an elementary fact that $|\nabla \times \mathbf{v}| \leqslant \sqrt{2}|\nabla \mathbf{v}|$, so

$$\begin{aligned} H(\mathbf{v}) &\geqslant \int_\Omega |\nabla \mathbf{v}|^2 + 2t\mathbf{v} \cdot \nabla \times \mathbf{v} - \left(\frac{\pi^2}{4} + t^2\right)|\mathbf{v}|^2 \, dx \\ &\geqslant \int_\Omega |\nabla \mathbf{v}|^2 - 2t|\mathbf{v}||\nabla \times \mathbf{v}| - \left(\frac{\pi^2}{4} + t^2\right)|\mathbf{v}|^2 \, dx \\ &\geqslant \int_\Omega |\nabla \mathbf{v}|^2 - 2t\sqrt{2}|\mathbf{v}||\nabla \mathbf{v}| - \left(\frac{\pi^2}{4} + t^2\right)|\mathbf{v}|^2 \, dx. \end{aligned}$$

From here we can use Cauchy's inequality, $ab \leqslant \frac{1}{2}(\epsilon a^2 + \frac{b^2}{\epsilon})$, with $\epsilon = 4t$ to obtain

$$H(\mathbf{v}) \geqslant \int_\Omega |\nabla \mathbf{v}|^2 \left(1 - \frac{1}{2\sqrt{2}}\right) - \left(\frac{\pi^2}{4} + t^2 + 4\sqrt{2}t^2\right)|\mathbf{v}|^2 \, dx. \tag{2.53}$$

As can be seen by the argument below, $\epsilon = 4t$ is not the optimal value to use in Cauchy's inequality for proving the global minimum property for the widest range of t values. A short calculation shows that $\epsilon = \left(\frac{4\sqrt{2}}{3} + \frac{2\sqrt{11}}{3}\right)t \approx 4.09t$ is in fact the optimal constant but we use $4t$ for ease here. Having established (2.53) we apply the Poincaré inequality we proved in Lemma 2.15 to deduce that

$$\begin{aligned} H(\mathbf{v}) &\geqslant \left[\pi^2\left(1 - \frac{1}{2\sqrt{2}}\right) - \left(\frac{\pi^2}{4} + t^2 + 4\sqrt{2}t^2\right)\right] \int_\Omega |\mathbf{v}|^2 \, dx \\ &=: \gamma_t \int_\Omega |\mathbf{v}|^2 \, dx \\ &\approx \left(3.91 - 6.65t^2\right) \int_\Omega |\mathbf{v}|^2 \, dx. \end{aligned} \tag{2.54}$$

Conclusion

We are now in a position to conclude the proof by drawing the two strands together. By taking an arbitrary $\mathbf{n} \in \mathcal{A}$ we know that

$$I(\mathbf{n}) - I(\mathbf{n}^*) = H(\mathbf{n} - \mathbf{n}^*) \geqslant \gamma_t \int_\Omega |\mathbf{n} - \mathbf{n}^*|^2 \, dx.$$

The definition of γ_t shows that if $t \leqslant 0.766$ then $\gamma_t > 0$. This means that there exists some $t^* > 0$ such that if $t < t^*$, $\mathbf{n}^*$ is indeed the unique global minimiser of the problem.

□

Theorem 2.18 is perhaps an unsurprising result. From the previous sections we had found the global minimum in the nematic one constant approximation case, and in some sense, small values of the cholesteric twist strength just represent a perturbation of that problem. So we are able to find the unique global minimum when the perturbation is small enough. What remains unclear however is whether for cases of high chirality (large values of t) we retain the property that a function of z remains the unique global minimum of the problem. What has become apparent in our subsequent investigations is that there may be a number of causes for our inability to penetrate the higher chirality situations. There is an argument to

be made that the Oseen-Frank director theory as we have used it in this chapter, is somewhat flawed because we are not truly respecting the head to tail symmetry of the molecules. We will return to this issue in Chapter 4. The second possibility is that perhaps our choice of boundary conditions on the lateral faces, periodicity, may be at the heart of the issue. In order to try and understand these problems, in the next chapter we focus on the local behaviour of cholesterics. We will use the tools that we developed in Chapter 1 to examine the local stability of specific states. We also investigate the relationship between the saddle-splay term and locally minimising the elastic free energy density. This particular connection seems to be crucial in finding and understanding multi-variable minimisers.

Chapter 3

Local minimisers for Liquid Crystal Problems

In the previous chapter we were principally interested in finding the global minimisers of our particular liquid crystal problem. We did so by finding solutions of the Euler-Lagrange equation and then using direct arguments to show that the solution was in fact the global minimum (Theorems 2.14 and 2.18). However we were only able to perform these analyses by using specific properties of the solutions. In general we will not be able to do this. It was briefly discussed in Chapter 1 that with a pointwise constraint, such as $|\mathbf{n}(x)| = 1$, we have a number of necessary conditions which are satisfied by a global minimiser. However, with a constraint there is no known set of sufficient conditions for any Lagrangian that we are aware of. This means that, in general, finding global minimisers for liquid crystals problems analytically will prove to be very difficult. In Chapter 1 however we were able to form a set of necessity and sufficiency results for weak and strong local minimisers. This is important because local minimisers still represent physically viable states which should be experimentally achievable given the correct conditions.

The framework established in Chapter 1 provides a concrete set of conditions to check in order to prove whether a state is a strong or weak local minimum, or neither. In this chapter we will study local minimisers for two particular liquid crystal problems. In Section 3.2 we will continue to study the problem from the previous chapter and investigate whether the minimiser of functions of z is a local minimiser over all admissible functions. To conclude the chapter we explore some of the potential shortcomings of the Oseen-Frank free energy. We focus in particular on a structure called the double-twist cylinder which, if the saddle splay term is non-zero, is locally more energetically favourable than the basic helical configuration. In addition, as a potential criticism of our own model, we will show that the periodicity actually ensures that there is no contribution from the saddle-splay term in the free energy density. Firstly however, we bring our analytical weight to bear on the cholesteric problem with homeotropic boundary conditions on both the top and bottom faces of the cell.

3.1 Homeotropic boundary conditions

Up to this point we have exclusively focused our attention on the problem with homeotropic anchoring applied to the top face and planar anchoring on the bottom face of the cell. However a more commonly studied problem is that of homeotropic boundary conditions on both faces. For the duration of this section we consider the problem of minimising

$$I(\mathbf{n}) = \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \, dx \tag{3.1}$$

over

$$\mathcal{A} := \left\{ \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right) \middle| \ \mathbf{n}|_{z=0} = \mathbf{n}|_{z=1} = \mathbf{e}_3, \ \mathbf{n}|_{x=-L_1} = \mathbf{n}|_{x=L_1}, \ \mathbf{n}|_{y=-L_2} = \mathbf{n}|_{y=L_2} \right\}. \tag{3.2}$$

This problem is slightly more approachable in that for every value of t we have a simple solution of the Euler-Lagrange equation. The constant function $\mathbf{n} = \mathbf{e}_3$ satisfies

$$\Delta \mathbf{n} - 2t\nabla \times \mathbf{n} + \mathbf{n}\left(|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n}\right) = 0,$$

for any t. This constant state is often called the unwound cholesteric state because of its deviation from the helical configuration

$$\mathbf{n}(z) := \begin{pmatrix} \cos(tz) \\ \sin(tz) \\ 0 \end{pmatrix}.$$

The stability of the unwound state has been approached both experimentally [39], and with simulations. However with our local minimiser results from Chapter 1 we can precisely quantify its stability as follows.

Theorem 3.1. *Consider the variational problem as described in* (3.1) *and* (3.2). *If $t < \pi$ then $\mathbf{n} = \mathbf{e}_3$ is a strict strong local minimiser of I. If $t > \pi$ then $\mathbf{n} = \mathbf{e}_3$ is not a weak local minimiser of I.*

Proof

The heart of the proof centres around showing that the second variation of I can be negative if $t > \pi$ and proving its positivity when $t < \pi$. Therefore when $t < \pi$ we are looking to show that for some $\delta > 0$

$$\frac{d^2}{d\epsilon^2} I\left(\frac{\mathbf{n} + \epsilon \mathbf{v}}{|\mathbf{n} + \epsilon \mathbf{v}|}\right)\bigg|_{\epsilon=0} = \frac{d^2}{d\epsilon^2} I\left(\mathbf{w}_\epsilon\right)\bigg|_{\epsilon=0} \geqslant \delta \|\mathbf{w}_0'\|_{1,2}^2 \tag{3.3}$$

for every $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$ where

$$\mathrm{Var}_{\mathcal{A}} := \left\{ \mathbf{v} \in C^\infty\left(\overline{\Omega}, \mathbb{R}^3\right) \middle| \ \mathbf{v}|_{z=0} = \mathbf{v}|_{z=1} = 0, \ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1}, \ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \right\}.$$

By referring to Theorem 1.14, we see that (3.3) is sufficient to show that the state is a strict strong local minimiser as the strengthened Weierstrass condition (1.26) is automatically satisfied. To accomplish this we need to find the exact form of the second variation. Let $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$

and $\mathbf{w}_\epsilon := \frac{\mathbf{n}+\epsilon\mathbf{v}}{|\mathbf{n}+\epsilon\mathbf{v}|}$, then

$$\begin{aligned}\frac{d^2}{d\epsilon^2} I(\mathbf{w}_\epsilon)\Big|_{\epsilon=0} =& 2\int_\Omega |\nabla \mathbf{w}_0'|^2 + 2t\mathbf{w}_0' \cdot \nabla \times \mathbf{w}_0'\, dx \\ &+ 2\int_\Omega \nabla \mathbf{w}_0'' : \nabla \mathbf{w}_0 + 2t\mathbf{w}_0'' \cdot \nabla \times \mathbf{w}_0\, dx \\ =& 2\int_\Omega |\nabla \mathbf{w}_0'|^2 + 2t\mathbf{w}_0' \cdot \nabla \times \mathbf{w}_0'\, dx \\ =& 2\int_\Omega |\nabla \mathbf{v}_1|^2 + |\nabla \mathbf{v}_2|^2 + 2t\left(\mathbf{v}_2\mathbf{v}_{1,3} - \mathbf{v}_1\mathbf{v}_{2,3}\right)\, dx.\end{aligned} \tag{3.4}$$

Note that only the derivatives in z can possibly make (3.4) negative since the other derivatives only appear as perfect squares. Therefore we proceed initially by proving that for $t < \pi$, $\mathbf{e}_3$ is a strict weak local minimiser of I over functions which just depend on z. Let

$$\mathbf{n}(z) := \begin{pmatrix} \cos\theta\cos\phi \\ \cos\theta\sin\phi \\ \sin\theta \end{pmatrix} \text{ where } \phi = \phi(z), \text{ and } \theta = \theta(z),$$

then we can perform the following energy estimate

$$\begin{aligned} I(\mathbf{n}) - I(\mathbf{e}_3) &= 4L_1L_2 \int_0^1 \theta'^2 + \cos^2\theta\left(\phi'^2 - 2t\phi'\right)\, dx \\ &\geqslant 4L_1L_2 \int_0^1 \theta'^2 - t^2\cos^2\theta\, dz. \end{aligned}$$

We let

$$J(\theta) := \int_0^1 \theta'^2 - t^2\cos^2\theta\, dz,$$

and we will show that $\theta = \frac{\pi}{2}$ is a strict weak local minimiser of J over

$$C := \left\{ f \in W^{1,2}(0,1) \,\middle|\, f(0) = f(1) = \frac{\pi}{2} \right\}$$

when $t < \pi$ and not a weak local minimiser when $t > \pi$. We prove the stability first. The constant $\frac{\pi}{2}$ clearly satisfies the Euler Lagrange equation for J and when we calculate the second variation we find

$$\frac{d^2}{d\epsilon^2} J\left(\frac{\pi}{2} + \epsilon g\right)\Big|_{\epsilon=0} = 2\int_0^1 g'^2 - t^2 g^2\, dz. \tag{3.5}$$

However we know that our test space is $W_0^{1,2}(0,1)$ and the Poincaré constant for those functions is precisely π^2 (see Lemma 2.15). Therefore if $t < \pi$, for any $g \in W_0^{1,2}(0,1)$

$$\frac{d^2}{d\epsilon^2} J\left(\frac{\pi}{2} + \epsilon g\right)\Big|_{\epsilon=0} \geqslant \frac{2\left(\pi^2 - t^2\right)}{\pi^2} \int_0^1 g'^2\, dz \geqslant \alpha \|g\|_{1,2}^2.$$

The standard 1-dimensional theory therefore implies that $\theta = \frac{\pi}{2}$ is a strict weak local minimiser of J. Now we take some $\mathbf{v} = (\mathbf{v}_1, \mathbf{v}_2, 0) \in \mathrm{Var}_{\mathcal{A}}$ such that $\mathbf{v} = \mathbf{v}(z)$ and $\|\mathbf{v}\|_{1,2} > 0$. A

small calculation, using a Taylor series expansion, shows that the Euler angle θ_ϵ associated with $\mathbf{w}_\epsilon$ is given by

$$\theta_\epsilon = \sin^{-1}\left(\frac{1}{\left(1+\epsilon^2(\mathbf{v}_1^2+\mathbf{v}_2^2)\right)^{\frac{1}{2}}}\right) = \frac{\pi}{2} - (\mathbf{v}_1^2+\mathbf{v}_2^2)^{\frac{1}{2}}\epsilon + \epsilon^3 f_\epsilon,$$

where $\|f_\epsilon\|_{1,\infty} \leqslant C$ uniformly around $\epsilon = 0$. This immediately implies that $\theta_\epsilon \to \frac{\pi}{2}$ in $W^{1,\infty}$. Thus for all non-zero ϵ values which are sufficiently small, $I(\mathbf{w}_\epsilon) - I(\mathbf{e}_3) \geqslant J(\theta_\epsilon) > 0$. As a result of these inequalities we know that

$$\left.\frac{d^2}{d\epsilon^2} I(\mathbf{w}_\epsilon)\right|_{\epsilon=0} \geqslant \left.\frac{d^2}{d\epsilon^2} J(\theta_\epsilon)\right|_{\epsilon=0}. \tag{3.6}$$

When we combine (3.6) with the alternative formulation of θ_ϵ we deduce

$$\left.\frac{d^2}{d\epsilon^2} J(\theta_\epsilon)\right|_{\epsilon=0} = \left.\frac{d^2}{d\epsilon^2} J\left(\frac{\pi}{2}+\epsilon g+\epsilon^3 f_\epsilon\right)\right|_{\epsilon=0} = \left.\frac{d^2}{d\epsilon^2} J\left(\frac{\pi}{2}+\epsilon g\right)\right|_{\epsilon=0} > 0.$$

Therefore we have proved that for any $\mathbf{v}(z) \in \mathrm{Var}_{\mathcal{A}}$, the second variation is strictly positive so long as $\mathbf{w}_0'$ is non-zero. Returning to the form of the second variation (3.4) we see that the perfect squares in the x and y variables imply that if we now take an arbitrary $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$ such that $\|\mathbf{w}_0'\|_{1,2} > 0$, then

$$\left.\frac{d^2}{d\epsilon^2} I(\mathbf{w}_\epsilon)\right|_{\epsilon=0} > 0. \tag{3.7}$$

To conclude stability we just need to show that (3.7) is in fact bounded below by $\delta\|\mathbf{w}_0'\|_{1,2}^2$ for some positive δ. We argue by contradiction. If this was not the case then we could find a sequence of functions $\left(\mathbf{v}^j\right)$ such that

$$\|\mathbf{w}_{0j}'\|_{1,2}^2 = \left\|\begin{pmatrix}\mathbf{v}_1^j\\ \mathbf{v}_2^j\\ 0\end{pmatrix}\right\|_{1,2}^2 = 1, \tag{3.8}$$

and the second variation about these functions tended to zero. Without loss of generality we can assume that $\mathbf{v}_1^j \rightharpoonup \mathbf{v}_1$ and $\mathbf{v}_2^j \rightharpoonup \mathbf{v}_2$ in $W^{1,2}(\Omega) \subset\subset L^2(\Omega)$ so that when we take the lim inf of the second variation we find

$$\begin{aligned} 0 &= \liminf_{j\to\infty} \int_\Omega |\nabla \mathbf{v}_1^j|^2 + |\nabla \mathbf{v}_2^j|^2 + 2t\left(-\mathbf{v}_1^j \mathbf{v}_{2,3}^j + \mathbf{v}_{1,3}^j \mathbf{v}_2^j\right) dx \\ &\geqslant \int_\Omega |\nabla \mathbf{v}_1|^2 + |\nabla \mathbf{v}_2|^2 + 2t\left(-\mathbf{v}_1 \mathbf{v}_{2,3} + \mathbf{v}_{1,3}\mathbf{v}_2\right) dx \\ &\geqslant 0. \end{aligned}$$

Hence $\mathbf{v}_1 = \mathbf{v}_2 = 0$ and so to have the second variation tend to zero we require that

$$\int_\Omega |\nabla \mathbf{v}_1^j|^2 + |\nabla \mathbf{v}_2^j|^2 \, dx \to 0,$$

and this clearly contradicts (3.8). Therefore we find

$$\left.\frac{d^2}{d\epsilon^2} I\left(\mathbf{w}(\epsilon)\right)\right|_{\epsilon=0} > \delta\|\mathbf{w}_0'\|_{1,2}^2$$

for some $\delta > 0$. So Theorem 1.14 implies $\mathbf{e}_3$ is a strict strong local minimiser of I if $t < \pi$. For the instability we return to the second variation of the functional J as given in (3.5). By setting $g(z) = \sin(\pi z)$ we see that the second variation is negative if $t > \pi$. Therefore there exists a sequence $\left(\theta_j\right) \subset C$, such that $\theta_j \to \frac{\pi}{2}$ in $W^{1,\infty}$ and $J(\theta_j) < 0$ for all j. Define

$$\mathbf{m}_j(z) := \begin{pmatrix} \cos\theta_j \cos(tz) \\ \cos\theta_j \sin(tz) \\ \sin\theta_j \end{pmatrix}$$

and we will show an upper bound for $\|\mathbf{m}_j - \mathbf{e}_3\|_{1,\infty}$ in terms of $\|\theta_j - \frac{\pi}{2}\|_{1,\infty}$. The mean value theorem allows us to say that

$$\begin{aligned} |\mathbf{m}_j - \mathbf{e}_3|^2 &= 2(1 - \sin\theta_j) \\ &\leqslant C_1 \left|\theta_j - \frac{\pi}{2}\right|. \end{aligned}$$

Similarly

$$|\nabla \mathbf{m}_j|^2 = \theta_j'^2 + t^2 \cos^2\theta_j \leqslant \theta_j'^2 + C_2 t^2 \left|\theta_j - \frac{\pi}{2}\right|,$$

therefore $\|\mathbf{m}_j - \mathbf{e}_3\|_{1,\infty} \to 0$ and

$$I(\mathbf{m}_j) - I(\mathbf{e}_3) = J(\theta_j) < 0.$$

This proves that $\mathbf{e}_3$ cannot be a weak local minimiser when $t > \pi$.

□

Remark 3.2. *It is not clear whether the constant state* $\mathbf{e}_3$ *is a local minimiser or not at the critical value of* $t = \pi$*. Although the problem is smooth in the twist parameter t, unless we know that* $\mathbf{e}_3$ *is a global minimiser for* $t < \pi$ *we do not know of a way to infer its stability at the critical value.*

3.2 Frustrated boundary conditions

The previous section shows how useful our local minimiser results from Chapter 1 can be when applied to liquid crystal problems. With this in mind we now turn our focus back to the problem that was studied in Chapter 2. We consider the same free energy, (3.1), as the previous section and the set of admissible functions is given by the set

$$\mathcal{A} := \left\{ \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right) \middle| \ \mathbf{n}|_{z=0} = \mathbf{e}_1, \ \mathbf{n}|_{z=1} = \mathbf{e}_3, \ \mathbf{n}|_{x=-L_1} = \mathbf{n}|_{x=L_1}, \ \mathbf{n}|_{y=-L_2} = \mathbf{n}|_{y=L_2} \right\}.$$

We would like to be able to prove a result similar to Theorem 3.1 for this situation, but without a more explicit form for the candidate minimiser $\mathbf{n}(z)$ (defined in (2.42), (2.43), and (2.44)) this remains an open analytical problem. We can however approach the problem with numerical methods. From Theorem 1.14 we have already proved that to show a C^1 solution of the Euler-Lagrange equation is a strong local minimiser, it is sufficient to show that

$$\frac{d^2}{d\epsilon^2} I\left(\frac{\mathbf{n} + \epsilon\mathbf{v}}{|\mathbf{n} + \epsilon\mathbf{v}|}\right)\bigg|_{\epsilon=0} \geqslant \gamma \left\|\mathbf{w}_0'\right\|_{1,2}^2 \tag{3.9}$$

for all test functions

$$\mathbf{v} \in \mathrm{Var}_{\mathcal{A}} := \left\{ \mathbf{v} \in C^{\infty}\left(\overline{\Omega}, \mathbb{R}^3\right) \,\middle|\, \mathbf{v}|_{z=0} = \mathbf{v}|_{z=1} = 0,\ \ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \right\}.$$

However the following lemma allows us to simplify this requirement in a way to make the subsequent computation much easier to handle.

Lemma 3.3. *Suppose* $\mathbf{n} \in \mathcal{A} \cap C^1\left(\overline{\Omega}, \mathbb{S}^2\right)$ *is a solution of the Euler-Lagrange equation. If there exists some* $\delta > 0$ *such that*

$$\left.\frac{d^2}{d\epsilon^2} I\left(\frac{\mathbf{n}+\epsilon\mathbf{v}}{|\mathbf{n}+\epsilon\mathbf{v}|}\right)\right|_{\epsilon=0} \geqslant \delta \|\mathbf{w}_0'\|_2^2, \tag{3.10}$$

for all $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$*, then* $\mathbf{n}$ *is a strong local minimiser of* I*.*

Proof

We will argue by contradiction in a similar vein to the proof of Theorem 3.1. However in this more general case we must first utilise the Euler-Lagrange equation to rewrite the second variation in a more convenient form. We remind the reader that

$$\mathbf{w}_0 = \mathbf{n}, \quad \mathbf{w}_0' = \mathbf{v} - \mathbf{n}(\mathbf{n}\cdot\mathbf{v}), \quad \mathbf{w}_0'' = -2\mathbf{v}(\mathbf{n}\cdot\mathbf{v}) - \mathbf{n}|\mathbf{v}|^2 + 3\mathbf{n}(\mathbf{n}\cdot\mathbf{v})^2. \tag{3.11}$$

From Chapter 1 we know that the second variation of (3.1) has the form

$$\begin{aligned}\left.\frac{d^2}{d\epsilon^2} I\left(\frac{\mathbf{n}+\epsilon\mathbf{v}}{|\mathbf{n}+\epsilon\mathbf{v}|}\right)\right|_{\epsilon=0} = 2\int_{\Omega} &|\nabla\mathbf{w}_0'|^2 + \nabla\mathbf{w}_0'' : \nabla\mathbf{w}_0 \\ &+ 2t(\mathbf{w}_0'\cdot\nabla\times\mathbf{w}_0' + \mathbf{w}_0''\cdot\nabla\times\mathbf{w}_0)\,dx.\end{aligned} \tag{3.12}$$

Additionally, since $\mathbf{n}$ satisfies the Euler-Lagrange equation, we know

$$\int_{\Omega} \nabla\boldsymbol{\phi} : \nabla\mathbf{n} + 2t\boldsymbol{\phi}\cdot\nabla\times\mathbf{n} - (\mathbf{n}\cdot\boldsymbol{\phi})\left(|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n}\right)dx = 0 \tag{3.13}$$

for all $\boldsymbol{\phi} \in \mathrm{Var}_{\mathcal{A}}$. The fact that $\mathbf{n} \in C^1\left(\overline{\Omega}, \mathbb{R}^3\right)$ means that with a simple limiting argument we can say that (3.13) is true for all $\boldsymbol{\phi} \in C$, where

$$C := \left\{ W^{1,1}\left(\Omega, \mathbb{R}^3\right) \,\middle|\, \mathbf{v}|_{z=0} = \mathbf{v}|_{z=1} = 0,\ \ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \right\}.$$

If we take some $\mathbf{v} \in \mathrm{Var}_{\mathcal{A}}$ then from (3.11) it is clear that $\mathbf{w}_0'' \in C$. Thus by substituting (3.13) into (3.12) we find that

$$\begin{aligned}\left.\frac{d^2}{d\epsilon^2} I\left(\frac{\mathbf{n}+\epsilon\mathbf{v}}{|\mathbf{n}+\epsilon\mathbf{v}|}\right)\right|_{\epsilon=0} &= 2\int_{\Omega} |\nabla\mathbf{w}_0'|^2 + 2t\mathbf{w}_0'\cdot\nabla\times\mathbf{w}_0' + \\ &\quad + \left(\mathbf{n}\cdot\mathbf{w}_0''\right)\left(|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n}\right)dx \\ &= 2\int_{\Omega} |\nabla\mathbf{w}_0'|^2 + 2t\mathbf{w}_0'\cdot\nabla\times\mathbf{w}_0' + \\ &\quad - |\mathbf{w}_0'|^2\left(|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n}\right)dx.\end{aligned}$$

The final equality simply uses the easily verifiable identity $|\mathbf{w}_0'|^2 = -\mathbf{n}\cdot\mathbf{w}_0''$. We suppose for contradiction that (3.10) holds but (3.9) does not. That means that we have a sequence $\left(\mathbf{v}_j\right) \in \mathrm{Var}_{\mathcal{A}}$ where

$$\|\mathbf{w}_{0\,j}'\|_{1,2} = \|\mathbf{v}_j - \mathbf{n}(\mathbf{n}\cdot\mathbf{v}_j)\|_{1,2} = 1 \tag{3.14}$$

for all j and

$$\int_\Omega |\nabla \mathbf{w}_{0\,j}'|^2 + 2t\mathbf{w}_{0\,j}'\cdot\nabla\times\mathbf{w}_{0\,j}' - \lambda(x)|\mathbf{w}_{0\,j}'|^2\,dx \to 0, \tag{3.15}$$

as $j\to\infty$. Equation (3.14) means that without loss of generality we can assume that $\mathbf{w}_{0\,j}' \rightharpoonup \mathbf{w}$. Using our assumption we know that

$$\int_\Omega |\nabla \mathbf{w}_{0\,j}'|^2 + 2t\mathbf{w}_{0\,j}'\cdot\nabla\times\mathbf{w}_{0\,j}' - \lambda(x)|\mathbf{w}_{0\,j}'|^2\,dx \geqslant \gamma\int_\Omega |\mathbf{w}_{0\,j}'|^2\,dx \to 0,$$

thus the sequence $\mathbf{w}_{0\,j}'$ coverges weakly to zero in $W^{1,2}$. Therefore since each of the functions has unit norm and $\|\lambda\|_\infty < \infty$ we deduce that

$$\begin{aligned}\int_\Omega |\nabla \mathbf{w}_{0\,j}'|^2\,dx &\to 1\\ \int_\Omega \mathbf{w}_j'(0)\cdot\nabla\times\mathbf{w}_{0\,j}'\,dx &\to 0\\ \int_\Omega \lambda(x)|\mathbf{w}_{0\,j}'|^2\,dx &\to 0\end{aligned}$$

and this directly contradicts equation (3.15).

□

Lemma 3.3 simplifies our problem. It shows that it is sufficient to prove that (3.10) holds to demonstrate that our candidate minimiser is a strong local minimiser. Now we turn our attention to the numerical methods used. Firstly since we know that $\mathbf{w}_0'\cdot\mathbf{n} = 0$ and

$$\mathbf{n}(x) = \begin{pmatrix}\cos\phi\cos\theta\\ \sin\phi\cos\theta\\ \sin\theta\end{pmatrix},$$

we can choose to write $\mathbf{w}_0'(x)$ in the following form.

$$\mathbf{w}_0'(x) = f(x)\begin{pmatrix}-\sin\phi\\ \cos\phi\\ 0\end{pmatrix} + g(x)\begin{pmatrix}-\cos\phi\sin\theta\\ -\sin\phi\sin\theta\\ \cos\theta\end{pmatrix}. \tag{3.16}$$

This is true because the three vectors in the above two equations form an orthonormal basis of $\mathbb{R}^3$. For the scalar functions $f, g : \Omega\to\mathbb{R}$, the fact that our candidate minimiser $\mathbf{n}(z)$ is smooth implies that

$$f, g \in \left\{\, h\in W^{1,2}(\Omega,\mathbb{R}) \,\middle|\, h|_{z=0} = h|_{z=1} = 0,\ h|_{x=-L_1} = h|_{x=L_1},\ h|_{y=-L_2} = h|_{y=L_2}\right\}.$$

Therefore f, g are unconstrained and satisfy periodicity conditions in all three variables. This means that they can be expanded as Fourier series. Unfortunately due to computational limitations we are unable to consider f, g as depending on all of x, y, and z, because if we consider N modes then the number of Fourier coefficients would be of the order N^3, which quickly

becomes too large to be handled. Therefore we will assume that $f = f(x,z)$ and $g = g(x,z)$. Their Fourier expansions are given by

$$f(x,z) = \sum_i \frac{a_i}{L^{\frac{1}{2}}} \sin(i\pi z) + \sum_{i,j} \frac{2}{L^{\frac{1}{2}}} \sin(i\pi z)\left[a_{i,j}\sin\left(\frac{j\pi x}{L_1}\right) + b_{i,j}\cos\left(\frac{j\pi x}{L_1}\right)\right]$$
$$g(x,z) = \sum_i \frac{\alpha_i}{L^{\frac{1}{2}}} \sin(i\pi z) + \sum_{i,j} \frac{2}{L^{\frac{1}{2}}} \sin(i\pi z)\left[\alpha_{i,j}\sin\left(\frac{j\pi x}{L_1}\right) + \beta_{i,j}\cos\left(\frac{j\pi x}{L_1}\right)\right].$$

3.2.1 Numerical Data

Our numerical method involves a number of variables. Firstly we choose a maximum number of modes for our Fourier series. This creates a finite number of variables (the Fourier coefficients) which need to be optimised. We substitute (3.16) into

$$\frac{d^2}{d\epsilon^2} I\left(\frac{\mathbf{n}+\epsilon\mathbf{v}}{|\mathbf{n}+\epsilon\mathbf{v}|}\right)\Big|_{\epsilon=0} = 2\int_\Omega |\nabla \mathbf{w}_0'|^2 + 2t\mathbf{w}_0' \cdot \nabla\times\mathbf{w}_0' - |\mathbf{w}_0'|^2\left(|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n}\right) dx \quad (3.17)$$

to obtain a quadratic function in the Fourier coefficients for f and g. Therefore if we let $\mathbf{v}$ be the vector containing the Fourier coefficients, (3.17) can be written as $\mathbf{v}^T\mathbf{A}\mathbf{v}$ where $\mathbf{A}$ is a real symmetric matrix. Now we can see the advantage of Lemma 3.3. Using the Fourier series decomposition of f and g we have that $\left\|\mathbf{w}_0'\right\|_2^2 = |\mathbf{v}|^2$. Hence we are looking to show that for some $\gamma > 0$

$$\mathbf{v}^T\mathbf{A}\mathbf{v} \geqslant \gamma|\mathbf{v}|^2,$$

for all $\mathbf{v} \in \mathbb{R}^M$, where we have M Fourier coefficients. In other words, if the minimum eigenvalue of A is strictly positive then $\mathbf{n}$ is a strong local minimiser for our problem. This is possible to determine. We use a two-dimensional trapezium rule to numerically calculate the the coefficient matrix A and the data collected is shown below. The variables that need to be considered are the number of modes, the mesh size in the x and z directions, the cholesteric twist strength t, and the width of the domain $2L_1$. The full Matlab code which was used for this algorithm is given in Appendix A.

$L_1 = 10$, Grid: 200 steps in x, 200 in z

Modes	λ_{min}: $t = 5$	λ_{min}: $t = 10$	λ_{min}: $t = 20$
2	4.0970994167	5.9453836876	7.9343341517
4	3.0979207277	4.2432620507	7.0833603864
6	2.5320829644	3.3947057217	6.0427540945
8	2.1955022258	3.1238121345	4.9822122355
10	2.1630895084	3.0571190385	4.1001024445
12	2.1630871805	3.0428794657	3.4887433157
14	2.1630868554	3.0400824359	3.1214861669
16	2.1630867759	3.0395620883	2.9224570673
18	2.1630867498	3.0394689614	2.8220197715
20	2.1630867397	3.0394527755	2.7737675109
22	2.1630867352	3.0394500264	2.7513756451
24	2.1630867331	3.0394495681	2.7412445095

$L_1 = 20$, Grid: 200 steps in x, 200 in z

Modes	λ_{min}: $t = 5$	λ_{min}: $t = 10$	λ_{min}: $t = 20$
2	4.2764919677	5.9453836876	7.9343341517
4	3.5974590100	4.2432620507	7.0833603864
6	3.3406764917	3.3947057217	6.0427540945
8	3.0694901052	3.1238121345	4.9822122355
10	2.7889998313	3.0571190385	4.1001024445
12	2.5310389275	3.0428794657	3.4887433157
14	2.3249145537	3.0400824359	3.1214861669
16	2.1954636527	3.0395620883	2.9224570673
18	2.1630867498	3.0394689614	2.8220197715
20	2.1630867397	3.0394527755	2.7737675109
22	2.1630867352	3.0394500264	2.7513756451
24	2.1630867331	3.0394495681	2.7412445095

$L_1 = 40$, Grid: 400 steps in x, 200 in z

Modes	λ_{min}: $t = 5$	λ_{min}: $t = 10$	λ_{min}: $t = 20$
2	4.3236194599	5.9453836876	7.9343341517
4	3.7486959997	4.2432620507	7.0833603864
6	3.6522850110	3.3947057217	6.0427540945
8	3.5649265823	3.1238121345	4.9822122355
10	3.4597992558	3.0571190385	4.1001024445
12	3.3394399350	3.0428794657	3.4887433157
14	3.2078976523	3.0400824359	3.1214861669
16	3.0694487615	3.0395620883	2.9224570673
18	2.9284067017	3.0394689614	2.8220197715
20	2.7889979726	3.0394527755	2.7737675109
22	2.6552716273	3.0394500264	2.7513756451
24	2.5310386810	3.0394495681	2.7412445095

From a naked eye inspection, with the exception of $t = 5$ and $L_1 = 40$, it certainly appears that as we increase the number of nodes the minimum eigenvalue converges to some strictly positive number. Moreover, particularly for $t = 10$ and $t = 20$, we see that varying the width L_1 seems to have no effect on the minimum eigenvalue for a given number of nodes. This implies that the optimal variation associated with this eigenvalue is most likely a function of z and we already know that $\mathbf{n}$ is the global minimiser amongst functions of z. The case $t = 5$ seems not to be so clear cut. However even in this case, for the width values $L_1 = 10$ or $L_1 = 20$, where convergence appears to happen, the limiting number seems to be the same and is well away from zero. For the case $t = 5$ and $L_1 = 40$, even though we do not see convergence we do not see anything to contradict our inclinations; our computational limitations simply became a factor before any convergence was seen. These conclusions are at odds with the experimental data which suggests that when $\frac{d}{P} = \frac{t}{2\pi} \approx 1$, cholesteric patterns begin to form [39].

On the other hand, these calculations do not prove anything in a mathematical sense, and my relative lack of expertise in numerical analysis dissuaded me from further study in this

area. However they do provide strong indications that, at least for a reasonable set of t and L_1, our function of z alone is a strong local minimiser of our problem in two dimensions. In fact we conjecture that the one variable minimiser is always the global minimiser of our problem, but we are unable to prove this claim. In the final sections of this chapter we explore the possibility that these global difficulties, and the predictions seemingly at odds with experiments, may arise because of either our modelling of the problem, or the fact that cholesterics are not even fully understood at a more local level.

3.3 Cholesteric Frustration

Although we have been able to discover much about the cholesteric problems we have heretofore been studying in Chapters 2 and 3, we are a long way from fully understanding all of the varied structures which can occur in cholesterics. Here we discuss some of the reasons for this difficulty, chief among which, is the notion of cholesteric frustration. We return to the general Oseen-Frank free-energy

$$w(\mathbf{n}, \nabla\mathbf{n}) = K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n} + t)^2 + K_3\,|\mathbf{n}\times\nabla\times\mathbf{n}|^2 + (K_2+K_4)\nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n}).$$

A very important part of the assumptions made by both Stewart [88] and Virga [92] in deriving their assumptions on the elastic constants, is that the "natural" state of a cholesteric liquid crystal is given by any fixed rotation of the helical configuration

$$\mathbf{n} = \begin{pmatrix} \cos(tz) \\ \sin(tz) \\ 0 \end{pmatrix}. \tag{3.18}$$

In both of these authors' derivations, this assumption mathematically leads to the following equation for any $|t| > 0$

$$K_2 + K_4 = 0. \tag{3.19}$$

This means that we assume that the saddle-splay term has no contribution to the free energy in cholesterics. However it is widely considered that quite a good approximation for the elastic constants in the nematic case is

$$K_1 = 2K_2 = K_3, \quad K_4 = 0.$$

Yet in some sense the nematic free energy is simply a limit of the cholesteric free energy as $t \to 0$, and one would definitely expect the elastic constants to have a continuous dependence on the twist strength t. Yet this is not borne out by the theoretical assumptions on the elastic constants. Other authors have performed alternative derivations of continuum liquid crystal theories and come to differing conclusions. Nehring & Saupe [73] showed that by using a different approach, the one constant approximation for cholesterics leads to $K_4 = 0$. This theoretical inconsistency about natural states and the elastic constants is also reflected by experimental data in certain conditions.

Physicists have long been aware of a number of phases of cholesteric liquid crystals which can occur particularly close to the isotropic transition temperature, usually within 2 or 3

Kelvin. Recently however new work [22] has demonstrated that these phases can be stable in a temperature range of up to 60 Kelvin. From a theoretical standpoint, Alexander & Yeomans [2] have shown how the values of the elastic constants K_i affect the stability range of these blue phases. These phases became known as blue phases because their structure was of a period which refracted visible light and the first such examples refracted blue light. If it were the case that (3.19) held for all cholesterics then any solution of the equation

$$\nabla \times \mathbf{n} = -t\mathbf{n},$$

would be the global minimiser of the free energy density, and this condition is certainly satisfied by (3.18). The simple fact that this is not the case shows that we should not adopt the approximation so readily. The case of $K_2 + K_4 \neq 0$ has been considered qualitatively by many physicists. Among the first were Meiboom, Sethna et al. [64] who showed that the saddle-splay term could give a negative contribution to the free energy.

Throughout the rest of this thesis, as we have been tacitly doing so already, we will be assuming that

$$K_2 + K_4 = K_2 \neq 0, \tag{3.20}$$

and seeing where that leads us with regards to minimisers, but we recognise that we have no method to prove that (3.20) holds. An appropriate question to ask if we assume this equation is: what is the minimiser of the free energy density? This question is the very centre of the idea of cholesteric frustration, because it transpires that in $\mathbb{R}^3$ there is no minimiser of the free energy density. The following proposition shows this for the one constant approximation using a particular rearrangement of the free energy from Sethna, Wright et al. [81].

Proposition 3.4. *Suppose $K_1 = K_2 = K_3 = K$ and $K_4 = 0$. Then*

$$w(\mathbf{n}, \nabla\mathbf{n}) \geqslant -Kt^2,$$

and no function $\mathbf{n} \in W^{1,2}(U, \mathbb{S}^2)$ can satisfy $w(\mathbf{n}, \nabla\mathbf{n}) = -Kt^2$ on any domain $U \subset \mathbb{R}^3$.

Proof

Applying the one constant approximation gives us a very convenient form of the free energy density, (2.4). However there is in fact another elegant form for this equation, which Sethna et. al. [81] used in their paper and which we will also employ

$$w(\mathbf{n}, \nabla\mathbf{n}) = K\left[\sum_{i,j}\left(\mathbf{n}_{i,j} - t\epsilon_{ijk}\mathbf{n}_k\right)^2 - t^2\right]. \tag{3.21}$$

In order to minimise this free energy density we look to solve

$$\mathbf{n}_{i,j} = t\epsilon_{ijk}\mathbf{n}_k. \tag{3.22}$$

The diagonal equations instantly imply that $\mathbf{n}_{1,1} = \mathbf{n}_{2,2} = \mathbf{n}_{3,3} = 0$. So that we can deduce

$$\mathbf{n}_1 = \mathbf{n}_1(y, z), \quad \mathbf{n}_2 = \mathbf{n}_2(x, z), \quad \mathbf{n}_3 = \mathbf{n}_3(x, y).$$

Now by looking at two more equations in (3.22) we have the following 3 equalities

$$\mathbf{n}_1 = \mathbf{n}_1(y,z) = \frac{1}{t}\mathbf{n}_{2,3}(x,z) = -\frac{1}{t}\mathbf{n}_{3,2}(x,y) \quad \Rightarrow \quad \mathbf{n}_1 = \text{Constant}.$$

By identical calculations we also deduce that $\mathbf{n}_2 = \text{Constant}$ and $\mathbf{n}_3 = \text{Constant}$, and the only constant function which satisfies (3.22) is $\mathbf{n} \equiv 0$ which is of course not a unit vector. This means the global minimiser of the free energy density cannot be achieved, but we can get arbitrarily close on cylinders of small radius. Consider the function given in cylindrical coordinates by

$$\mathbf{n}^* = \sin(tr)\underline{\phi} + \cos(tr)\underline{z} \qquad \text{where} \qquad \underline{z} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \underline{\phi} = \begin{pmatrix} \sin\phi \\ -\cos\phi \\ 0 \end{pmatrix}. \tag{3.23}$$

This particular state has been dubbed the double twist cylinder, and what is important about it is that

$$w(\mathbf{n}^*, \nabla\mathbf{n}^*) = -Kt^2$$

along the line $r = 0$. So because this state is smooth in all of its arguments, by considering cylinders of arbitrarily small radius we find that the bound of $-Kt^2$ is sharp.

□

Remark 3.5. *This means that when $K_2 + K_4 \neq 0$ there is no "natural" state the liquid crystal prefers to take; on a local level there is always a more preferable state. It is how these local structures fit together to determine a minimiser over a non-local area that appears to be the key to the problem.*

Remark 3.6. *In their paper [81], Sethna et al. actually showed that the free energy is not frustrated in a special case, on the surface of $\mathbb{S}^3$ (the sphere in $\mathbb{R}^4$). They showed that the double twist function, such as in* (3.23)*, is indeed the minimum of the free energy, meaning in that example there is no cholesteric frustration. This gives credence to the notion that these double twist structures are genuinely worthy of study as local low-energy structures.*

We can prove an analogous proposition in the case when the elastic constants are non-equal. However it is a long calculation and no extra insight is gained into cholesterics, so we omit it.

3.4 Blue Phases and the Double Twist Cylinder

Now that the idea of cholesteric frustration has been introduced we address the question of how these double twist cylinders fit into the pantheon of cholesteric structures and how they could arise. Hence we return to the problem of minimising the integral functional rather than the problem of minimising the integrand. We have learned from Section 3.3 that the double twist function, given in Cartesian coordinates by

$$\mathbf{n} = \begin{pmatrix} \sin\left(t(x^2+y^2)^{\frac{1}{2}}\right)\frac{y}{(x^2+y^2)^{\frac{1}{2}}} \\ -\sin\left(t(x^2+y^2)^{\frac{1}{2}}\right)\frac{x}{(x^2+y^2)^{\frac{1}{2}}} \\ \cos\left(t(x^2+y^2)^{\frac{1}{2}}\right) \end{pmatrix},$$

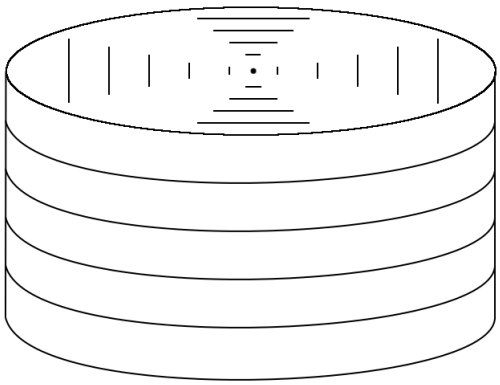


Figure 3.1: Line field representation of the Double Twist Cylinder

locally gives a lower energy than what is generally considered to be the natural cholesteric state (as long as $K_2 + K_4 \neq 0$). From here we write this function in the following form

$$\mathbf{n} = \begin{pmatrix} \sin(tr)\frac{y}{r} \\ -\sin(tr)\frac{x}{r} \\ \cos(tr) \end{pmatrix},$$

where $r^2 = x^2 + y^2$. Figure 3.1 gives a pictorial representation of the line field which this state represents. The director is vertical through the center of the cylinder and along each fixed radial line, the director rotates at a constant rate about this radial line. To see how much energy benefit could be achieved with this structure we carry out some routine calculations and find the following equalities:

$$\nabla \cdot \mathbf{n} = 0 \qquad \mathbf{n} \cdot \nabla \times \mathbf{n} = -t - \frac{\cos(tr)\sin(tr)}{r}$$

$$|\mathbf{n} \times \nabla \times \mathbf{n}|^2 = \frac{\sin^4(tr)}{r^2} \quad \nabla \cdot ((\mathbf{n} \cdot \nabla)\mathbf{n} - (\nabla \cdot \mathbf{n})\mathbf{n}) = -2t\frac{\cos(tr)\sin(tr)}{r}.$$

By substituting these equalities into the free energy density we find

$$\begin{aligned} w(\mathbf{n}, \nabla\mathbf{n}) &= K\left(\left(\frac{\cos(tr)\sin(tr)}{r}\right)^2 + \frac{\sin^4(tr)}{r^2} - 2t\frac{\cos(tr)\sin(tr)}{r}\right) \\ &= K\left(\frac{\sin^2(tr)}{r^2} - 2t\frac{\cos(tr)\sin(tr)}{r}\right). \end{aligned} \tag{3.24}$$

This form of the free energy density immediately implies (using L'Hôpital's rule) that along the line $r = 0$ this function achieves the lower bound $-Kt^2$. However the double twist cylinder only has a negative elastic energy up to a radius of approximately $\frac{3\pi}{8t}$. Thus if t is large then we would need many of these structures to fill our domain. This negative elastic energy is in stark contrast to the case when $\mathbf{n}$ is a function of z only and satisfies the following lower bound

Lemma 3.7. *Let* $\mathbf{n} = \mathbf{n}(z)$. *If* $K_1, K_2, K_3 \geqslant 0$, *then* $w(\mathbf{n}, \nabla\mathbf{n}) \geqslant 0$.

Proof

The free energy density is given by

$$w(\mathbf{n}, \nabla\mathbf{n}) = K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n}+t)^2 + K_3\,|\mathbf{n}\times\nabla\times\mathbf{n}|^2 + (K_2+K_4)\nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n}).$$

However the final term is simply zero for functions of z only since

$$\nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n}) = \nabla\cdot\left(\mathbf{n}_3\begin{pmatrix}\mathbf{n}_{1,3}\\ \mathbf{n}_{2,3}\\ \mathbf{n}_{3,3}\end{pmatrix} - \mathbf{n}_{3,3}\begin{pmatrix}\mathbf{n}_1\\ \mathbf{n}_2\\ \mathbf{n}_3\end{pmatrix}\right) = 0.$$

This clearly implies that $w(\mathbf{n}, \nabla\mathbf{n}) \geqslant 0$.

□

Problem with Periodicity

So what we can conclude from the previous section is that if we remove the assumption that $K_2 + K_4 = 0$ for cholesterics, then this double twist structure is more energetically favourable than the traditional twist by an order of t^2. Importantly this double twist structure makes good use of the saddle-splay term in the free energy. Ideally we would have liked to try and construct a solution using these sort of structures to give a lower energy value than any function of z alone. However an issue arises with the boundary conditions that we have been using. Periodicity in x and y, leads to the following proposition which effectively scuppers any chance of using these double twist structures in our problem as it stands. In the final chapter we will implicitly show that the following proposition does not hold for special functions of bounded variation so that we are able to construct a suitable array of double twist cylinders in that situation.

Proposition 3.8. *Let*

$$\mathbf{n}\in\mathcal{A} := \left\{\, \mathbf{v}\in W^{1,2}(\Omega,\mathbb{S}^2) \,\middle|\, \mathbf{v}|_{z=0} = \mathbf{e}_1,\ \mathbf{v}|_{z=1} = \mathbf{e}_3,\ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \,\right\},$$

where $\Omega = (-L_1, L_1)\times(-L_2, L_2)\times(0,1)$. *Then*

$$\int_\Omega \nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n})\ dx = 0.$$

Proof

To avoid technical issues over density of smooth functions in Sobolev spaces between manifolds we will show the slightly stronger statement that the following integral is zero

$$J(\mathbf{n}) := \int_\Omega \nabla\cdot((\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n})\,dx, \tag{3.25}$$

for all unconstrained functions

$$\mathbf{n}\in\mathcal{A}' := \left\{\, \mathbf{v}\in W^{1,2}(\Omega,\mathbb{R}^3) \,\middle|\, \mathbf{v}|_{z=0} = \mathbf{e}_1,\ \mathbf{v}|_{z=1} = \mathbf{e}_3,\ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \,\right\}.$$

First we look to show that expression (3.25) is zero for a dense subset $\mathcal{B}$, of $\mathcal{A}'$.

$$\mathcal{B} := \left\{ \mathbf{v} \in C^\infty\left(\overline{\Omega}, \mathbb{R}^3\right) \,\middle|\, \mathbf{v}|_{z=0} = \mathbf{e}_1,\ \mathbf{v}|_{z=1} = \mathbf{e}_3,\ \mathbf{v}|_{x=-L_1} = \mathbf{v}|_{x=L_1},\ \mathbf{v}|_{y=-L_2} = \mathbf{v}|_{y=L_2} \right\}.$$

So we take an arbitrary element $\mathbf{v} \in \mathcal{B}$ and we observe that since we are in the special case of a rectangular domain, the periodic boundary conditions imply that for arbitrary $y \in (-L_2, L_2)$, $z \in (0, 1)$ (differentiability up to the boundary is ensured because the domain is Lipschitz, see [9, p. 705] or [57, Thm 10.29].)

$$\begin{aligned}\frac{\partial \mathbf{v}}{\partial y}(-L_1, y, z) &= \lim_{h\to 0} \frac{\mathbf{v}(-L_1, y+h, z) - \mathbf{v}(-L_1, y, z)}{h} \\ &= \lim_{h\to 0} \frac{\mathbf{v}(L_1, y+h, z) - \mathbf{v}(L_1, y, z)}{h} = \frac{\partial \mathbf{v}}{\partial y}(L_1, y, z).\end{aligned}$$

By very similar arguments we conclude the following set of equalities

$$\begin{aligned}\left.\frac{\partial \mathbf{v}}{\partial y}\right|_{x=-L_1} &= \left.\frac{\partial \mathbf{v}}{\partial y}\right|_{x=L_1}, \quad \left.\frac{\partial \mathbf{v}}{\partial z}\right|_{x=-L_1} = \left.\frac{\partial \mathbf{v}}{\partial z}\right|_{x=L_1}, \\ \left.\frac{\partial \mathbf{v}}{\partial x}\right|_{y=-L_2} &= \left.\frac{\partial \mathbf{v}}{\partial x}\right|_{y=L_2}, \quad \left.\frac{\partial \mathbf{v}}{\partial z}\right|_{y=-L_2} = \left.\frac{\partial \mathbf{v}}{\partial z}\right|_{y=L_2}.\end{aligned} \tag{3.26}$$

This puts us in a position where we can calculate the integral; we use the divergence theorem to obtain

$$\begin{aligned}J(\mathbf{v}) &= \int_{\partial\Omega} ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot\mathbf{N}dS \\ &= \int_{x=-L_1} ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot(-\mathbf{e}_1) + \int_{x=L_1} ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot\mathbf{e}_1 \\ &\quad + \int_{y=-L_2} ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot(-\mathbf{e}_2) + \int_{y=L_2} ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot\mathbf{e}_2 \\ &\quad + \int_{z=0} ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot(-\mathbf{e}_3) + \int_{z=1} ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot\mathbf{e}_3.\end{aligned} \tag{3.27}$$

In order to deduce that each of the above lines in the previous equation are equal to zero we note that

$$\begin{aligned}((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot\mathbf{e}_1 &= \mathbf{v}_2\mathbf{v}_{1,2} + \mathbf{v}_3\mathbf{v}_{1,3} - \mathbf{v}_1\mathbf{v}_{2,2} - \mathbf{v}_1\mathbf{v}_{3,3} \\ ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot\mathbf{e}_2 &= \mathbf{v}_1\mathbf{v}_{2,1} + \mathbf{v}_3\mathbf{v}_{2,3} - \mathbf{v}_2\mathbf{v}_{1,1} - \mathbf{v}_2\mathbf{v}_{3,3} \\ ((\mathbf{v}\cdot\nabla)\mathbf{v} - (\nabla\cdot\mathbf{v})\mathbf{v})\cdot\mathbf{e}_3 &= \mathbf{v}_1\mathbf{v}_{3,1} + \mathbf{v}_2\mathbf{v}_{3,2} - \mathbf{v}_3\mathbf{v}_{1,1} - \mathbf{v}_3\mathbf{v}_{2,2}.\end{aligned} \tag{3.28}$$

The first two equalities in (3.28) show that the first two lines of (3.27) are indeed zero by utilising the set of equalities in (3.26). Finally we note that since $\mathbf{v}$ is prescribed and constant in the $z = 0, 1$ faces, we must have that

$$\left.\frac{\partial \mathbf{v}}{\partial x}\right|_{z=0} = \left.\frac{\partial \mathbf{v}}{\partial y}\right|_{z=0} = \left.\frac{\partial \mathbf{v}}{\partial x}\right|_{z=1} = \left.\frac{\partial \mathbf{v}}{\partial y}\right|_{z=1} = 0,$$

meaning that the final line in (3.27) is zero as both of the integrands are identically zero. So we have that

$$J(\mathbf{v}) = 0 \quad \forall\, \mathbf{v} \in \mathcal{B}.$$

So now if we take an arbitrary element $\mathbf{n} \in \mathcal{A}'$, the density of $\mathcal{B}$ implies that

$$\exists(\mathbf{v}^j) \subset \mathcal{B} \text{ such that } \|\mathbf{v}^j - \mathbf{n}\|_{1,2} \longrightarrow 0 \; as \; j \to \infty.$$

With this information it is clear when writing (3.25) in component form and using the fact that

$$f^j \to f \text{ in } L^2 \quad \text{and} \quad g^j \to g \text{ in } L^2 \quad \Rightarrow \quad f^j g^j \to fg \quad in \quad L^1,$$

we deduce the convergence of the integral values so that

$$0 = J(\mathbf{v}^j) \longrightarrow J(\mathbf{n}).$$

Therefore $J(\mathbf{n}) = 0$ for all $\mathbf{n} \in \mathcal{A}'$ and $\mathcal{A} \subset \mathcal{A}'$, so the statement is proved.

□

This brings our study of cholesterics within the classical Oseen-Frank framework to a close. We have proved that our one variable minimisers are the global minimisers for our canonical cholesteric problem so long as the cholesteric pitch is suitably long. The numerical data presented in Section 3.2.1 suggests that they are also strong local minimisers for shorter cholesteric pitches. However, both experimentally and analytically, we know that for shorter pitch lengths, structures such as cholesteric fingers and double twist cylinders are more favourable on a local level by utilising the saddle-splay energy. But we have just shown in Proposition 3.8 that our assumption of periodicity prevents any utilisation of the saddle-splay term. A possible reason for this is the fundamental problem, which we mentioned earlier, that the traditional Oseen-Frank model does not fully respect the head to tail symmetry of the molecules. This may be restricting the kinds of behaviour that it can predict. In the next chapter we prove that for the Oseen-Frank model to respect the symmetry, we must change the function space of the director $\mathbf{n}$. When we do so, we can prove the existence of multi-dimensional cholesteric patterns.

Chapter 4

Links between Continuum Theories

4.1 Introduction

In the study of the calculus of variations, modelling any physical problem has two basic aspects. The Lagrangian represents the mathematical model for the free energy density of the system being studied. The second aspect is the regularity of the mappings being considered: the function space. Even though this is well known, usually the majority of the focus is given over to the exact form of the Lagrangian, even though with a fixed Lagrangian choosing a different function space can give rise to a different minimum energy for the functional. This idea was first observed by Lavrentiev [55] and has since been known as the Lavrentiev phenomenon. We noted in the introduction that this has particular relevance in the study of liquid crystals because of the abudance of continuum theories. We recall the basics of three continuum theories in particular.

In the previous two chapters we studied liquid crystals using the oldest continuum theory based on the Oseen-Frank energy

$$I_O(\mathbf{n}) := \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \, dx,$$

where $\mathbf{n} : \Omega \to \mathbb{S}^2$. The liquid crystal molecules are rod-like, and this theory was developed on the supposition that the energy of the system can be modelled through the elastic strains of their principal axis $\mathbf{n}$. In the 1990s Ericksen proposed an extension of this theory with the addition of a scalar order parameter $s : \Omega \to \mathbb{R}$ to represent the degree of orientation of the molecules. The director represents an average local orientation, and the scalar order parameter represents the local variance from this mean. In this setting the free energy has the form [92]

$$I_E(\mathbf{n}, s) = \int_\Omega 2s^2 \left(|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \right) + \frac{2}{3} |\nabla s|^2 + \sigma(s) \, dx,$$

where $\sigma(s) := \frac{a}{2}s^2 + \frac{b}{3}s^3 + \frac{c}{4}s^4$. The function σ is the bulk energy which represents the competition between the isotropic and ordered phases. The function must be bounded below, so that $c > 0$. Furthermore, well below the nematic-isotropic transition temperature, $s = 0$ should not be a local minimum of σ, hence $a < 0$. A third approach comes in the form of the Landau-de Gennes theory. Their idea was to use a matrix order parameter $\mathbf{Q} : \Omega \to \mathbb{R}^{3\times3}$

which is traceless and symmetric. We will use a specific formulation of their proposed free energy (see for example [2, 52])

$$I_L(\mathbf{Q}) = \int_\Omega |\nabla \mathbf{Q}|^2 + 4t\mathbf{Q} \cdot \nabla \times \mathbf{Q} + 3t^2|\mathbf{Q}|^2 + \psi_B(\mathbf{Q})\, dx, \tag{4.1}$$

where $(\nabla \times \mathbf{Q})_{ij} = \sum_{a,b} \epsilon_{jab} \mathbf{Q}_{ib,a}$ and $\psi_B(\mathbf{Q}) := \frac{\overline{a}}{2}\mathrm{Tr}\left(\mathbf{Q}^2\right) + \frac{\overline{b}}{3}\mathrm{Tr}\left(\mathbf{Q}^3\right) + \frac{\overline{c}}{4}\left(\mathrm{Tr}\left(\mathbf{Q}^2\right)\right)^2$. Physical constraints ensure that $\overline{c} > 0$ and $\overline{a} < 0$ well below the transition temperature for the same reasons as in Ericksen's theory. If in addition we impose the condition that two of the three eigenvalues of $\mathbf{Q}$ must be equal, then we reduce (4.1) to the case of uniaxial states. With this restriction, $\mathbf{Q}$ can be written as

$$\mathbf{Q} := s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I\right), \tag{4.2}$$

for some $s \in \mathbb{R}$, and $\mathbf{n} \in \mathbb{S}^2$. Through a simple calculation, if we substitute (4.2) into the bulk energy ψ_B we get exactly the Ericksen bulk energy provided that

$$\overline{a} = \frac{3a}{2},\ \overline{b} = \frac{9b}{2},\ \overline{c} = \frac{9c}{4}. \tag{4.3}$$

Throughout this chapter we will be assuming that (4.3) holds. An immediate advantage of using a matrix order parameter is that the symmetry issues of the molecules do not arise because line fields of the form $\mathbf{n} \otimes \mathbf{n}$ are used. Our goal in this chapter is to try and bring this advantage over to a director based theory to determine whether the predictions of the classical Oseen-Frank theory are restricted by not respecting this symmetry. By writing the matrix order parameter $\mathbf{Q}$ in the uniaxial form we clearly see that it is highly plausible that there will be some relationship between these three continuum theories. Here we precisely determine some of these links by considering different choices of function spaces for the variables $s, \mathbf{n}$, and $\mathbf{Q}$. This idea has received some attention in recent years. In papers by Majumdar, Zarnescu, and Nguyen [63, 75], minimisers of the Landau-de Gennes free energy were shown to converge to minimisers of the Oseen-Frank free energy in the vanishing elastic constant limit. This limit essentially forces the matrix order parameter to become uniaxial in order to minimise the dominant bulk energy term. We will consider a similar limit at the end of this chapter which we can use to justify an Oseen-Frank model using director fields which are special functions of bounded variation.

The main technical issue which needs to be considered for our results is finding a unit vector field $\mathbf{m}$ which corresponds to a given line field $\mathbf{n} \otimes \mathbf{n}$. This lifting question in Sobolev and BV spaces has been studied in its own right in a number of papers [16, 28]. We will prove four lifting results, Propositions 4.8, 4.14, 4.19 and 4.20. The different results are needed because the problem can be very different depending on the ambient dimension and the domain topology. Propositions 4.19 and 4.20 in particular illustrate the fact that the vector field cannot always retain the same regularity as the line field. However, unlike in other studies, we will use these results as a vehicle to prove the connections between the Landau-de Gennes theory

and Ericksen's theory. For reasons which will become clearer later in the chapter, we will also define the following free energy which we will term the biaxial Ericksen free energy

$$\begin{aligned} I_{BE}(\mathbf{n},\mathbf{m},s_1,s_2) = \int_\Omega & 2s_1^2\left(|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2\right) + 2s_2^2\left(|\nabla\mathbf{m}|^2 + 2t\mathbf{m}\cdot\nabla\times\mathbf{m} + t^2\right) \\ & - 2s_1s_2\left(|\mathbf{m}^T\nabla\mathbf{n} - t\mathbf{n}\times\mathbf{m}|^2 + |\mathbf{n}^T\nabla\mathbf{m} - t\mathbf{m}\times\mathbf{n}|^2 - t^2\right) \\ & + \frac{|\nabla(s_1-s_2)|^2}{3} + \frac{1}{3}\left(|\nabla s_1|^2 + |\nabla s_2|^2\right) + \sigma(s_1,s_2)\,dx, \end{aligned} \tag{4.4}$$

where $s_1 \geqslant 0$, $s_2 \leqslant 0$, $\mathbf{n},\mathbf{m} \in \mathbb{S}^2$, and $\mathbf{n}\cdot\mathbf{m} = 0$. In this chapter we will begin to seriously consider functions of bounded variation and we remind the reader that their basic definitions and properties were outlined in the introduction (or refer to [5]). However the space of admissible functions that we will require is a slightly smaller space than SBV. Therefore if $\Omega \subset \mathbb{R}^d$ is an open set, we define

$$SBV^2\left(\Omega,\mathbb{R}^k\right) := \left\{ \mathbf{n} \in SBV\left(\Omega,\mathbb{R}^k\right) \,\middle|\, \nabla\mathbf{n} \in L^2\left(\Omega,\mathbb{R}^{k\times d}\right),\ \mathcal{H}^{d-1}\left(S_{\mathbf{n}}\right) < \infty \right\}.$$

4.2 Preliminary Lemmas

In order to prove the main results of this chapter we require a number of relatively simple preliminary lemmas. Therefore we prove them in this section in isolation, then we will apply them when appropriate in the subsequent theorems. Lemmas 4.3, 4.4, and 4.5 concern specific facts about Sobolev spaces and Lemmas 4.6 and 4.7 are central to deriving the appropriate function space for the scalar order parameters. It should be noted that when we are dealing with Sobolev functions we always assume that we have chosen the precise representative amongst the equivalence class of functions equal almost everywhere. Using this precise representative [35, Section 4.8] it is important to define a little notation that we will be using in this chapter. If $f \in W^{1,p}(\Omega)$ then we define

$$C_f := \bigcap_{\epsilon>0} \overline{\{|f| \leqslant \epsilon\}}.$$

This might just seem like an unnecessarily complicated method of defining the set where f vanishes. However this is not true in general. If f is continuous then $C_f = \{f = 0\}$, but the converse is false. Clearly C_f is closed and contains $\{f = 0\}$, therefore

$$\overline{\{f = 0\}} \subset C_f.$$

In this chapter we will need to use two different characterisations of Sobolev spaces. The first is the absolute continuity on lines (see for example [35, Section 4.9.2]) and the second is the difference quotient characterisation [57, Thm 10.55].

Theorem 4.1 (Absolute continuity)**.** *Let $p \in [1,\infty)$ and $\Omega \subset \mathbb{R}^d$ be an open set. If $f \in W^{1,p}(\Omega)$ (and is the precise representative) then for each $k = 1,\dots,d$*

$$f_k^*(x_0,t) = f(\dots,x_{k-1},t,x_{k+1},\dots)$$

is absolutely continuous in t for $\mathcal{L}^{d-1}$ *almost every* $x_0 = (x_1, \dots, x_{k-1}, x_{k+1}, \dots, x_d) \in \mathbb{R}^{d-1}$. *Additionally* $\left(f_k^*\right)' \in L^p(\Omega)$.

Conversely, if $f \in L^p(\Omega)$ *and* $f = g$ *almost everywhere, where for each* $k = 1, \dots, d$, *the functions*

$$g_k(x_0, t) = g(\dots, x_{k-1}, t, x_{k+1}, \dots)$$

are absolutely continuous in t for $\mathcal{L}^{d-1}$ *almost every* $x_0 \in \mathbb{R}^{d-1}$ *and* $g_k' \in L^p(\Omega)$. *Then* $f \in W^{1,p}(\Omega)$.

Proposition 4.2 (Difference quotient)**.** *Let* $p \in [1, \infty)$ *and* $\Omega \subset \mathbb{R}^d$ *be an open set and* $u \in L^p(\Omega)$. *Then*

$$u \in W^{1,p}(\Omega) \iff \forall\, i = 1, \dots, d\ \exists K > 0 \text{ such that } \forall\, \Omega' \subset\subset \Omega \text{ and } |h| \leqslant \operatorname{dist}(\Omega', \partial\Omega) \text{ we have } \|u(\cdot + h\mathbf{e}_i) - u(\cdot)\|_{p,\Omega'} \leqslant K$$

Lemma 4.3. *Let* $p \in [1, \infty)$ *and* $\Omega \subset \mathbb{R}^d$ *be an open and bounded set. Suppose* $f \in W^{1,p}(\Omega)$, *and* $g : \Omega \to \mathbb{R}$ *are maps such that*

$$|f(x)| \geqslant \delta > 0\ \mathcal{H}^{d-1}\ a.e.\ x \in \Omega, \quad fg \in W^{1,p}(\Omega) \quad \text{and} \quad |g(x)| \leqslant C\ a.e.\ x \in \Omega.$$

Then $g \in W^{1,p}(\Omega)$.

Proof

In the spirit of using Theorem 4.1, we take some $x_0 \in \mathbb{R}^{d-1}$. Then by our assumptions, without loss of generality we can assume that f and fg are absolutely continuous on the set

$$U_{x_0} := \{\, (t, x_0) \in \Omega \,|\, t \in \mathbb{R} \,\}.$$

and $|f(x)| \geqslant \delta$ on U_{x_0}. Hence we can use the standard facts that the reciprocal of a non-zero absolutely continuous function and the product of two absolutely continuous functions are still absolutely continuous to deduce that

$$g_1(t, x_0) := \frac{(fg)(t, x_0)}{f(t, x_0)}$$

is absolutely continuous on U_{x_0}. Furthermore

$$\frac{d}{dt} g_1(t, x_0) = \frac{\frac{\partial}{\partial x_1}(fg)(x)}{f(x)} - \frac{g(x)\frac{\partial}{\partial x_1} f(x)}{f(x)}. \tag{4.5}$$

Our assumptions imply that $\frac{1}{f}, g \in L^\infty(\Omega)$ and $\nabla f, \nabla(fg) \in L^p(\Omega)$. Hence from (4.5) we deduce

$$g_1' \in L^p(\Omega).$$

This logic applies for all line segments parallel to the coordinate axes, hence by Theorem 4.1 $g \in W^{1,p}(\Omega)$.

□

Lemma 4.4. *Let $p \in [1, \infty)$ and $\Omega \subset \mathbb{R}^d$ be an open set. Suppose that $f \in W^{1,p}(\Omega)$, and $g : \Omega \setminus C_f \to \mathbb{R}$ are maps such that $fg \in W^{1,p}(\Omega)$ and $|g(x)| \leqslant D$ for almost every $x \in \Omega \setminus C_f$. Then*

$$g \in W^{1,p}_{loc}\left(\Omega \setminus C_f\right).$$

Proof

We take some $U \subset\subset \Omega \setminus C_f$ and we just need to show that $|f(x)|$ is bounded below away from zero on U in order to apply Lemma 4.3. This is where the importance of the definition of C_f becomes clear. We can use it to deduce that

$$\inf_{x \in \overline{U}} |f(x)| > 0. \tag{4.6}$$

If this were not the case then $\overline{U} \cap \{|f| \leqslant \epsilon\}$ is non-empty for all $\epsilon > 0$. Then $V_\epsilon := \overline{U} \cap \overline{\{|f| \leqslant \epsilon\}}$ is a nested sequence of non-empty closed sets. Thus its intersection contains a point. This contradicts $U \subset\subset \Omega \setminus C_f$. Once we know that (4.6) holds we can simply apply Lemma 4.3 to find that

$$g \in W^{1,p}(U) \Longrightarrow g \in W^{1,p}_{loc}\left(\Omega \setminus C_f\right).$$

□

Lemma 4.5. *Let $p \in [1, \infty)$ and $\Omega \subset \mathbb{R}^d$ be an open set. Suppose that $f, g : \Omega \to \mathbb{R}$ are two maps such that $f \in W^{1,p}(\Omega) \cap C(\Omega)$,*

$$g \in W^{1,p}_{loc}(\Omega \setminus \{f = 0\}) \cap L^\infty(\Omega \setminus \{f = 0\}) \text{ and } fg \in W^{1,p}(\Omega \setminus \{f = 0\}).$$

Then $fg \in W^{1,p}(\Omega)$.

Proof

For ease of notation we let $\Omega' := \Omega \setminus \{f = 0\}$. If we let $h : \Omega \to \mathbb{R}$ be defined by

$$h(x) := \begin{cases} f(x)g(x) & \text{if } x \in \Omega' \\ 0 & \text{otherwise} \end{cases},$$

then clearly we have $h, \nabla h \in L^p(\Omega)$, where

$$\nabla h := \begin{cases} \nabla(fg)(x) & \text{if } x \in \Omega' \\ 0 & \text{otherwise} \end{cases}.$$

Therefore we just need to show that the integration by parts formula holds in order to deduce the result. To that end, we take a $\psi \in C^\infty_0(\Omega)$ and we need to show that

$$\int_{\Omega'} f(x)g(x)\frac{\partial \psi}{\partial x_j}(x)\,dx = -\int_{\Omega'} \frac{\partial}{\partial x_j}\left[f(x)g(x)\right]\psi(x)\,dx. \tag{4.7}$$

We know that Sobolev functions are absolutely continuous on almost every line segment parallel to the coordinate axes (Theorem 4.1). Therefore fg is absolutely continuous on $\Omega'_{y_0} := \Omega' \cap \{(x, y_0) \,|\, x \in \mathbb{R}\}$ for almost every $y_0 \in \mathbb{R}^{d-1}$. Then by splitting up Ω'_{y_0} into its

connected components U_i, which will be open 1-dimensional intervals of the form (a_i, b_i), we see that

$$\begin{aligned}\int_{\Omega'_{y_0}} (fg)\,\psi_{,j}\,dx &= \sum_i \int_{U_i} (fg)\,\psi_{,j}\,dx \\ &= -\int_{\Omega'_{y=0}} (fg)_{,j}\,\psi\,dx + \sum_i \left[fg\psi(b_i, y_0) - fg\psi(a_i, y_0)\right].\end{aligned} \tag{4.8}$$

Here we have two possibilities. If $(a_i, y_0) \in \partial\Omega$ then $\psi(a_i, y_0) = 0$ since $\psi \in C_0^\infty(\Omega)$. Alternatively if $(a_i, y_0) \in \partial\{f = 0\}$ then $f(a_i, y_0) = 0$. Therefore in either case we see that each element of the sum in (4.8) must be zero. Hence

$$\int_{\Omega'_{y_0}} (fg)\,\psi_{,j}\,dx = -\int_{\Omega'_{y=0}} (fg)_{,j}\,\psi\,dx,$$

for almost every $y_0 \in \mathbb{R}^{d-1}$, so that by performing the remaining $d-1$ integrations we immediately find (4.7). Therefore we have shown

$$\int_\Omega h\psi_{,j}\,dx = -\int_\Omega h_{,j}\psi\,dx \quad \forall\psi \in C_0^\infty(\Omega),\ \ j = 1, \ldots, n.$$

Hence $h \in W^{1,p}(\Omega)$ and $h = fg\ \mathcal{L}^n$ almost everywhere which gives us our conclusion.

□

Lemma 4.6. *Using the Frobenius matrix norm $|A|^2 = \sum_{i,j} a_{ij}^2$, we have the following inequality.*

$$\left| s_1 \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} Id \right) - s_2 \left(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3} Id \right) \right|^2 \geqslant \frac{1}{6} |s_1 - s_2|^2 \tag{4.9}$$

for any $s_1, s_2 \in \mathbb{R}$ and $\mathbf{n}, \mathbf{m} \in \mathbb{S}^2$.

Proof

The proof is simply by direct calculation. When we multiply out the left-hand side of (4.9) we obtain

$$\begin{aligned} LHS &= \sum_{i,j} s_1^2 \left(\mathbf{n}_i\mathbf{n}_j - \frac{1}{3}\delta_{ij} \right)\left(\mathbf{n}_i\mathbf{n}_j - \frac{1}{3}\delta_{ij} \right) + s_2^2 \left(\mathbf{m}_i\mathbf{m}_j - \frac{1}{3}\delta_{ij} \right)\left(\mathbf{m}_i\mathbf{m}_j - \frac{1}{3}\delta_{ij} \right) \\ &\quad - \sum_{i,j} 2s_1 s_2 \left(\mathbf{n}_i\mathbf{n}_j - \frac{1}{3}\delta_{ij} \right)\left(\mathbf{m}_i\mathbf{m}_j - \frac{1}{3}\delta_{ij} \right) \\ &= \frac{2}{3}\left(s_1^2 + s_2^2 \right) - 2s_1 s_2 \left((\mathbf{n} \cdot \mathbf{m})^2 - \frac{1}{3} \right). \end{aligned}$$

Now we split the proof into the two cases of $s_1 s_2 \geqslant 0$ and $s_1 s_2 < 0$ and show that we have the result in either situation. If we are in the first case then

$$LHS \geqslant \frac{2}{3}\left(s_1^2 + s_2^2 \right) - \frac{4s_1 s_2}{3} = \frac{2}{3}(s_1 - s_2)^2 \geqslant \frac{1}{6}(s_1 - s_2)^2.$$

In the second case we have

$$\begin{aligned} LHS &\geqslant \frac{2}{3}\left(s_1^2+s_2^2\right)+\frac{2s_1s_2}{3} \\ &= \frac{2}{3}\left(s_1^2+s_2^2\right)+\frac{2s_1s_2}{3}-\frac{1}{6}(s_1-s_2)^2+\frac{1}{6}(s_1-s_2)^2 \\ &= \frac{1}{2}(s_1+s_2)^2+\frac{1}{6}(s_1-s_2)^2 \\ &\geqslant \frac{1}{6}(s_1-s_2)^2 . \end{aligned}$$

□

Lemma 4.7. *Suppose that*

$$\begin{aligned} \mathbf{Q}_1 &= s_1\left(\mathbf{n}_1\otimes\mathbf{n}_1-\frac{1}{3}I\right)+s_2\left(\mathbf{n}_2\otimes\mathbf{n}_2-\frac{1}{3}I\right) \\ \mathbf{Q}_2 &= t_1\left(\mathbf{m}_1\otimes\mathbf{m}_1-\frac{1}{3}I\right)+t_2\left(\mathbf{m}_2\otimes\mathbf{m}_2-\frac{1}{3}I\right) \end{aligned}$$

for $s_1, t_1 \geqslant 0$, $s_2, t_2 \leqslant 0$ *and* $\mathbf{n}_1, \mathbf{n}_2, \mathbf{m}_1, \mathbf{m}_2 \in \mathbb{S}^2$ *where* $\mathbf{n}_1\cdot\mathbf{n}_2 = \mathbf{m}_1\cdot\mathbf{m}_2 = 0$. *Then*

$$\begin{aligned} |\mathbf{Q}_1-\mathbf{Q}_2|^2 \geqslant & \frac{1}{6}\left[(s_1-t_1)^2+(s_2-t_2)^2\right] \\ & +\frac{1}{6}\left[|s_1\mathbf{n}_1\otimes\mathbf{n}_1-t_1\mathbf{m}_1\otimes\mathbf{m}_1|^2+|s_2\mathbf{n}_2\otimes\mathbf{n}_2-t_2\mathbf{m}_2\otimes\mathbf{m}_2|^2\right]. \end{aligned} \tag{4.10}$$

Proof

As in the previous lemma, (4.10) is understood using the Frobenius matrix norm $|A|^2 = \sum_{i,j} a_{ij}^2$. We multiply out the left hand side of (4.10) to find

$$\begin{aligned} |\mathbf{Q}_1-\mathbf{Q}_2|^2 &= \sum_{i,j}\Bigg[s_1\left(\mathbf{n}_{1i}\mathbf{n}_{1j}-\frac{1}{3}\delta_{ij}\right)+s_2\left(\mathbf{n}_{2i}\mathbf{n}_{2j}-\frac{1}{3}\delta_{ij}\right) \\ &\qquad -t_1\left(\mathbf{m}_{1i}\mathbf{m}_{1j}-\frac{1}{3}\delta_{ij}\right)-t_2\left(\mathbf{m}_{2i}\mathbf{m}_{2j}-\frac{1}{3}\delta_{ij}\right)\Bigg]^2 \\ &= \frac{2}{3}\left(s_1^2+s_2^2+t_1^2+t_2^2\right)-\frac{2}{3}(s_1s_2+t_1t_2)-2\sum_{i,j=1}^{2}s_it_j\left((\mathbf{n}_i\cdot\mathbf{m}_j)^2-\frac{1}{3}\right). \end{aligned}$$

However we know that $s_1t_2, s_2t_1 \leqslant 0$ and for any two unit vectors $\mathbf{n}$ and $\mathbf{m}$, $|\mathbf{n}\otimes\mathbf{n}-\mathbf{m}\otimes\mathbf{m}|^2 = 2-2(\mathbf{n}\cdot\mathbf{m})^2$. These two facts allow us to estimate the above expression and complete the

assertion with the following calculation

$$
\begin{aligned}
&|\mathbf{Q}_1 - \mathbf{Q}_2|^2 \\
&\geqslant \frac{2}{3}\left(s_1^2 + s_2^2 + t_1^2 + t_2^2 - s_1 s_2 - t_1 t_2\right) + \frac{2}{3}\left(s_1 t_2 + s_2 t_1\right) \\
&\quad - 2 s_1 t_1 \left((\mathbf{n}_1 \cdot \mathbf{m}_1)^2 - \frac{1}{3}\right) - 2 s_2 t_2 \left((\mathbf{n}_2 \cdot \mathbf{m}_2)^2 - \frac{1}{3}\right) \\
&= \frac{2}{3}\left(s_1^2 + s_2^2 + t_1^2 + t_2^2 - s_1 s_2 - t_1 t_2 + s_1 t_2 + s_2 t_1 - 2 s_1 t_1 - 2 s_2 t_2\right) \\
&\quad + s_1 t_1 \left|\mathbf{n}_1 \otimes \mathbf{n}_1 - \mathbf{m}_1 \otimes \mathbf{m}_1\right|^2 + s_2 t_2 |\mathbf{n}_2 \otimes \mathbf{n}_2 - \mathbf{m}_2 \otimes \mathbf{m}_2|^2 \\
&= \frac{1}{6}\left[(s_1 - t_1)^2 + (s_2 - t_2)^2 + |s_1 \mathbf{n}_1 \otimes \mathbf{n}_1 - t_1 \mathbf{m}_1 \otimes \mathbf{m}_1|^2 + |s_2 \mathbf{n}_2 \otimes \mathbf{n}_2 - t_2 \mathbf{m}_2 \otimes \mathbf{m}_2|^2\right] \\
&\quad + \frac{5}{6}\left[s_1 t_1 \left|\mathbf{n}_1 \otimes \mathbf{n}_1 - \mathbf{m}_1 \otimes \mathbf{m}_1\right|^2 + s_2 t_2 |\mathbf{n}_2 \otimes \mathbf{n}_2 - \mathbf{m}_2 \otimes \mathbf{m}_2|^2\right] + \frac{1}{3}(s_1 - s_2 - t_1 + t_2)^2 \\
&\geqslant \frac{1}{6}\left[(s_1 - t_1)^2 + (s_2 - t_2)^2 + |s_1 \mathbf{n}_1 \otimes \mathbf{n}_1 - t_1 \mathbf{m}_1 \otimes \mathbf{m}_1|^2 + |s_2 \mathbf{n}_2 \otimes \mathbf{n}_2 - t_2 \mathbf{m}_2 \otimes \mathbf{m}_2|^2\right].
\end{aligned}
$$

□

4.3 One-dimensional Results

We begin the main portion of the chapter with the first of our results about the lifting of line fields to vector fields. As the following proposition makes clear, in one-dimensional Sobolev spaces we can find a vector field lifting with the same regularity as the original line field.

Proposition 4.8. *Suppose that $\Omega \subset \mathbb{R}$ is a bounded domain and that $p \in [1, \infty)$. If*

$$\mathbf{n} \otimes \mathbf{n} \in W^{1,p}_{loc}\left(\Omega, \mathbb{R}^{3\times 3}\right)$$

where $|\mathbf{n}| = 1$ then there exists some

$$\mathbf{m} \in W^{1,p}_{loc}\left(\Omega, \mathbb{S}^2\right)$$

such that $\mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n}$ on Ω.

Proof

Through the Sobolev embedding theorem our assumptions imply

$$\mathbf{n} \otimes \mathbf{n} \in C\left(\overline{U}, \mathbb{R}^{3\times 3}\right)$$

for any open set $U \subset\subset \Omega$. This certainly implies that $\mathbf{n} \otimes \mathbf{n} \in C\left(\Omega, \mathbb{R}^{3\times 3}\right)$. If we take any $x \in \Omega$, it is contained in some $U \subset\subset \Omega$, then we choose $\mathbf{m}(x)$ to be one of the two possible unit vectors to ensure that $\mathbf{m}(x) \otimes \mathbf{m}(x) = \mathbf{n} \otimes \mathbf{n}(x)$. The uniform continuity of $\mathbf{n} \otimes \mathbf{n}$ on $\overline{U}$ then ensures that this one choice at x defines a mapping $\mathbf{m} \in C\left(\overline{U}, \mathbb{S}^2\right)$. Hence

$$\mathbf{m} \in C\left(\Omega, \mathbb{S}^2\right).$$

To prove its differentiability, we note that for $h > 0$ we have the relation

$$\begin{aligned}&\left[\frac{\mathbf{m}_i(x+h)\mathbf{m}_j(x+h) - \mathbf{m}_i(x)\mathbf{m}_j(x)}{h}\right]\left[\frac{\mathbf{m}_j(x+h) + \mathbf{m}_j(x)}{2}\right]\\ =&\frac{\mathbf{m}_i(x+h)}{2}\left[\frac{\mathbf{m}_j(x+h)^2 - \mathbf{m}_j(x)^2}{h}\right] + \mathbf{m}_j(x)\left[\frac{\mathbf{m}_i(x+h) - \mathbf{m}_i(x)}{h}\right]\left[\frac{\mathbf{m}_j(x+h) + \mathbf{m}_j(x)}{2}\right].\end{aligned}$$

If we sum this expression over j and take the limit as $h \to 0$, we find

$$\lim_{h\to 0}\frac{\mathbf{m}_i(x+h) - \mathbf{m}_i(x)}{h} = \sum_j (\mathbf{m}_i\mathbf{m}_j)'(x)\mathbf{m}_j(x) = \sum_j (\mathbf{n}_i\mathbf{n}_j)'(x)\mathbf{m}_j(x).$$

Therefore the derivative of $\mathbf{m}_i$ exists almost everywhere and is equal to $\sum_j (\mathbf{n}_i\mathbf{n}_j)'(x)\mathbf{m}_j(x) \in L^p_{loc}(\Omega)$, which implies

$$\mathbf{m} \in W^{1,p}_{loc}\left(\Omega, \mathbb{S}^2\right).$$

□

Corollary 4.9. *Suppose $\Omega \subset \mathbb{R}$ is a bounded domain and that $p \in [1, \infty)$. If $\mathbf{n} \otimes \mathbf{n} \in W^{1,p}\left(\Omega, \mathbb{R}^{3\times 3}\right)$ where $|\mathbf{n}| = 1$, then there exists some $\mathbf{m} \in W^{1,p}\left(\Omega, \mathbb{S}^2\right)$ such that $\mathbf{m}\otimes\mathbf{m} = \mathbf{n}\otimes\mathbf{n}$.*

This corollary immediately follows from the proof of Proposition 4.8. This lifting result together with the lemmas from Section 4.2 mean we can now move ahead and prove our two equivalence results in one dimension. However we must first define our notion of equivalence between minimisation problems.

Definition 4.10. *We say that the problem of minimising the integral functional $I(\mathbf{n})$ over the set of admissible functions $\mathcal{A}$ is equivalent to minimising the integral functional $J(\mathbf{m})$ over the set of admissible functions $\mathcal{B}$ if and only if there is a bijective map $p : \mathcal{A} \to \mathcal{B}$ such that $I(\mathbf{n}) = J(p(\mathbf{n}))$ for every $\mathbf{n} \in \mathcal{A}$.*

4.3.1 Uniaxial Landau-de Gennes

Theorem 4.11. *Suppose $\Omega \subset \mathbb{R}$ is a bounded domain. Then minimising $I_L(\mathbf{Q})$ over*

$$\mathcal{A} := \left\{ \mathbf{Q} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right) \,\middle|\, \mathbf{Q} = \mathbf{Q}^T,\ \operatorname{Tr}\mathbf{Q} = 0,\ \mathbf{Q}\ \textit{uniaxial} \right\},$$

is equivalent to minimising $I_E(\mathbf{n}, s)$ over

$$\mathcal{B} := \left\{ s \in W^{1,2}(\Omega),\ \mathbf{n} \in W^{1,2}_{loc}\left(\Omega \setminus \{s = 0\}, \mathbb{S}^2\right) \,\middle|\, \int_\Omega s^2|\nabla\mathbf{n}|^2\, dx < \infty \right\}.$$

Proof

The main idea of the proof, as with each of the subsequent equivalence results, is to show a one-to-one correspondence between the sets of admissible functions. A quick formal calculation can then show that the two Lagrangians are in fact equal so that the minimisation

problems are equivalent in the sense of Definition 4.10. We begin by taking some $\mathbf{Q} \in \mathcal{A}$. Then we know that this matrix has the form

$$\mathbf{Q}(x) = s(x)\left(\mathbf{n} \otimes \mathbf{n}(x) - \frac{1}{3}I\right) \tag{4.11}$$

for some $|\mathbf{n}| = 1$. We apply Lemma 4.6 to deduce that

$$|\mathbf{Q}(x) - \mathbf{Q}(y)|^2 \geqslant \frac{1}{6}|s(x) - s(y)|^2, \tag{4.12}$$

for any $x, y \in \Omega$. This immediately implies that $s \in L^2(\Omega)$ and to show it is in the required Sobolev space we use the difference quotient characterisation of $W^{1,2}$. Equation (4.12) implies

$$\|\mathbf{Q}(\cdot + h) - \mathbf{Q}(\cdot)\|_{2,U} \geqslant 6^{-\frac{1}{2}}\|s(\cdot + h) - s(\cdot)\|_{2,U} \tag{4.13}$$

for any $U \subset\subset \Omega$ and $|h| \leqslant d(U, \partial\Omega)$. Therefore by Proposition 4.2 we infer that $s \in W^{1,2}(\Omega)$. Coupling this fact with (4.11) directly implies that $s\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$. If we take any $U \subset\subset \Omega \setminus \{s = 0\}$ then by the continuity of s, it is clear that

$$\inf_{x\in U} |s(x)| > 0.$$

This means that we can apply Lemma 4.3 to $s\mathbf{n} \otimes \mathbf{n}$ and deduce

$$\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(U, \mathbb{R}^{3\times 3}\right).$$

Therefore $\mathbf{n} \otimes \mathbf{n} \in W^{1,2}_{loc}\left(\Omega \setminus \{s = 0\}, \mathbb{R}^{3\times 3}\right)$. Now we can apply our lifting result, Proposition 4.8, to find the vector field corresponding to $\mathbf{n} \otimes \mathbf{n}$. There exists some

$$\mathbf{m} \in W^{1,2}_{loc}\left(\Omega \setminus \{s = 0\}, \mathbb{S}^2\right)$$

such that $\mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n}$ almost everywhere. To show the joint regularity we note that $s(\mathbf{n} \otimes \mathbf{n}) = s(\mathbf{m} \otimes \mathbf{m}) \in W^{1,2}(\Omega, \mathbb{R}^{3\times 3})$, hence

$$\int_\Omega |\nabla [s(\mathbf{m} \otimes \mathbf{m})]|^2 \, dx = \int_\Omega 2s^2|\nabla \mathbf{m}|^2 + |\nabla s|^2 \, dx < \infty. \tag{4.14}$$

This concludes the first inclusion; we took some $\mathbf{Q} \in \mathcal{A}$ and found a pair $(s, \mathbf{m}) \in \mathcal{B}$ such that $\mathbf{Q} = s\left(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3}I\right)$ almost everywhere. The reverse inclusion is a little more straightforward, we take some $(s, \mathbf{n}) \in \mathcal{B}$ and we just need to show that $s\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$. Since $W^{1,2}_{loc} \cap L^\infty$ is an algebra of functions, it is closed under products, so that

$$\mathbf{n} \otimes \mathbf{n} \in W^{1,2}_{loc}\left(\Omega \setminus \{s = 0\}, \mathbb{R}^{3\times 3}\right). \tag{4.15}$$

Using the joint regularity assumption we know that for any open set $U \subset\subset \Omega \setminus \{s = 0\}$

$$\int_U |\nabla(s\mathbf{n} \otimes \mathbf{n})|^2 \, dx = \int_U 2s^2|\nabla \mathbf{n}|^2 + |\nabla s|^2 \, dx \leqslant \int_\Omega 2s^2|\nabla \mathbf{n}|^2 + |\nabla s|^2 \, dx < \infty. \tag{4.16}$$

As the upper bound in (4.16) is independent of U, the above equation clearly demonstrates that $s\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(\Omega \setminus \{s = 0\}, \mathbb{R}^{3\times 3}\right)$. Finally we apply Lemma 4.5 to deduce $s\mathbf{n} \otimes \mathbf{n} \in$

$W^{1,2}\left(\Omega, \mathbb{R}^{3\times3}\right)$. This establishes the bijective correspondence between $\mathcal{A}$ and $\mathcal{B}$. For the formal equivalence of the Lagrangians we just need to take some $\mathbf{Q} \in \mathcal{A}$ and compute its Lagrangian in terms of s and $\mathbf{n}$.

$$
\begin{aligned}
&= |\nabla \mathbf{Q}|^2 + 4t\mathbf{Q} \cdot \nabla \times \mathbf{Q} + 3t^2|\mathbf{Q}|^2 \\
&= \sum_{i,j,k} \left(s_{,k} \left(\mathbf{n}_i \mathbf{n}_j - \frac{1}{3}\delta_{ij} \right) + s\left(\mathbf{n}_{i,k}\mathbf{n}_j + \mathbf{n}_i \mathbf{n}_{j,k} \right) \right)^2 \\
&+ 4t \sum_{i,j,a,b} \epsilon_{jab} s \left(\mathbf{n}_i \mathbf{n}_j - \frac{1}{3}\delta_{ij} \right) \left[s_{,a} \left(\mathbf{n}_i \mathbf{n}_b - \frac{1}{3}\delta_{ib} \right) + s\left(\mathbf{n}_{i,b}\mathbf{n}_j + \mathbf{n}_i \mathbf{n}_{j,b} \right) \right] \\
&+ 2t^2 \sum_{i,j} s^2 \left(\mathbf{n}_i \mathbf{n}_j - \frac{1}{3}\delta_{ij} \right)^2 \\
&= 2s^2 \left(|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2 \right) + \frac{2}{3}|\nabla s|^2.
\end{aligned}
$$

Therefore if we have some $\mathbf{Q} \in \mathcal{A}$ we have the relation that $I_L(\mathbf{Q}) = I_E(\mathbf{n}, s)$ if $(\mathbf{n}, s)$ is the pair of functions in $\mathcal{B}$ associated with $\mathbf{Q}$. Therefore any $\mathbf{Q} \in \mathcal{A}$ which minimises I_L will yield a pair $(\mathbf{n}, s) \in \mathcal{B}$ which minimises I_E and vice versa.

□

4.3.2 Biaxial Landau-de Gennes

Theorem 4.12. *Suppose $\Omega \subset \mathbb{R}$ is a bounded domain. Then minimising $I_L(\mathbf{Q})$ over*

$$
\mathcal{A} := \left\{ \mathbf{Q} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times3}\right) \,\middle|\, \mathbf{Q}^T = \mathbf{Q},\ \operatorname{Tr}\mathbf{Q} = 0 \right\}
$$

is equivalent to minimising $I_{BE}(\mathbf{n}, \mathbf{m}, s_1, s_2)$ over

$$
\mathcal{B} := \left\{ \begin{array}{c} s_1, -s_2 \in W^{1,2}\left(\Omega, [0,\infty)\right), \\ \mathbf{n} \in W^{1,2}_{loc}\left(\Omega \setminus \{s_1 = 0\}, \mathbb{S}^2\right), \\ \mathbf{m} \in W^{1,2}_{loc}\left(\Omega \setminus \{s_2 = 0\}, \mathbb{S}^2\right) \end{array} \,\middle|\, \begin{array}{c} \int_\Omega s_1|\nabla \mathbf{n}|^2 + s_2|\nabla \mathbf{m}|^2\, dx < \infty, \\ \mathbf{n} \cdot \mathbf{m} = 0 \end{array} \right\}.
$$

Proof

The basic form of this proof follows that of the previous theorem but using more general biaxial forms. We take some $\mathbf{Q} \in \mathcal{A}$. Then we know that we can write

$$
\mathbf{Q} = \sum_1^3 \lambda_i \mathbf{v}_i \otimes \mathbf{v}_i,
$$

where $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3$ are the eigenvalues and $\mathbf{v}_i$ are the eigenvectors of $\mathbf{Q}$. Using the relations $\sum_1^3 \lambda_i = 0$ and $\sum_1^3 \mathbf{v}_i \otimes \mathbf{v}_i = Id$ we can eliminate λ_2 and $\mathbf{v}_2$ to find

$$
\mathbf{Q} = s_1 \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I \right) + s_2 \left(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3} I \right)
$$

for $\mathbf{n} = \mathbf{v}_1$, $\mathbf{m} = \mathbf{v}_3$, $s_1 = (2\lambda_1 + \lambda_3) \geqslant 0$ and $s_2 = (2\lambda_3 + \lambda_1) \leqslant 0$. Applying Lemma 4.7 to this function $\mathbf{Q}(x)$, we deduce that

$$\begin{aligned} |\mathbf{Q}(x) - \mathbf{Q}(y)|^2 \geqslant & \frac{1}{6}\left[(s_1(x) - s_1(y))^2 + (s_2(x) - s_2(y))^2\right] \\ & + \frac{1}{6}\left[|s_1\mathbf{n}\otimes\mathbf{n}(x) - s_1\mathbf{n}\otimes\mathbf{n}(y)|^2 + |s_2\mathbf{m}\otimes\mathbf{m}(x) - s_2\mathbf{m}\otimes\mathbf{m}(y)|^2\right]. \end{aligned} \tag{4.17}$$

As in the previous proof, using the difference quotient characterisation of Sobolev spaces, from (4.17) we infer that

$$s_1, s_2 \in W^{1,2}(\Omega), \;\; s_1\mathbf{n}\otimes\mathbf{n}, s_2\mathbf{m}\otimes\mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right).$$

In order to find the correct function space for $\mathbf{n}$ we can simply apply Lemma 4.4 in conjunction with Proposition 4.8 to deduce the existence of a mapping

$$\mathbf{n}_1 \in W^{1,2}_{loc}\left(\Omega \setminus C_{s_1}, \mathbb{S}^2\right) = W^{1,2}_{loc}\left(\Omega \setminus \{s_1 = 0\}, \mathbb{S}^2\right)$$

such that $\mathbf{n}_1 \otimes \mathbf{n}_1 = \mathbf{n}\otimes\mathbf{n}$ whenever $s_1 \neq 0$. By identical reasoning we can also find a mapping $\mathbf{m}_1 \in W^{1,2}_{loc}\left(\Omega \setminus \{s_2 = 0\}, \mathbb{S}^2\right)$ such that $\mathbf{m}_1 \otimes \mathbf{m}_1 = \mathbf{m}\otimes\mathbf{m}$ whenever $s_2 \neq 0$. The joint regularity condition for the two pairs of functions is clear by using the same argument as from (4.14). For the reverse inclusion we take a set of mappings $(\mathbf{n}, \mathbf{m}, s_1, s_2) \in \mathcal{B}$ and we just need to show that $s_1\mathbf{n}\otimes\mathbf{n}, s_2\mathbf{m}\otimes\mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$ to ensure that

$$\mathbf{Q} := s_1\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right) + s_2\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}I\right) \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right). \tag{4.18}$$

However we can use the same logic from the previous proof (see (4.15) and (4.16)) to each of the pairs $(s_1, \mathbf{n})$ and $(s_2, \mathbf{m})$ separately to arrive at (4.18). This proves the equivalence between the sets $\mathcal{A}$ and $\mathcal{B}$. To conclude the proof it is a simple but somewhat long calculation to show that if we have some $\mathbf{Q}$ in the form of (4.18), then substituting this into the Landau-de Gennes energy (4.1) will precisely produce the biaxial Ericksen energy (4.4). Using the form of $\mathbf{Q}$ as given in (4.18) we find

$$\begin{aligned} |\nabla\mathbf{Q}|^2 = & \sum_{i,j,k}\left(s_{1,k}\left(\mathbf{n}_i\mathbf{n}_j - \frac{\delta_{ij}}{3}\right) + s_1\left(\mathbf{n}_{i,k}\mathbf{n}_j + \mathbf{n}_i\mathbf{n}_{j,k}\right)\right. \\ & \left. + s_{2,k}\left(\mathbf{m}_i\mathbf{m}_j - \frac{\delta_{ij}}{3}\right) + s_2\left(\mathbf{m}_{i,k}\mathbf{m}_j + \mathbf{m}_i\mathbf{m}_{j,k}\right)\right)^2 \\ = & \frac{|\nabla(s_1 - s_2)|^2}{3} + \frac{|\nabla s_1|^2 + |\nabla s_2|^2}{3} + 2\left(s_1^2|\nabla\mathbf{n}|^2 + s_2^2|\nabla\mathbf{m}|^2\right) + 4s_1s_2\left(\mathbf{m}^T\nabla\mathbf{n}\right)\cdot\left(\mathbf{n}^T\nabla\mathbf{m}\right), \end{aligned}$$

and

$$\begin{aligned} \mathbf{Q}\cdot\nabla\times\mathbf{Q} = & \sum_{i,j,a,b}\epsilon_{jab}\left[s_1\left(\mathbf{n}_i\mathbf{n}_j - \frac{\delta_{ij}}{3}\right) + s_2\left(\mathbf{m}_i\mathbf{m}_j - \frac{\delta_{ij}}{3}\right)\right]\mathbf{Q}_{ib,a} \\ = & \; s_1^2\mathbf{n}\cdot\nabla\times\mathbf{n} + s_2^2\mathbf{m}\cdot\nabla\times\mathbf{m} + s_1s_2\left[\left(\mathbf{n}^T\nabla\mathbf{m}\right)\cdot(\mathbf{m}\times\mathbf{n}) + \left(\mathbf{m}^T\nabla\mathbf{n}\right)\cdot(\mathbf{n}\times\mathbf{m})\right], \end{aligned}$$

and

$$|\mathbf{Q}|^2 = \sum_{i,j} \left[s_1 \left(\mathbf{n}_i \mathbf{n}_j - \frac{\delta_{ij}}{3} \right) + s_2 \left(\mathbf{m}_i \mathbf{m}_j - \frac{\delta_{ij}}{3} \right) \right]^2$$
$$= \frac{2}{3} \left(s_1^2 + s_2^2 - s_1 s_2 \right).$$

By combining these three equations we can show that the free energy densities are indeed formally equivalent so that $I_L(\mathbf{Q}) = I_{BE}(\mathbf{n}, \mathbf{m}, s_1, s_2)$. Therefore the two problems are equivalent.

□

4.4 Two and Three-dimensional Results

In higher dimensions the lifting results involve a greater number of intricacies, primarily because of the fact that not all connected domains are simply connected, unless we are in dimension one. The importance of simply-connected domains when looking to turn a line field into a vector field is crucial. On the simplest level, given a line field $\mathbf{n} \otimes \mathbf{n}$, at every point of the domain there are two possible choices for the vector field: $\mathbf{n}$ and $-\mathbf{n}$. A choice is made at some given point $x \in \Omega$ and we want to use this decision to choose what the vector field should be at every other point. This is more easily done in simply-connected domains because any two continuous curves in Ω connecting two points $x, y \in \Omega$ are homotopic. As an example to illustrate this, in Figure 4.1 the smooth line field as denoted by the dashed lines cannot be converted into a smooth vector field because of the holes in the domain.

We will prove three lifting results analogous to Proposition 4.8 about the regularity of line fields and vectors fields in two and three dimensions. For the first we extend a result of Ball and Zarnescu.

Theorem 4.13. *[13, Theorem 2] Suppose that $d = 2$ or 3 and $\Omega \subset \mathbb{R}^d$ is an open, bounded and simply connected set with continuous boundary. Suppose there is a mapping $\mathbf{n} : \Omega \to \mathbb{S}^2$ such that $\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$. Then*

$$\exists\, \mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right) \text{ s.t. } \mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n} \text{ a.e.}$$

This result assumes that the simply connected domain has a continuous boundary. Our extension will remove this assumption. Therefore we will show that it is possible to convert line fields to vector fields in the space $W^{1,2}$ when the domain is simply connected.

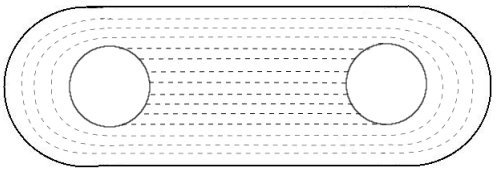


Figure 4.1: Non-simply connected domain example

Proposition 4.14. *Suppose that $d = 2$ or 3 and $\Omega \subset \mathbb{R}^d$ is an open, bounded and simply connected set. Suppose there is a mapping $\mathbf{n} : \Omega \to \mathbb{S}^2$ such that $\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$. Then*

$$\exists\, \mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right) \text{ s.t. } \mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n} \text{ a.e.}$$

Proof

Since Ω is an open set we know that for all $x \in \Omega$ there exists a maximal radius $\epsilon_x > 0$, such that

$$U_x := B(x, \epsilon_x) \subseteq \Omega.$$

The result of Ball-Zarnescu [13, Theorem 2] applies in any simply connected domain which has a continuous boundary, so certainly we can apply their result to each of these balls U_x to deduce that

$$\exists\, \mathbf{m} \in W^{1,2}(U_x, \mathbb{S}^2) \text{ s.t. } \mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n} \text{ a.e. on } U_x. \tag{4.19}$$

We also know that whenever we apply this result there are two possible choices for the vector field: $\mathbf{m}$ and $-\mathbf{m}$. The main issue in this proof is how to choose the orientations in each ball U_x so that at the finish we have a function with $W^{1,2}$ regularity on the whole of Ω.

We fix an arbitrary point $x \in \Omega$. Applying [13, Theorem 2] precisely gives us the statement (4.19). Now we proceed to show that this one choice uniquely defines the choice that we must make in every other ball U_y in Ω. We take $y \in \Omega$, $y \neq x$, and we suppose we have a continuous injective curve f such that

$$f : [0, 1] \to \Omega \text{ and } f(0) = x, \;\; f(1) = y.$$

We use this curve to motivate the following definition. For $t \in [0, 1]$ let

$$t_+ := \inf\left\{ \mu \geq t \;\middle|\; \mu \in [0, 1], \;\; f(\mu) \notin U_{f(t)} \right\} \wedge \{1\}. \tag{4.20}$$

This simply defines the first point on the curve to leave the set $U_{f(t)}$ (or 1 if there is no such point). Using this notion we define a sequence (t_j) as follows:

$$t_1 := 0_+ \quad t_2 := (t_1)_+ \quad t_3 := (t_2)_+ \;\; \ldots$$

Lemma 4.15. *$\exists\, N \in \mathbb{N}$ such that $t_N = 1$.*

Proof

It is clear from (4.20) that if $t \in [0, 1)$ then $t < t_+ \leq 1$ so that this sequence is a monotonically increasing sequence which is bounded above by 1. Such a sequence must converge. For a contradiction we suppose

$$t_j \to t < 1.$$

Consider the set $U_{f(t)}$; we know that $\epsilon_{f(t)} > 0$. We also know f is a continuous function so $f(t_j) \to f(t)$. Hence

$$\exists J \text{ s.t. } \forall j \geq J \quad f(t_j) \subset B\Big(f(t), \frac{\epsilon_{f(t)}}{2}\Big).$$

As we defined the radii of our balls to be maximal it must be that

$$\epsilon_{f(t_J)} > \frac{\epsilon_{f(t)}}{2},$$

thus

$$t_{J+1} = (t_J)_+ > t,$$

which is a contradiction. So we must have that $t_j \to 1$ as $j \to \infty$. Using this argument again we deduce that there can only be finitely many different terms. We know

$$\exists M \text{ s.t. } \forall j \geq M \quad f(t_j) \subset B\Big(f(1), \frac{\epsilon_{f(1)}}{2}\Big) = B\Big(y, \frac{\epsilon_y}{2}\Big).$$

This time maximality allows us to deduce that it must be the case that $(t_M)_+ = t_{M+1} = 1$.

□

It is also necessary to note a second property before we continue onto the main portion of the proof.

Lemma 4.16.

$$\inf_{t\in[0,1]} \epsilon_{f(t)} > 0 \tag{4.21}$$

Proof

This statement is simple because the explicit form for ϵ_x is $d(x, \partial\Omega)$. The continuity of the distance function ensures that ϵ_x is a continuous function of x. Combining this with the fact that it is positive on the compact set $f([0, 1])$, gives (4.21).

□

Now that we have established these lemmas we can move on to the choice construction. For all $t \in [0, t_1]$ we know

$$\mathcal{L}^d\left(U_x \cap U_{f(t)}\right) > 0,$$

so that we can uniquely choose the orientation in $U_{f(t)}$ by ensuring that on the set $U_x \cap U_{f(t)}$, it agrees with the orientation already chosen for U_x. We continue this process for the finite number of intervals $[t_j, t_{j+1}]$. This construction ensures that we have uniquely chosen an orientation at each point along the curve using the orientation at its starting point. Now we need to show that the orientation chosen for U_y is independent of the path chosen. To do this we take a second continuous injective curve $g : [0, 1] \to \Omega$ such that $g(0) = x$ and $g(1) = y$. At this juncture we use the crucial assumption that Ω is simply connected which has the following formulation.

A set is simply connected if and only if it is path connected and any two continuous curves with the same endpoints are homotopic.

This means that our two curves f and g must be homotopic in the sense that there exists a continuous map H, with the following properties

$$H : [0,1] \times [0,1] \to \Omega \quad \text{s.t.} \quad H(t,0) = f(t),\ H(t,1) = g(t),\ H(0,\lambda) = x \text{ and } H(1,\lambda) = y.$$

For a contradiction we assume that using this second path we arrive at the other orientation on the set U_y. Then we can define

$$\lambda^* := \inf \{ \mu \,|\, H(1,\mu) \text{ gives the opposite orientation to } H(1,0) = f(1) \}.$$

The fact that H is continuous on a compact set means that it is uniformly continuous, therefore

$$\forall\, \epsilon > 0 \quad \exists\, \delta > 0 \text{ s.t. } |(t_1,\lambda_1) - (t_2,\lambda_2)| < \delta \ \Rightarrow\ |H(t_1,\lambda_1) - H(t_2,\lambda_2)| < \epsilon. \tag{4.22}$$

Keeping Lemma 4.16 in mind, we set

$$\lambda_2 := \max\left\{\lambda^* - \frac{\delta}{2}, 0\right\} \quad \text{and} \quad \epsilon := \frac{1}{4} \inf_{t\in[0,1]} \epsilon_{H(t,\lambda^*)} > 0,$$

and choose $\lambda_1 \in \left(\lambda^*, \lambda^* + \frac{\delta}{2}\right)$ such that $H(1,\lambda_1)$ gives the opposite orientation to $H(1,0)$. This means we have $0 \leqslant \lambda_2 < \lambda_1 \leqslant 1$ and $|\lambda_1 - \lambda_2| < \delta$. Then using (4.22) we can easily deduce

$$|H(t,\lambda_1) - H(t,\lambda_2)| < \epsilon \quad \forall\, t \in [0,1].$$

By the definition of ϵ we must also have that

$$\mathcal{L}^d \left(U_{H(t,\lambda_1)} \cap U_{H(t,\lambda_2)}\right) > 0 \quad \forall\, t \in [0,1]. \tag{4.23}$$

Our assumption is that the two paths $H(t,\lambda_1)$ and $H(t,\lambda_2)$ begin with the same orientation and finish with different ones. Therefore we can find two points $a, b \in [0,1]$, arbitrarily close together, such that the two paths have the same orientation at a and the converse at b. However by choosing a and b sufficiently close, the definition of ϵ and (4.23) tell us that the four sets

$$U_{H(a,\lambda_1)},\ U_{H(b,\lambda_1)},\ U_{H(a,\lambda_2)},\ U_{H(b,\lambda_2)}$$

all have a common intersection. Thus by our choice construction they must all agree on this intersection, a contradiction. Therefore,

$$\{ \mu \,|\, H(1,\mu) \text{ has the opposite orientation to } H(1,0) = f(1) \} = \emptyset,$$

meaning the choice of orientation on U_y is path independent. To conclude we need to show that by this process we have defined a function $\mathbf{m}$, which has $W^{1,2}$ regularity everywhere in the domain. Take any two points $x \neq y$, $x, y \in \Omega$, then if

$$\mathcal{L}^d \left(U_x \cap U_y\right) = 0 \ \Rightarrow\ \mathbf{m} \in W^{1,2}\left(U_x \cup U_y, \mathbb{S}^2\right).$$

Equally, by our construction, if $\mathcal{L}^d\left(U_x \cap U_y\right) > 0$ then the orientations chosen in U_x and U_y agree on $U_x \cap U_y$. Thus in either case we have

$$\mathbf{m} \in W^{1,2}\left(U_x \cup U_y, \mathbb{S}^2\right).$$

Using this as a base case it is clear that a simple induction gives us

$$\mathbf{m} \in W^{1,2}\left(\bigcup_{i=1}^{N} U_{x_i}, \mathbb{S}^2\right), \tag{4.24}$$

for any finite union. Now take any $U \subset\subset \Omega$; $\left\{ U_x \,|\, x \in \overline{U} \right\}$ is an open cover for $\overline{U}$. This has a finite subcover $\left\{ U_{x_i} \;\middle|\; 1 \leq i \leq N,\ x_i \in \overline{U} \right\}$. Then equation (4.24) tells us

$$\mathbf{m} \in W^{1,2}\left(\bigcup_{1}^{M} U_{x_i}, \mathbb{S}^2\right) \;\Rightarrow\; \mathbf{m} \in W^{1,2}\left(U, \mathbb{S}^2\right) \;\Rightarrow\; \mathbf{m} \in W^{1,2}_{\text{loc}}\left(\Omega, \mathbb{S}^2\right). \tag{4.25}$$

In order to remove the local condition from (4.25) we note that $\mathbf{m}\otimes\mathbf{m} = \mathbf{n}\otimes\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$ and

$$\infty > \int_\Omega |\nabla\left(\mathbf{n}\otimes\mathbf{n}\right)|^2\, dx = \int_\Omega |\nabla\left(\mathbf{m}\otimes\mathbf{m}\right)|^2\, dx = \int_\Omega 2|\nabla\mathbf{m}|^2\, dx. \tag{4.26}$$

Combining (4.26) with (4.25) we finally see that

$$\mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right).$$

□

Remark 4.17. *This proposition shows that in a bounded simply connected domain in $\mathbb{R}^2$ or $\mathbb{R}^3$, uniaxial Landau-de Gennes theory with a constant scalar order parameter is directly equivalent to the Oseen-Frank theory.*

This lifting result is a nice extension of the result of Ball & Zarnescu but we cannot restrict ourselves to just studying simply-connected domains because for a function $s \in W^{1,2}(\Omega)$ we do not know in general that $\Omega \setminus C_s$ is simply-connected. Hence we will now prove the lifting result which is analogous to Proposition 4.14 in a general domain. However in order to do so we will require the Whitney decomposition theorem.

Theorem 4.18. *[87, Theorem 3, p.16] Let $F \subset \mathbb{R}^n$ be a non-empty closed set and $\Omega := F^c$. Then there is a set of closed cubes $\left\{ Q_j \subset \Omega \,|\, 1 \leqslant j \right\}$ such that*

- $\Omega = \bigcup_1^\infty Q_j$
- $int(Q_j) \cap int\left(Q_k\right) = \emptyset$ *if* $j \neq k$
- $diam\left(Q_j\right) \leqslant d\left(Q_j, \partial\Omega\right) \leqslant 4diam\left(Q_j\right)$.

Proposition 4.19. *Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded domain where $d = 2, 3$ and suppose that*

$$\mathbf{n} \otimes \mathbf{n} \in W^{1,2}_{loc}\left(\Omega, \mathbb{R}^{3\times 3}\right)$$

where $|\mathbf{n}| = 1$ almost everywhere in Ω. Then there exists an

$$\mathbf{m} \in SBV^2_{loc}\left(\Omega, \mathbb{S}^2\right)$$

such that $\mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n}$ almost everywhere, and $\mathbf{m}_+ = -\mathbf{m}_-$ $\mathcal{H}^{d-1}$ almost everywhere on $S_{\mathbf{m}}$.

Proof

We immediately apply the decomposition theorem, Theorem 4.18. This instantly gives us a set of cubes $\left\{ Q_j \subset \Omega \,\middle|\, 1 \leqslant j \right\}$ with the given properties. For ease of notation we will denote the interior of each of these closed cubes by U_j. We can certainly say that

$$\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(U_j, \mathbb{R}^{3\times 3}\right).$$

The interior of each cube is clearly simply-connected so we can apply Theorem 4.14 to find some $\mathbf{m} \in W^{1,2}\left(U_j, \mathbb{S}^2\right)$ such that $\mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n}$ almost everywhere. We can do this in each of the cubes to find some

$$\mathbf{m} \in W^{1,2}\left(\bigcup_1^\infty U_j, \mathbb{S}^2\right).$$

All we need to do to complete the proof is to investigate the behaviour of $\mathbf{m}$ over the boundaries of these cubes to show that it is in SBV^2_{loc}. To do that we take some $V \subset\subset \Omega$ and begin by showing

$$\inf\left\{ \mathrm{diam} Q_j \,\middle|\, Q_j \cap V \neq \emptyset \right\} > 0. \tag{4.27}$$

We suppose for a contradiction that (4.27) doesn't hold. Then that means we can find a sequence of cubes Q_{j_k} such that $\mathrm{diam}\left(Q_{j_k}\right) \to 0$ and $Q_{j_k} \cap V \neq \emptyset$. However because V is compactly contained in Ω

$$d(V, \partial\Omega) \geqslant \epsilon,$$

for some $\epsilon > 0$. The convergence of the diameters means that there is some K such that for all $k \geqslant K$, $\mathrm{diam}\left(Q_{j_k}\right) \leqslant \frac{\epsilon}{2}$, and therefore $d\left(Q_{j_k}, \partial\Omega\right) \geqslant \frac{\epsilon}{2}$ as well. However we can see that this contradicts the third property of these cubes. Therefore (4.27) holds. Crucially this means that because our domain Ω is bounded, the set V only intersects finitely many of these cubes and therefore

$$V \subset \bigcup_1^N Q_j.$$

We define $U := \bigcup_1^N \left(V \cap U_j\right) = V \setminus \left(\bigcup_1^N \partial Q_j\right)$, and we note that

$$\mathbf{m} \in W^{1,2}\left(U, \mathbb{S}^2\right) = W^{1,2}\left(V \setminus \left(\bigcup_1^N \partial Q_j\right), \mathbb{S}^2\right). \tag{4.28}$$

Equation (4.28) together with the fact that $\mathcal{H}^{d-1}\left(\bigcup_1^N \partial Q_j\right) < \infty$ means we can apply Ambrosio's result, Proposition 0.8, to deduce that

$$\mathbf{m} \in SBV^2\left(V, \mathbb{S}^2\right)$$

with $\mathcal{H}^{d-1}\left(S_{\mathbf{m}} \setminus \bigcup_1^N \partial Q_j\right) = 0$. Finally we just need to prove that $\mathbf{m}_+ = -\mathbf{m}_-$ on the jump set $S_{\mathbf{m}}$. We know that $\mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(V, \mathbb{R}^{3\times 3}\right)$, thus $S_{\mathbf{m}\otimes\mathbf{m}} = \emptyset$. Therefore it is the case that $\mathbf{m}_+ = \pm\mathbf{m}_-$, $\mathcal{H}^{d-1}$ almost everywhere on $S_{\mathbf{m}}$. If this were not the case then the line field $\mathbf{m} \otimes \mathbf{m}$ would have a non-trivial jump set. However by definition, the approximate discontinuity set, $S_{\mathbf{m}}$, consists of points such that $\mathbf{m}_+ \neq \mathbf{m}_-$. Hence $\mathbf{m}_+ = -\mathbf{m}_-$ $\mathcal{H}^{d-1}$ almost everywhere on $S_{\mathbf{m}}$.

□

We shall see that this lifting result will be the crucial one when proving the equivalence between the uniaxial Landau-de Gennes theory and Ericksen's theory. We would however like to have an appropriate analogue to Corollary 4.9 in the two and three dimensional case where we remove the locality assumptions from the previous result. Unfortunately we cannot do this because the Whitney decomposition theorem breaks up the domain into infinitely many simply connected pieces. The union of the boundaries of these components may have infinite $\mathcal{H}^{d-1}$ measure meaning that we are unable to apply Proposition 0.8. However our final lifting result shows that with a Lipschitz boundary for our domain, we can cover an open neighbourhood of the boundary with finitely many simply connected pieces. This allows us to overcome the difficulties.

Proposition 4.20. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain, where $d = 2, 3$. Suppose that*

$$\mathbf{n} \otimes \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$$

where $|\mathbf{n}| = 1$ almost everywhere. Then there exists an $\mathbf{m} \in SBV^2\left(\Omega, \mathbb{S}^2\right)$ such that $\mathbf{m} \otimes \mathbf{m} = \mathbf{n} \otimes \mathbf{n}$ almost everywhere and $\mathbf{m}_+ = -\mathbf{m}_-$ $\mathcal{H}^{d-1}$ almost everywhere on $S_{\mathbf{m}}$.

Proof

As Ω is a Lipschitz domain [25, Definition 1.40], for every $x \in \partial\Omega$ there exists some $r > 0$ and map $h_x : B(x, r) \to Q$, where $Q = (-1, 1)^d$, such that

1. h_x is bijective.
2. h_x and h_x^{-1} are Lipschitz continuous.
3. $h_x(\partial\Omega \cap B(x, r)) = A_0 := \{\, x \in Q \,|\, x_d = 0 \,\}$
4. $h_x(\Omega \cap B(x, r)) = A_+ := \{\, x \in Q \,|\, x_d > 0 \,\}$

Combining properties 1, 2, and 4 tells us that h_x is a homeomorphism between $\Omega \cap B(x, r)$ and A_+. Furthermore a homeomorphism defines a homotopy-equivalence so that these two sets are homotopy equivalent. If a set X is simply-connected and homotopy equivalent to Y,

then Y is also simply connected. Clearly A_+ is simply connected, hence $B(x,r)\cap\Omega$ is simply connected. For each $x\in\partial\Omega$, we define

$$U_x := B(x,r)\cap\Omega.$$

Then $(U_x)_{x\in\partial\Omega}$ is an open cover for the compact set $\partial\Omega$. Hence it has a finite subcover $(U_{x_\alpha})_1^J$. This is the main idea of the proof, by covering the boundary with a finite number of sets which are simply connected, we can begin to construct our SBV function. Beginning with U_{x_1} we can find some $\mathbf{m}_1\in W^{1,2}\left(U_{x_1},\mathbb{S}^2\right)$ such that $\mathbf{m}\otimes\mathbf{m}=\mathbf{n}\otimes\mathbf{n}$ on U_{x_1}. Then we progress to U_{x_2}: there exists some $\mathbf{v}\in W^{1,2}\left(U_{x_2},\mathbb{S}^2\right)$ such that $\mathbf{v}\otimes\mathbf{v}=\mathbf{n}\otimes\mathbf{n}$ on U_{x_2}. Then we define

$$\mathbf{m}_2(x) := \begin{cases} \mathbf{v}(x) & \text{if} \quad x\in U_{x_2} \\ \mathbf{m}_1(x) & \text{if} \quad x\in U_{x_1}\setminus U_{x_2}. \end{cases}$$

Using Proposition 0.8, this defines a function $\mathbf{m}_2\in SBV^2\left(U_{x_1}\cup U_{x_2},\mathbb{S}^2\right)$ with the desired properties. By continuing this process finitely many times for each $2\leqslant i\leqslant J$, and defining

$$\mathbf{m}_i(x) := \begin{cases} \mathbf{v}(x) & \text{if} \quad x\in U_{x_i} \\ \mathbf{m}_{i-1}(x) & \text{if} \quad x\in\left(\bigcup_{\alpha=1}^{i-1}U_{x_\alpha}\right)\setminus U_{x_i}. \end{cases} \tag{4.29}$$

we obtain a function $\mathbf{m}_J\in SBV^2\left(\bigcup_{\alpha=1}^J U_{x_\alpha},\mathbb{S}^2\right)$. This deals with the regularity requirements near the boundary and so we proceed onto the interior. Let

$$\delta := d\left(\partial\Omega,\Omega\setminus\bigcup_1^J U_{x_\alpha}\right)>0.$$

Then we can cover $\Omega\setminus\bigcup_{\alpha=1}^J U_{x_\alpha}$ with a mesh of cubes with disjoint interiors and side length $\frac{\delta}{4}$. There can only be finitely many such cubes because $|\Omega|<\infty$. These cubes are like those in the Whitney decomposition theorem except that they are all of the same size and we enumerate them $(Q_\beta)_1^K$. Now we can use the same construction idea as from (4.29). For each $i=1,\dots,K$ we know that there exists some $\mathbf{v}\in W^{1,2}\left(Q_i,\mathbb{S}^2\right)$ such that $\mathbf{v}\otimes\mathbf{v}=\mathbf{n}\otimes\mathbf{n}$. Hence we define

$$\mathbf{m}_{J+i}(x) := \begin{cases} \mathbf{v}(x) & \text{if} \quad x\in Q_i \\ \mathbf{m}_{J+i-1}(x) & \text{if} \quad x\in\left[\left(\bigcup_{\alpha=1}^J U_{x_\alpha}\right)\cup\left(\bigcup_{\beta=1}^{i-1}Q_\beta\right)\right]\setminus Q_i, \end{cases}$$

and $\mathbf{m}_{J+i}\in SBV^2\left(\left[\left(\bigcup_{\alpha=1}^J U_{x_\alpha}\right)\cup\left(\bigcup_{\beta=1}^i Q_\beta\right)\right],\mathbb{S}^2\right)$. Having repeated this process finitely many times (for $i=1,\dots,K$) we will have found

$$\mathbf{m}_{J+K}\in SBV^2\left(\left[\bigcup_{\alpha=1}^J U_{x_\alpha}\cup\bigcup_{\beta=1}^K Q_\beta\right],\mathbb{S}^2\right).$$

Define the closed set C by

$$C := \bigcup_{\alpha=1}^J\partial B(x_\alpha,r_\alpha)\cup\bigcup_{\beta=1}^K\partial Q_\beta.$$

We have constructed our function $\mathbf{m}_{J+K}$ so that its discontinuity set must be contained within C and $\mathcal{H}^{d-1}(C)<\infty$. It is worth noting that we chose to define C using the boundaries of

$B(x_\alpha, r_\alpha)$ rather than U_{x_α} as we did not want to include $\partial\Omega$ in C. As the discontinuity set must be contained within C we have that

$$\mathbf{m} := \mathbf{m}_{J+K} \in W^{1,2}\left(\Omega \setminus C, \mathbb{S}^2\right).$$

Therefore by again applying Proposition 0.8, we deduce that $\mathbf{m} \in SBV^2\left(\Omega, \mathbb{S}^2\right)$ and $\mathbf{m}\otimes\mathbf{m} = \mathbf{n}\otimes\mathbf{n}$. The equivalence of these two tensors immediately implies that $\mathbf{m}_+ = -\mathbf{m}_-$ $\mathcal{H}^{d-1}$ almost everywhere on $S_{\mathbf{m}}$.

□

Just as in Section 4.3, now that we have established our lifting results we can use them to prove two equivalence results between the Landau-de Gennes theory and Ericksen's theory. However there is a very subtle but thorny technicality in multiple dimensions which needs to be addressed.

Technicality

In the following result, Theorem 4.21, we will show the relationship between the uniaxial Landau-de Gennes theory and Ericksen's theory. By comparison with the one-dimensional result, Theorem 4.11, it would not be unreasonable to suppose that the set of admissible functions for the Ericksen problem should be

$$\mathcal{B} := \left\{ s \in W^{1,2}(\Omega),\ \mathbf{n} \in SBV^2_{loc}\left(\Omega \setminus C_s, \mathbb{S}^2\right) \,\middle|\, \int_\Omega s^2|\nabla\mathbf{n}|^2\,dx < \infty,\ \mathbf{n}_+ = -\mathbf{n}_- \text{ on } S_{\mathbf{n}} \right\}.$$

If we were to take a pair $(s, \mathbf{n}) \in \mathcal{B}$, in order to prove the equivalence of the admissible functions, we would need to show that $s\mathbf{n}\otimes\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times3}\right)$. Since $SBV^2_{loc} \cap L^\infty$ is closed under products we would find $\mathbf{n}\otimes\mathbf{n} \in SBV^2_{loc}\left(\Omega \setminus C_s, \mathbb{R}^{3\times3}\right)$. The fact that $\mathbf{n}_+ = -\mathbf{n}_-$ on $S_{\mathbf{m}}$ would then indicate that $\mathbf{n}\otimes\mathbf{n} \in W^{1,2}_{loc}\left(\Omega \setminus C_s, \mathbb{R}^{3\times3}\right)$. Finally the joint regularity would imply that

$$s\mathbf{n}\otimes\mathbf{n} \in W^{1,2}\left(\Omega \setminus C_s, \mathbb{R}^{3\times3}\right). \tag{4.30}$$

From an intuitive point of view it is only a short step to deduce that (4.30) implies $s\mathbf{n}\otimes\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times3}\right)$. However lots of subtle points about the fine regularity of Sobolev functions come into play. We would need Lemma 4.5 to hold without the additional continuity assumption. This would be true if we could show, for example, that for $f \in W^{1,p}(\Omega)$

$$\mathcal{H}^{d-1}\left(C_f \setminus \{f = 0\}\right) = 0. \tag{4.31}$$

We conjecture that (4.31) always holds because Sobolev functions should not have a discontinuity set with Hausdorff dimension greater than or equal to $d-1$. However presently we are unable to prove this claim. Therefore in the multi-dimensional results below we will simply assume that $s(\mathbf{n}\otimes\mathbf{n}) \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times3}\right)$ as our joint regularity condition. The reasoning above shows that this is not an oversimplification; it is only used to deal with this small technicality which we believe to be true in any case.

4.4.1 Uniaxial Landau-de Gennes

Theorem 4.21. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with $d = 2, 3$. Then minimising $I_L(\mathbf{Q})$ over*

$$\mathcal{A} := \left\{ \mathbf{Q} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right) \,\middle|\, \mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right) \right\}$$

is equivalent to minimising $I_E(s, \mathbf{n})$ over

$$\mathcal{B} := \left\{ s \in W^{1,2}(\Omega),\ \mathbf{n} \in SBV^2_{loc}\left(\Omega \setminus C_s, \mathbb{S}^2\right) \,\middle|\, s\mathbf{n}\otimes\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right) \right\}.$$

Proof

This proof closely follows that of Theorem 4.11 so we will skim over the details of this proof which have already been addressed there. We take a $\mathbf{Q} \in \mathcal{A}$ then we know that we can write $\mathbf{Q}$ as $s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right)$. We can immediately use the logic from (4.12) and (4.13) to deduce that

$$s \in W^{1,2}(\Omega).$$

Therefore $s\mathbf{n}\otimes\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)$. Then by using Lemma 4.4 we find

$$\mathbf{n}\otimes\mathbf{n} \in W^{1,2}_{loc}\left(\Omega \setminus C_s, \mathbb{R}^{3\times 3}\right).$$

We are now in a position to use our previous lifting result to convert this line field into a vector field. Applying Proposition 4.19 to $\mathbf{n}\otimes\mathbf{n}$ tells us that there exists some mapping

$$\mathbf{m} \in SBV^2_{loc}\left(\Omega \setminus C_s, \mathbb{S}^2\right) \text{ such that } \mathbf{m}\otimes\mathbf{m} = \mathbf{n}\otimes\mathbf{n} \ a.e.$$

and $\mathbf{m}_+ = -\mathbf{m}_-$ $\mathcal{H}^{d-1}$ almost everywhere on the jump set $S_{\mathbf{m}}$. This completes the inclusion as we have shown that $(s, \mathbf{m}) \in \mathcal{B}$. The reverse inclusion is trivial; we take a pair $(s, \mathbf{n}) \in \mathcal{B}$ and then it is clear from their definitions that

$$\mathbf{Q} := s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right) \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right).$$

This establishes the link between the sets of admissible functions and the formal equivalence of the Lagrangians is exactly the same as in Theorem 4.11.

□

4.4.2 Biaxial Landau-de Gennes

Theorem 4.22. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with $d = 2, 3$. Then minimising $I_L(\mathbf{Q})$ over*

$$\mathcal{A} := \left\{ \mathbf{Q} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right) \,\middle|\, \mathbf{Q} = s_1\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right) + s_2\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}I\right) \right\}$$

is equivalent to minimising $I_{BE}(\mathbf{n}, \mathbf{m}, s_1, s_2)$ over

$$\mathcal{B} := \left\{ \begin{array}{c} s_1, -s_2 \in W^{1,2}(\Omega, [0,\infty)), \\ \mathbf{n} \in SBV^2_{loc}\left(\Omega \setminus C_{s_1}, \mathbb{S}^2\right), \\ \mathbf{m} \in SBV^2_{loc}\left(\Omega \setminus C_{s_2}, \mathbb{S}^2\right) \end{array} \,\middle|\, \begin{array}{c} s_1\mathbf{n}\otimes\mathbf{n}, s_2\mathbf{m}\otimes\mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right), \\ \mathbf{n}\cdot\mathbf{m} = 0 \end{array} \right\}.$$

Proof

The proof of this result follows similar lines to that of Theorem 4.12. We begin by taking $\mathbf{Q} \in \mathcal{A}$. The variable $\mathbf{Q}$ can be written as

$$\mathbf{Q} := s_1\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right) - s_2\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}I\right),$$

where $s_1 \geqslant 0$, $s_2 \leqslant 0$, $|\mathbf{n}| = |\mathbf{m}| = 1$ and $\mathbf{n}\cdot\mathbf{m} = 0$. By following the same arguments as from the beginning of the proof of Theorem 4.12, straight away we deduce

$$s_1, s_2 \in W^{1,2}(\Omega), \;\; s_1\mathbf{n}\otimes\mathbf{n}, s_2\mathbf{m}\otimes\mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right).$$

Then, just as in the proof of Theorem 4.12, we can apply both Lemma 4.4 and Proposition 4.19 to each of the matrix valued functions above, and find

$$\mathbf{u} \in SBV^2_{loc}\left(\Omega \setminus C_{s_1}, \mathbb{S}^2\right) \text{ and } \mathbf{v} \in SBV^2_{loc}\left(\Omega \setminus C_{s_2}, \mathbb{S}^2\right).$$

where $\mathbf{u}\otimes\mathbf{u} = \mathbf{n}\otimes\mathbf{n}$ and $\mathbf{v}\otimes\mathbf{v} = \mathbf{m}\otimes\mathbf{m}$ almost everywhere. This concludes the first inclusion. For the reverse one we take some $(\mathbf{n}, \mathbf{m}, s_1, s_2) \in \mathcal{B}$ then using the joint regularity assumptions that

$$s_1\mathbf{n}\otimes\mathbf{n}, s_2\mathbf{m}\otimes\mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right),$$

we clearly see that we have

$$\mathbf{Q} := s_1\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right) + s_2\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}I\right) \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right).$$

This finalises the one-to-one correspondence of $\mathcal{A}$ and $\mathcal{B}$. The formal equivalence of the Lagrangians was already established in the proof of Theorem 4.12, so the assertion is complete. □

4.5 A Different Approach

These theorems provide an interesting insight into the precise function space equivalences between the Landau-de Gennes, Ericksen and Oseen-Frank theories. However as we see from the statement of Theorem 4.21 for example, it would be a very great analytical exercise to find minimisers of the Ericksen energy given that the director $\mathbf{n}$ and the scalar order parameter s are not independent. The biaxial energy (4.4) is yet another order of magnitude more difficult if one were looking for any sort of explicit minimiser. If, in isolation, we were to try and minimise

$$I_E(\mathbf{n}, s) = \int_\Omega 2s^2\left(|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2\right) + \frac{2}{3}|\nabla s|^2 + \sigma(s)\,dx, \tag{4.32}$$

over

$$\mathcal{B} := \left\{ s \in W^{1,2}(\Omega), \; \mathbf{n} \in SBV^2_{loc}\left(\Omega \setminus C_s, \mathbb{S}^2\right) \;\middle|\; s\mathbf{n}\otimes\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{R}^{3\times 3}\right)\right\}, \tag{4.33}$$

it would not even be clear whether we could show the existence of a global minimiser through the direct method of the calculus of variations. In fact, Theorem 4.21 ensures that a global minimiser does exist. Therefore in this final section we will use the above results as motivation to justify a new liquid crystal continuum model which is tractable for an analytical approach. For example, with the scalar order parameter we are not so much interested in its exact value, but where it vanishes, as this represents a change in phase of the liquid crystal sample. Therefore we are principally interested in the two different states of s: where it is zero, and where it is non-zero. Using this idea we can use a Γ-convergence result to retain the phase change information whilst simplifying the energy greatly. As we will quantify later, the Γ-convergence is a suitable approximation to make because the size of the elastic constants for the liquid crystal are many orders of magnitude smaller than the bulk constants. In the paper of Ambrosio & Tortorelli [6] a similar Γ-convergence idea was explored. They considered the Ericksen free energy for a nematic liquid crystal and used a single well potential for the function σ. Interestingly the Γ-limit of the functional was of the form

$$I(\mathbf{n}) = \begin{cases} \int_\Omega \alpha|\nabla \mathbf{n}|^2\,dx + K\mathcal{H}^{d-1}(S_{\mathbf{n}}) & \text{if } \mathbf{n} \in SBV\left(\Omega, \mathbb{S}^2\right) \text{ and } s = 1, \\ \infty & \text{otherwise.} \end{cases}$$

Their result was possible to prove because in the classical Ericksen theory, the order parameters s and $\mathbf{n}$ are independent. However our situation is more difficult. The complexity of the set of admissible functions means that we shall only be able to take a partial Γ-limit of (4.32) and (4.33) to discuss and justify a cholesteric free energy density which uses SBV functions in a similar manner to the equation above. We recall the definition of Γ-convergence.

Definition 4.23 (Γ-convergence)**.** *Let X be a metric space. Then $f_j : X \to \mathbb{R} \cup \{\pm\infty\}$ Γ-converges to $f : X \to \mathbb{R} \cup \{\pm\infty\}$, if for every $x \in X$ we have the following two properties.*

1. *If $x_j \to x$ in X then*
$$f(x) \leqslant \liminf_j f_j(x_j).$$

2. *There exists some sequence $x_j \to x$ in X such that*
$$f(x) \geqslant \limsup_j f_j(x_j).$$

4.5.1 Γ-Convergence Result

Suppose that $d \in \{1, 2, 3\}$ and $\Omega \subset \mathbb{R}^d$ is an open set, with Lipschitz boundary. Suppose that $\sigma : \mathbb{R} \to [0, \infty)$ is a continuous function with exactly two distinct zeroes at s_- and s_+. Let $\epsilon > 0$ and $F_\epsilon, F : L^1(\Omega, \mathbb{R}) \to \overline{\mathbb{R}}$ be defined by

$$F_\epsilon(v) := \begin{cases} \int_\Omega \frac{2\epsilon}{3}|\nabla v|^2 + \frac{1}{\epsilon}\sigma(v)\,dx & v \in W^{1,2}(\Omega) \\ \infty & \text{otherwise} \end{cases}$$

and

$$F(v) := \begin{cases} C\mathcal{H}^{d-1}(S_v) & v \in SBV^2(\Omega, \{s_-, s_+\}) \\ \infty & \text{otherwise} \end{cases}$$

where $C = 2\sqrt{\frac{2}{3}}\int_{s_-}^{s_+} \sqrt{\sigma(\lambda)}\, d\lambda$.

Theorem 4.24. *The functional F_ϵ Γ-converges to F with the strong topology on $L^1(\Omega, \mathbb{R})$. Furthermore if u_ϵ is a minimiser of F_ϵ and $u_\epsilon \to u$ as $\epsilon \to 0$ in $L^1(\Omega)$ then u is a minimiser of F.*

Proof

The proof has three main steps. We show the two inequalities required for Γ-convergence and then address the convergence of minimisers statement. This result is similar to one proved by Modica [68, Theorem 1] and therefore we will utilise some results from his paper to shorten our proof.

We begin by showing the lower bound for Γ-convergence. Let (v_ϵ) be a sequence of $L^1(\Omega)$ functions such that $v_\epsilon \to v \in L^1(\Omega)$ as $\epsilon \to 0$. We need to show that

$$\liminf_{\epsilon\to 0} F_\epsilon(v_\epsilon) \geqslant F(v).$$

Without loss of generality we can assume that $\liminf_{\epsilon\to 0} F_\epsilon(v_\epsilon) = \lim_{\epsilon\to 0} F_\epsilon(v_\epsilon) < \infty$. As $v_\epsilon \to v$ in $L^1(\Omega)$, up to a subsequence we may also assume that $v_\epsilon \to v$ almost everywhere. Then the continuity of σ, together with Fatou's Lemma implies

$$\int_\Omega \sigma(v)\, dx \leqslant \liminf_{\epsilon\to 0} \int_\Omega \sigma(v_\epsilon)\, dx \leqslant \liminf_{\epsilon\to 0} C_1\epsilon = 0.$$

Therefore $v(x) = s_-$ or s_+ almost everywhere. As the function $\overline{v_\epsilon} = s_- \vee v_\epsilon \wedge s_+ \in H^1(\Omega)$, without loss of generality we can assume that $v_\epsilon(x) \in [s_-, s_+]$ since $F_\epsilon(\overline{v_\epsilon}) \leqslant F_\epsilon(v_\epsilon)$. Then by using Young's inequality and Hölder's inequality we find

$$\begin{aligned} F_\epsilon(v_\epsilon) &\geqslant 2\left(\int_\Omega \frac{2}{3}|\nabla v_\epsilon|^2\, dx\right)^{\frac{1}{2}}\left(\int_\Omega \sigma(v_\epsilon)\, dx\right)^{\frac{1}{2}} \\ &\geqslant 2\sqrt{\frac{2}{3}}\int_\Omega |\nabla v_\epsilon|\sqrt{\sigma(v_\epsilon)}\, dx. \end{aligned}$$

If we introduce the function $\psi(t) = \int_{s_-}^t \sqrt{\sigma(\lambda)}\, d\lambda$, as it is continuous, $v_\epsilon \to v$ in $L^1(\Omega)$, and $s_- \leqslant v_\epsilon \leqslant s_+$, we deduce from the dominated convergence theorem that $\psi(v_\epsilon) \to \psi(v)$ in $L^1(\Omega)$. We also know that

$$\infty > \liminf_{\epsilon\to 0} F_\epsilon(v_\epsilon) \geqslant 2\sqrt{\frac{2}{3}}\liminf_{\epsilon\to 0}\int_\Omega |\nabla(\psi(v_\epsilon))|\, dx.$$

These deductions allow us infer that $\psi(v) \in BV(\Omega)$ [7, Proposition 10.1.1] and

$$\liminf_{\epsilon\to 0} F_\epsilon(v_\epsilon) \geqslant 2\sqrt{\frac{2}{3}}\int_\Omega |D(\psi(v))|. \tag{4.34}$$

However v only takes two possible values. Therefore we can find the exact form of (4.34) and conclude

$$\liminf_{\epsilon\to 0} F_\epsilon(v_\epsilon) \geqslant \left(2\sqrt{\frac{2}{3}}\int_{s_-}^{s_+} \sqrt{\sigma(\lambda)}\, d\lambda\right)\mathcal{H}^{d-1}(S_v).$$

For the upper bound in the definition of Γ-convergence we take some $v \in L^1(\Omega)$ and we need a sequence $v_\epsilon \to v$ in $L^1(\Omega)$ such that

$$\limsup_{\epsilon\to 0} F_\epsilon(v_\epsilon) = \lim_{\epsilon\to 0} F_\epsilon(v_\epsilon) = F(v). \tag{4.35}$$

Without loss of generality we can assume $v \in SBV^2(\Omega, \{s_-, s_+\})$. As v only takes two values we can write it as $s_- + (s_+ - s_-)\chi_{\{v=s_+\}}$. Following Modica's argument, initially we assume a smoothness property, then prove (4.35) in general by approximation. Suppose there exists some open set $A \subset \mathbb{R}^d$ such that ∂A is non-empty, compact, smooth, $\mathcal{H}^{d-1}(\partial A \cap \partial\Omega) = 0$ and $v = s_- + (s_+ - s_-)\chi_A$. Then we can find a set of Lipschitz functions $v_\epsilon \to v$ in $L^1(\Omega)$ which satisfy (4.35) [68, Proposition 2]. Now we take a general $v \in SBV^2(\Omega, \{s_-, s_+\})$ and [68, Lemma 1] implies that we can find sets (A_j) satisfying the above regularity conditions such that

$$\mathcal{H}^{d-1}(\partial A_j) \to \mathcal{H}^{d-1}(S_v).$$

For ease we can assume that $\mathcal{H}^{d-1}(\partial A_j) \leqslant \mathcal{H}^{d-1}(S_v) + \frac{1}{j}$ for every j. If we define $v^j := s_- + (s_+ - s_-)\chi_{A_j}$, then by our initial step, we can find Lipschitz functions (v^j_ϵ) such that

$$\limsup_{\epsilon\to 0} F_\epsilon(v^j_\epsilon) \leqslant C\mathcal{H}^{d-1}(\partial A_j) \leqslant C\left(\mathcal{H}^{d-1}(S_v) + \frac{1}{j}\right). \tag{4.36}$$

Using a simple diagonalisation argument we can find some sequence $\epsilon(j) \to 0$ as $j \to \infty$ such that

$$\limsup_{j\to\infty} F_{\epsilon(j)}\left(v^j_{\epsilon(j)}\right) \leqslant C\mathcal{H}^{d-1}(S_v).$$

Therefore F_ϵ does Γ-converge to F in the appropriate sense. So to finish the proof we just need to show the standard Γ-convergence property: convergence of minimisers. Suppose that we have a sequence of minimisers (u_ϵ) such that $u_\epsilon \to u$ in $L^1(\Omega)$. We first show that

$$F(u) \leqslant F(v)$$

for every $v \in SBV^2(\Omega, \{s_-, s_+\})$ which satisfies the above smoothness property. However this is clear because if (v_ϵ) is the series of Lipschitz functions approximating v in $L^1(\Omega)$ then

$$F(u) \leqslant \liminf_{\epsilon\to 0} F_\epsilon(u_\epsilon) \leqslant \liminf_{\epsilon\to 0} F_\epsilon(v_\epsilon) \leqslant \limsup_{\epsilon\to 0} F_\epsilon(v_\epsilon) \leqslant F(v).$$

Now if we take an arbitrary $v \in SBV^2(\Omega, \{s_-, s_+\})$, we can use a very similar approximation argument (using equation (4.36)) as above to deduce

$$F(u) \leqslant F(v).$$

Thus u is indeed a minimiser of F.

□

In order to be able to use Theorem 4.24 as a suitable approximation we need to employ some knowledge about the bulk energy σ. We know that it has the form

$$\sigma(s) := \frac{a}{2}s^2 + \frac{b}{3}s^3 + \frac{c}{4}s^4$$

where $c > 0$, and a is temperature dependent. It is often assumed that $a = \alpha(T - T^*)$ where $\alpha > 0$ and T^* is the temperature at which the isotropic state becomes unstable. If we follow this convention on the form of a then there is a critical temperature, $T_c > T^*$ (following the notation of Virga [92]), such that σ has exactly two global minimisers: 0 and s_+. By the addition of a constant, without loss of generality we can assume that $\sigma(0) = \sigma(s_+) = 0$ at or near this critical temperature.

Finally, and most importantly, we need to consider the size of the bulk constants relative to the elastic constants to ensure that taking a Γ-limit is a physically appropriate limit to take. As was discussed in Chapter 2, an example set of measured values of the Frank elastic constants of the liquid crystal MBBA at 25°C [88] is

$$K_1 = 6 \times 10^{-12}N, \quad K_2 = 3.8 \times 10^{-12}N, \quad K_3 = 7.5 \times 10^{-12}N.$$

Of course exact values vary between liquid crystals but they are certainly of the order of $10^{-11}N$ or less. On the other hand the bulk constants α, b, and c are very much larger. They have been measured fewer times but a set of values for MBBA was experimentally found to be [93]

$$\alpha = 0.042 \times 10^6 Nm^{-2}K^{-1}, \quad b = -0.64 \times 10^6 Nm^{-2}, \quad c = 0.35 \times 10^6 Nm^{-2}.$$

Throughout this chapter we have been tacitly using the one constant approximation for our elastic energies with an elastic constant of the order $10^{-11}N$. However, as can be seen from (4.32) we have been considering energies where we have divided through by this Frank constant. Therefore the value of the bulk constants in our functional (4.32) will be of the order 10^{15} or 10^{16}. This validates the idea of using a Γ-convergence result to provide an approximation to our variational problem. Theorem 4.24 therefore implies that our variational problem could be considered to be approximated by the following problem: minimising

$$I_E(\mathbf{n}, s) = \int_\Omega 2s^2 \left(|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2\right) dx + K\mathcal{H}^{d-1}(S_s) \tag{4.37}$$

over

$$\mathcal{B} := \left\{ s \in SBV^2(\Omega, \{0, s_+\}), \mathbf{n} \in SBV^2\left(\Omega \setminus C_s, \mathbb{S}^2\right) \,\middle|\, \mathbf{n}_- = -\mathbf{n}_+ \ \mathcal{H}^{d-1} \ a.e. \text{ on } S_{\mathbf{n}} \right\}.$$

This is simpler but we still have the issue of two variables which are not independent from each other. So now if we consider the variable $\mathbf{m} := s\mathbf{n}$ then because we know that

$$s = s_+\chi_{\{s=s_+\}} \in SBV^2(\Omega), \text{ and } \mathbf{n}\chi_{\{s=s_+\}} \in SBV^2\left(\{s = s_+\}, \mathbb{S}^2\right)$$

and $SBV \cap L^\infty$ is an algebra of functions, we find

$$\mathbf{m} \in \mathcal{A} := \left\{ SBV^2\left(\Omega, s_+\mathbb{S}^2 \cup \{0\}\right)\right\}. \tag{4.38}$$

Therefore if we now consider the free-energy (4.37) to be just a function of $\mathbf{m}$ we arrive at the form

$$\begin{aligned} I(\mathbf{m}) &:= \int_{\{\mathbf{m}\neq 0\}} |\nabla \mathbf{m}|^2 + 2t\mathbf{m}\cdot\nabla\times\mathbf{m} + t^2|\mathbf{m}|^2\,dx + K\mathcal{H}^{d-1}(A) \\ &= \int_\Omega |\nabla \mathbf{m}|^2 + 2t\mathbf{m}\cdot\nabla\times\mathbf{m} + t^2|\mathbf{m}|^2\,dx + K\mathcal{H}^{d-1}(A), \end{aligned} \tag{4.39}$$

where $A = \{\, x \in S_{\mathbf{m}} \,|\, \mathbf{m}_- = 0 \text{ or } \mathbf{m}_+ = 0\,\}$. We now find ourselves with a free-energy which is strongly related to the Oseen-Frank free energy. The set $\{\mathbf{m} \neq 0\}$ corresponds to the liquid crystal phase of the sample, whereas $\{\mathbf{m} = 0\}$ represents wherever the molecules are isotropic. Even though this appears to be an Oseen-Frank energy, because it was derived from the uniaxial Landau-de Gennes model it has some immediate advantages.

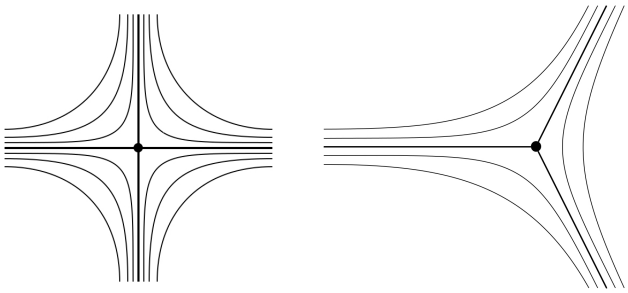


Figure 4.2: Two defect profiles

The defects shown in Figure 4.2 can be given a finite energy in this model by inserting a small core of isotropic region in the center. Secondly, weak anchoring is automatically included in the model because with variational problems set in BV, it cannot be guaranteed that a minimiser satisfies imposed boundary conditions. Unfortunately, the variational problem as given by (4.38) and (4.39) is not well-posed in SBV. This is because we do not have a control on the entirety of the jump set of $\mathbf{m}$, only the part which bounds the isotropic region. Therefore if we were to apply the direct method to (4.39) we cannot show that a minimiser exists. Hence we need make a mathematical approximation in order to allow us to properly study this problem. We propose minimising

$$I(\mathbf{m}) := \int_\Omega |\nabla \mathbf{m}|^2 + 2t\mathbf{m}\cdot\nabla\times\mathbf{m} + t^2|\mathbf{m}|^2\,dx + K\mathcal{H}^{d-1}(S_{\mathbf{m}}) \tag{4.40}$$

over $\mathcal{B}$ as given by (4.38). Then if we let $\mathbf{n} := \frac{\mathbf{m}}{s_+}$ and $J = \frac{1}{s_+^2} I$ it is clear that (4.40) can be written as

$$J(\mathbf{n}) := \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2|\mathbf{n}|^2\,dx + \tilde{K}\mathcal{H}^{d-1}(S_{\mathbf{n}})$$

over the set of admissible functions

$$\mathbf{n} \in SBV^2\left(\Omega, \mathbb{S}^2 \cup \{0\}\right). \tag{4.41}$$

This discussion has brought us to an Oseen-Frank style, free energy functional whose admissible mappings lie in SBV. We are aware that this is not a rigorous derivation but by comparison with the results of Ambrosio & Tortorelli [6], if the full Γ-limit of (4.32) and (4.33) could be found, we believe that it would be in a comparable form to (4.41).

Chapter 5

Bounded Variation Variational Problems

5.1 Introduction

When trying to model nematic or cholesteric liquid crystals, we know that many of the commonly used molecules are rod-like. Therefore any model should respect this invariance of the molecules. The Landau-de Gennes theory does this by utilising a matrix order parameter with terms such as $\mathbf{n} \otimes \mathbf{n}$ to ensure the symmetry. What we saw conclusively in the previous chapter was if we wish to use the director as a simpler order parameter, then we must consider director fields of bounded variation for full generality. We are not the first to propose the use of functions of bounded variation to apply to liquid crystal problems (see [5, 8]). However we go further than simply proposing a model. We prove the existence of a minimiser, we find various forms of the Euler-Lagrange equation, we discover solutions in simple cases, and we find minimisers for specific liquid crystal problems.

Although the analysis of SBV functions is more technical than Sobolev functions, we will show in this chapter that by studying models with director fields of such regularity, we can actually extend our more classical Sobolev space analysis from Chapters 2 and 3. For example, we will show that for large values of the cholesteric twist, the minimiser of the Oseen-Frank energy must depend on more than a single variable. Furthermore any function of z alone cannot even be a local minimiser for the SBV problem with a large enough cholesteric twist. Both of these results are consistent with the experimental data of cholesteric patterns but proved elusive in previous chapters when $\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right)$. In addition to the bounded variation material outlined in the introduction, in order to study such problems it is important to introduce some results in SBV to show that it is an appropriate space in which to set variational problems. Suppose that $\Omega \subset \mathbb{R}^d$ is an open and bounded set.

Theorem 5.1 (Closure of SBV [5])**.** *Let $\phi : [0, \infty) \to [0, \infty]$, $\theta : (0, \infty) \to (0, \infty]$ be two lower-semicontinuous, increasing functions which satisfy*

$$\lim_{t \to \infty} \frac{\phi(t)}{t} = \infty, \quad \lim_{t \to 0} \frac{\theta(t)}{t} = \infty.$$

If $(u_j) \subset SBV(\Omega, \mathbb{R})$ is a sequence such that

$$\sup_j \left\{ \int_\Omega \phi\left(|\nabla u_j|\right) \, dx + \int_{S_{u_j}} \theta\left(|u_{j+} - u_{j-}|\right) \, d\mathcal{H}^{d-1} \right\} < \infty. \tag{5.1}$$

Then if (u_j) is weak* convergent in $BV(\Omega, \mathbb{R})$ then its limit $u \in SBV(\Omega, \mathbb{R})$. Additionally

$$\liminf_{j\to\infty} \int_\Omega \phi\left(|\nabla u_j|\right) \, dx \geqslant \int_\Omega \phi\left(|\nabla u|\right) \, dx$$
$$\liminf_{j\to\infty} \int_{S_{u_j}} \theta\left(|u_{j+} - u_{j-}|\right) \, dx \geqslant \int_{S_u} \theta\left(|u_+ - u_-|\right) \, dx$$

if ϕ is convex and θ is concave.

Theorem 5.2 (Compactness of SBV [5])**.** *If $(u_j) \subset SBV(\Omega, \mathbb{R})$ is a sequence satisfying* (5.1) *and $\sup_j \|u_j\|_\infty < \infty$ then there exists some $u \in SBV(\Omega, \mathbb{R})$ such that for some subsequence $u_{j_k} \overset{*}{\rightharpoonup} u$ in BV.*

We note that these closure and compactness notions are also true in the vectorial case. See for example [36, Thm 2.1]. These two results are precisely the type of results which allow the direct method of the calculus of variations to be applied to problems involving SBV functions. Therefore from a mathematical point of view it is a sensible framework within which to study liquid crystal problems. Over the next three sections we will define our SBV variational problem and establish the existence of a minimiser and various forms of the Euler-Lagrange equation which are satisfied by a minimiser. In the final sections we will begin to show the usefulness of this SBV approach by applying it to some example nematic and cholesteric problems. In doing so we show that theoretical predictions made using an SBV framework rectify important deficiencies that exist in the Oseen-Frank setting. Section 5.5 focuses on some of the different minimiser predictions made by using SBV director fields for classic nematic problems. Then towards the end of the chapter we turn our attention back to the main cholesteric problem of this thesis and prove the existence of multidimensional minimisers (Proposition 5.16). This result is a significant step forward from what we were able to achieve without functions of bounded variation. At the end of the chapter we briefly turn our attention to smectic liquid crystals and discuss how the ideas we are using here could also be usefully applied to them, in addition to nematic and cholesteric liquid crystals.

5.2 The Problem

There are a number of small technical issues which need to be considered when setting up variational problems with functions of bounded variation. Throughout this chapter, our domain $\Omega \subset \mathbb{R}^d$ will be a bounded Lipschitz domain. We will of course want to apply boundary conditions to our problem, but this creates an issue. Using the direct method of the calculus of variations, we will be able to extract a subsequence from the minimising sequence $\left(\mathbf{n}_j\right)$ which converges weakly* in SBV. However traces are not preserved under weak* convergence. Therefore we will actually consider our variational problem over an enlarged domain Ω_ϵ in the following sense. We look to minimise the integral functional

$$I(\mathbf{n}) = \int_{\Omega_\epsilon} w(\mathbf{n}, \nabla\mathbf{n}) \, dx + K\mathcal{H}^2(S_\mathbf{n}), \tag{5.2}$$

over the set of admissible functions

$$\mathcal{A} := \left\{ \mathbf{n} \in SBV^2\left(\Omega_\epsilon, \mathbb{S}^2 \cup \{0\}\right) \,\middle|\, \mathbf{n} = \mathbf{g} \text{ on } \Omega_\epsilon \backslash \overline{\Omega} \right\}, \tag{5.3}$$

where Ω_ϵ is an open set containing Ω and $\mathbf{g} \in W^{1,2}\left(\Omega_\epsilon \setminus \Omega, \mathbb{S}^2\right)$. As we shall see, this extended domain idea allows us to prove the existence of a minimiser for our problem while at the same time incorporating weak boundary conditions since $S_{\mathbf{n}}$ is allowed to intersect $\partial\Omega$. After this section, when there is no room for confusion we will drop the subscript on the extended domain Ω_ϵ. However we maintain the understanding that we are studying an extended domain and the jump set can lie on the portion of the boundary $\partial\Omega$ where boundary conditions are applied. In terms of liquid crystal theory our Lagrangian will be the familiar one-constant Oseen-Frank free energy

$$w(\mathbf{n}, \nabla\mathbf{n}) = \left[|\nabla\mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2\right].$$

The only critical properties of the free energy density that we require for the existence proof is that it is bounded below and for any $\mathbf{n} \in \mathbb{R}^3$, $w(\mathbf{n}, \cdot)$ is a convex function.

5.3 Existence of a Minimiser

Theorem 5.3. *Consider the minimisation problem given by* (5.2) *and* (5.3)*. Then there exists an* $\mathbf{n} \in \mathcal{A}$ *such that*

$$I(\mathbf{n}) = \inf_{\mathbf{m} \in \mathcal{A}} I(\mathbf{m}).$$

Proof

This result is an adaptation of [5, Thm 5.24] to our specific setup. We have that $\inf_{\mathbf{m}\in\mathcal{A}} I(\mathbf{m}) > -\infty$, so by taking a minimising sequence $\mathbf{n}^j$, the structure of the functional itself implies

$$\int_\Omega |\nabla\mathbf{n}^j|^2 \, dx + K\mathcal{H}^{d-1}\left(S_{\mathbf{n}^j}\right) \leqslant M \tag{5.4}$$

for every j. This means we can apply Theorem 5.2 to deduce that there is a subsequence (which we relabel) such that

$$\mathbf{n}^j \overset{*}{\rightharpoonup} \mathbf{n} \quad \text{in } BV, \text{ where } \mathbf{n} \in SBV(\Omega, \mathbb{R}^3).$$

Furthermore, since $I(\mathbf{n}) < \infty$ we infer that $\mathbf{n} \in SBV^2(\Omega, \mathbb{R}^3)$. Now we can simply apply two results from the literature. The first is that under the assumption (5.4), we have that [7, Remark 13.4.2]

$$\liminf_{j\to\infty} \mathcal{H}^{d-1}(S_{\mathbf{n}^j}) \geqslant \mathcal{H}^{d-1}(S_{\mathbf{n}}). \tag{5.5}$$

The second result, Ioffe's Theorem [5, Thm 5.8], gives us the lower semicontinuity of the elastic terms so that

$$\liminf_{j\to\infty} \int_\Omega w(\mathbf{n}^j, \nabla\mathbf{n}^j)\, dx \geqslant \int_\Omega w(\mathbf{n}, \nabla\mathbf{n})\, dx. \tag{5.6}$$

Combining (5.5) and (5.6) proves the lower semicontinuity

$$\liminf_{j\to\infty} I(\mathbf{n}^j) \geqslant I(\mathbf{n}).$$

So to conclude existence we just need that $\mathbf{n} \in \mathcal{A}$. Firstly we require that $\mathbf{n} \in \mathbb{S}^2 \cup \{0\}$. This is true because weak* convergence in BV implies convergence in L^1 so there is a subsequence converging almost everywhere. The set $\mathbb{S}^2 \cup \{0\}$ is closed, hence $\mathbf{n}(x) \in \mathbb{S}^2 \cup \{0\}$. We also need to prove that

$$\mathbf{n} = \mathbf{g} \quad \text{on} \quad \Omega_\epsilon \backslash \overline{\Omega}. \tag{5.7}$$

The same reasoning applies here. The L^1 convergence of $\mathbf{n}^j$ implies pointwise convergence for a subsequence, this readily implies (5.7). Hence $\mathbf{n} \in \mathcal{A}$ and $I(\mathbf{n}) = \inf_{\mathbf{m}\in\mathcal{A}} I(\mathbf{m})$.

□

This establishes the existence of a minimiser of this problem for all values of the cholesteric twist t. It is clear that this proof easily applies to our standard liquid crystal problem where we have a cuboid domain and boundary conditions on the top and bottom faces. In other words when

$$\Omega_\epsilon = (-L_1, L_1) \times (-L_2, L_2) \times (-\epsilon, 1+\epsilon)$$

and

$$\mathcal{A} = \left\{ \mathbf{n} \in SBV^2(\Omega_\epsilon, \mathbb{S}^2 \cup \{0\}) \,\middle|\, \mathbf{n} = \mathbf{e}_1 \text{ if } z \in (-\epsilon, 0),\ \mathbf{n} = \mathbf{e}_3 \text{ if } z \in (1, 1+\epsilon) \right\}.$$

Note that we have not been including periodicity in the lateral directions for the admissible functions. We do so for simplicity but periodicity could be included for this problem by using another extended domain idea and requiring that $\mathbf{n}(x, y, z) = \mathbf{n}(x + 2L_1, y, z) = \mathbf{n}(x, y + 2L_2, z)$.

5.4 Euler-Lagrange Equation

The logical progression, once we know that minimisers exist, is to find the Euler-Lagrange equation for this problem so that we can begin to find candidate minimisers. This is a relatively simple affair when studying problems in Sobolev spaces; we use an outer variation to derive an integral equation which is the weak form of some set of partial differential equations. However the discontinuity set $S_\mathbf{n}$ creates additional issues. For example if we were to perform an outer variation with some smooth function ϕ the discontinuity set would remain unchanged. To overcome this problem we will be using an inner variation to derive a form of the Euler-Lagrange equation. Then we will show that if the discontinuity set $\overline{S}_\mathbf{n}$ has sufficient regularity we can write the Euler-Lagrange equation in other forms.

The following progression of results mirrors those found in [5, Section 7.4] but we are investigating a different Lagrangian. Therefore we will utilise some results from their work and adapt their arguments to our situation as necessary. The functional we will be using throughout this section is given by

$$I(\mathbf{n}) = \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2 \, dx + K\mathcal{H}^{d-1}(S_\mathbf{n}), \tag{5.8}$$

with the set of admissible functions as given in (5.3).

Theorem 5.4. *Let* $\mathbf{n} \in \mathcal{A}$ *be a minimiser of* (5.8)*. Then*

$$\begin{aligned} 0 = &\int_\Omega \left[|\nabla \mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2|\mathbf{n}|^2\right]\operatorname{div}\phi - 2\nabla\mathbf{n} : (\nabla\mathbf{n}\nabla\phi) - 2t\nabla\phi : \mathbf{A}\, dx \\ &+ K\int_{S_\mathbf{n}} div^{S_\mathbf{n}}\,\phi\, d\mathcal{H}^{d-1} \end{aligned} \tag{5.9}$$

for any $\phi \in C_0^1\left(\Omega, \mathbb{R}^d\right)$*, where* $\mathbf{A}_{i,j} = \left(\frac{\partial \mathbf{n}}{\partial x_i}\times\mathbf{n}\right)_j$.

Proof

As mentioned above we will be using an inner variation to derive (5.9). Take a $\phi \in C_0^1\left(\Omega, \mathbb{R}^d\right)$. Then for $\epsilon > 0$ sufficiently small, the map $\psi_\epsilon(x) := x + \epsilon\phi(x)$ is a diffeomorphism of Ω onto itself. Therefore if we let $y = \psi_\epsilon(x)$ and define $\mathbf{n}_\epsilon(y) := \mathbf{n}\left(\psi_\epsilon^{-1}(y)\right)$, we know that

$$I(\mathbf{n}_\epsilon) \geqslant I(\mathbf{n}).$$

In other words

$$\frac{d}{d\epsilon} I(\mathbf{n}_\epsilon)\Big|_{\epsilon=0} = 0. \tag{5.10}$$

In order to use (5.10) we will find an expression for $I(\mathbf{n}_\epsilon) - I(\mathbf{n})$. By performing a change of variables we find

$$\begin{aligned} &\int_\Omega |\nabla\mathbf{n}_\epsilon(y)|^2 + 2t\mathbf{n}_\epsilon(y)\cdot\nabla\times\mathbf{n}_\epsilon(y) + t^2|\mathbf{n}_\epsilon(y)|^2\, dy - \int_\Omega |\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2|\mathbf{n}|^2\, dx \\ &= \int_\Omega \left[\left|\nabla\mathbf{n}(x)\nabla\psi_\epsilon^{-1}\left(\psi_\epsilon(x)\right)\right|^2 + 2t\mathbf{n}_i(x)\epsilon_{ijk}\left(\nabla\mathbf{n}\nabla\psi_\epsilon^{-1}\left(\psi_\epsilon(x)\right)\right)_{kj} + t^2|\mathbf{n}(x)|^2\right]\left|\det\nabla\psi_\epsilon(x)\right|\, dx \\ &\quad - \int_\Omega |\nabla\mathbf{n}|^2 - 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2|\mathbf{n}|^2\, dx. \end{aligned} \tag{5.11}$$

But we only need to consider terms up to order ϵ and we can easily calculate that

$$\begin{aligned} \nabla\psi_\epsilon^{-1}\left(\psi_\epsilon(x)\right) &= \left(I + \epsilon\nabla\phi(x)\right)^{-1} = I - \epsilon\nabla\phi(x) + O(\epsilon^2) \\ \det\nabla\psi_\epsilon(x) &= \det\left(I + \epsilon\nabla\phi(x)\right) = 1 + \epsilon\operatorname{div}\phi(x) + O(\epsilon^2). \end{aligned}$$

Applying these approximations to (5.11) allows us to deduce that

$$\begin{aligned} &I(\mathbf{n}_\epsilon) - I(\mathbf{n}) \\ &= \int_\Omega \left[|\nabla\mathbf{n}(I - \epsilon\nabla\phi)|^2 + 2t\mathbf{n}_i\epsilon_{ijk}\left(\nabla\mathbf{n}(1 - \epsilon\nabla\phi)\right)_{kj} + t^2|\mathbf{n}|^2\right](1 + \epsilon\operatorname{div}\phi)\, dx \\ &\quad - \int_\Omega |\nabla\mathbf{n}|^2 - 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2|\mathbf{n}|^2\, dx + O(\epsilon^2) + K\left(\mathcal{H}^{d-1}(S_{\mathbf{n}_\epsilon}) - \mathcal{H}^{d-1}(S_\mathbf{n})\right) \\ &= \epsilon\int_\Omega \left[|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2|\mathbf{n}|^2\right]\operatorname{div}\phi - 2\nabla\mathbf{n} : (\nabla\mathbf{n}\nabla\phi) - 2t\nabla\phi : \mathbf{A}\, dx + O(\epsilon^2) \\ &\quad + K\left(\mathcal{H}^{d-1}(S_{\mathbf{n}_\epsilon}) - \mathcal{H}^{d-1}(S_\mathbf{n})\right), \end{aligned} \tag{5.12}$$

where $\mathbf{A}$ is given in the statement. To finish the proof we just need to apply [5, Thm 7.31] concerning the first variation of the area to deduce that

$$K\left(\mathcal{H}^{d-1}(S_{\mathbf{n}_\epsilon}) - \mathcal{H}^{d-1}(S_\mathbf{n})\right) = \epsilon K\int_{S_\mathbf{n}} \operatorname{div}^{S_\mathbf{n}}\phi\, d\mathcal{H}^{d-1} + O(\epsilon^2).$$

Then dividing (5.12) by ϵ and taking the limit as $\epsilon \to 0$ gives us the statement.

□

We cannot easily formulate (5.9) as the weak form of some strong equation due to the unknown regularity of the discontinuity set $S_{\mathbf{n}}$. Therefore in the following results we will assume some *a-priori* regularity of the discontinuity set, or the function itself, and find equivalent forms of the Euler-Lagrange equation given the regularity condition.

Proposition 5.5. *Suppose* $\mathbf{n} \in \mathcal{A}$ *is a minimiser of* (5.8)*. Let* $A \subset\subset \Omega$ *and suppose that*

$$\overline{S}_{\mathbf{n}} \cap A = \{ (z, \phi(z)) \mid z \in D \}, \tag{5.13}$$

where $D \subset \mathbb{R}^{d-1}$ *is an open set and* $\phi \in C^1(D, \mathbb{R})$*. Then*

$$\int_{A \setminus \overline{S}_{\mathbf{n}}} \nabla \mathbf{v} : \nabla \mathbf{n} + t(\mathbf{v} \cdot \nabla \times \mathbf{n} + \mathbf{n} \cdot \nabla \times \mathbf{v}) - (\mathbf{n} \cdot \mathbf{v}) \left(|\nabla \mathbf{n}|^2 + 2t \mathbf{n} \cdot \nabla \times \mathbf{n} \right) dx = 0,$$

for all $\mathbf{v} \in C_0^\infty \left(A, \mathbb{R}^k \right)$.

Proof

The local regularity of the discontinuity gives us the decomposition that

$$A = A^+ \cup A^- \cup \left(A \cap \overline{S}_{\mathbf{n}} \right)$$

where $A^+ = \{ (z,t) \in A \mid t > \phi(z) \}$ and $A^- = \{ (z,t) \in A \mid t < \phi(z) \}$ are open sets. We take some $\mathbf{v} \in C_0^\infty \left(A, \mathbb{R}^k \right)$ and we will consider the outer variation

$$\mathbf{n}_\epsilon(x) := \begin{cases} P(\mathbf{n} + \epsilon \mathbf{v}) & x \in A^+ \\ \mathbf{n}(x) & x \in A^- \end{cases},$$

where

$$P(x) = \begin{cases} \frac{x}{|x|} & |x| \in \left(\frac{2}{3}, \frac{4}{3} \right) \\ 0 & |x| < \frac{1}{3} \end{cases}$$

is the projection map onto $\mathbb{S}^2 \cup \{0\}$. Using this variation we can certainly say that $\frac{d}{d\epsilon} I(\mathbf{n}_\epsilon)\Big|_{\epsilon=0} = 0$. So by arguing in the same manner as variational problems in Sobolev spaces we find

$$\begin{aligned} 0 &= \int_{\{\mathbf{n} \in \mathbb{S}^2\} \cap A^+} \nabla \mathbf{v} : \nabla \mathbf{n} + t(\mathbf{v} \cdot \nabla \times \mathbf{n} + \mathbf{n} \cdot \nabla \times \mathbf{v}) - (\mathbf{n} \cdot \mathbf{v}) \left(|\nabla \mathbf{n}|^2 + 2t \mathbf{n} \cdot \nabla \times \mathbf{n} \right) dx \\ &= \int_{A^+} \nabla \mathbf{v} : \nabla \mathbf{n} + t(\mathbf{v} \cdot \nabla \times \mathbf{n} + \mathbf{n} \cdot \nabla \times \mathbf{v}) - (\mathbf{n} \cdot \mathbf{v}) \left(|\nabla \mathbf{n}|^2 + 2t \mathbf{n} \cdot \nabla \times \mathbf{n} \right) dx. \end{aligned}$$

We obtain a similar equation in A^- using the same logic. Integrating by parts on the terms involving the gradients of $\mathbf{v}$ we find that this is the weak form of

$$\begin{aligned} \Delta \mathbf{n} - 2t \nabla \times \mathbf{n} &= -\mathbf{n} \left(|\nabla \mathbf{n}|^2 + 2t \mathbf{n} \cdot \nabla \times \mathbf{n} \right) && \text{in } A^+ \\ \frac{\partial \mathbf{n}}{\partial \boldsymbol{\nu}} + t \mathbf{n} \times \boldsymbol{\nu} &= 0 && \text{on } \partial A^+ \cap \overline{S}_{\mathbf{n}}, \end{aligned} \tag{5.14}$$

where $\boldsymbol{\nu}$ is the normal to the set $\partial A^+ \cap \overline{S_{\mathbf{n}}}$.

□

This is a reassuring proposition since it proves that away from the jump set, the minimiser $\mathbf{n}$ must satisfy the same equation as would be satisfied by a Sobolev director field on the entirety of the domain. However by assuming a little more regularity for the function and its jump set we can strengthen the Euler-Lagrange equation still further.

Theorem 5.6. *Suppose* $\mathbf{n} \in \mathcal{A}$ *is a minimiser of* (5.8). *Let* $A \subset\subset \Omega$ *and suppose that* $\mathbf{n} \in W^{2,2}\left(A \setminus \overline{S_{\mathbf{n}}}\right)$ *and* $\overline{S}_{\mathbf{n}} \cap A$ *is given as in* (5.13), *where* $D \subset \mathbb{R}^{d-1}$ *is an open set and* $\phi \in C^{1,\gamma}(D, \mathbb{R})$. *Then for every* $\boldsymbol{\eta} \in C_0^\infty(A, \mathbb{R}^d)$

$$\int_{S_{\mathbf{n}} \cap A} \left[|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2\right]^{\pm} \boldsymbol{\nu} \cdot \boldsymbol{\eta}\, d\mathcal{H}^{d-1} = K \int_{S_{\mathbf{n}} \cap A} div^{S_{\mathbf{n}}} \boldsymbol{\eta}\, d\mathcal{H}^{d-1}, \tag{5.15}$$

where $\boldsymbol{\nu}$ *is the upper normal to* $\overline{S}_{\mathbf{n}} \cap A$.

Proof

The essence of the proof is to use integration by parts on equation (5.9). We recall that the matrix $\mathbf{A}$ is defined by $\mathbf{A}_{i,j} = \sum_{a,b} \epsilon_{jab} \mathbf{n}_{a,i} \mathbf{n}_b$. In order to perform the integration by parts we note initially that $\mathbf{n} \in W^{2,2}(A^+) \cap W^{2,2}(A^-) \cap \mathcal{A}$. We begin with the following calculation

$$\begin{aligned}
&\int_{A^+} \left[|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2\right] \mathrm{div}\boldsymbol{\eta} - 2\nabla \mathbf{n} : (\nabla \mathbf{n} \nabla \boldsymbol{\eta}) - 2t\nabla \boldsymbol{\eta} : \mathbf{A}\, dx \\
&= \int_{S_{\mathbf{n}} \cap A} -\left[|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2\right]^+ \boldsymbol{\nu} \cdot \boldsymbol{\eta} + 2\mathbf{n}_{i,j} \mathbf{n}_{i,a} \eta_a \nu_j + 2t\eta_a \mathbf{A}_{a,j} \nu_j\, d\mathcal{H}^{d-1} \\
&\quad + \int_{A^+} -\eta_a \frac{\partial}{\partial x_a}\left(\mathbf{n}_{i,j}\mathbf{n}_{i,j} + 2t\mathbf{n}_i \epsilon_{ijk} \mathbf{n}_{k,j} + t^2 \mathbf{n}_i \mathbf{n}_i\right) + \eta_a \frac{\partial}{\partial x_j}\left(2\mathbf{n}_{i,j}\mathbf{n}_{i,a} + 2t\mathbf{A}_{a,j}\right) dx.
\end{aligned}$$

In order to simplify this we note that on $\partial A^+ \cap \overline{S_{\mathbf{n}}}$

$$\mathbf{n}_{i,j}\mathbf{n}_{i,a}\eta_a\nu_j + t\eta_a \mathbf{A}_{a,j}\nu_j = \mathbf{n}_{i,a}\eta_a\left(\frac{\partial \mathbf{n}_i}{\partial \boldsymbol{\nu}} + t(\mathbf{n} \times \boldsymbol{\nu})_i\right) = 0.$$

This holds because of the natural boundary condition from equation (5.14). Furthermore, using the Euler-Lagrange equation from (5.14) we can also deduce

$$\begin{aligned}
&\frac{\partial}{\partial x_a}\left(\mathbf{n}_{i,j}\mathbf{n}_{i,j} + 2t\mathbf{n}_i \epsilon_{ijk}\mathbf{n}_{k,j}\right) + \frac{\partial}{\partial x_j}\left(2\mathbf{n}_{i,j}\mathbf{n}_{i,a} + 2t\mathbf{A}_{a,j}\right) \\
&= 2(\mathbf{n}_{i,jj}\mathbf{n}_{i,a} - 2t\mathbf{n}_{i,a}\epsilon_{ijk}\mathbf{n}_{k,j}) \\
&= 2\left[|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n}\right] \sum_i \mathbf{n}_{i,a}\mathbf{n}_i = 0.
\end{aligned}$$

Therefore

$$\begin{aligned}
&\int_{A^+} \left[|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2\right] \mathrm{div}\boldsymbol{\eta} - 2\nabla \mathbf{n} : (\nabla \mathbf{n} \nabla \boldsymbol{\eta}) - 2t\nabla \boldsymbol{\eta} : \mathbf{A}\, dx \\
&= \int_{S_{\mathbf{n}} \cap A} -\left[|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2\right]^+ \boldsymbol{\nu} \cdot \boldsymbol{\eta} dx,
\end{aligned}$$

and a similar equation holds in the region A^-. This gives us the assertion.

□

Remark 5.7. *In [5] they were able to extend Proposition 5.6 without assuming the extra regularity that* $\mathbf{n} \in W^{2,2}(A \setminus \overline{S_{\mathbf{n}}})$*. In order to be able to do the same here we would require some a-priori knowledge about the regularity of weak solutions to* (5.14) *which we do not have.*

Our final remark on the Euler-Lagrange equation comes courtesy of the divergence theorem on manifolds.

Remark 5.8. *[5, Remark 7.39] If in addition to the assumptions of Theorem 5.6, the set* $A \cap \overline{S}_{\mathbf{n}}$ *can be written as the graph of a* C^2 *function* ϕ*, then we find that* (5.15) *can be written as*

$$-Kdiv\left(\frac{\nabla\phi}{\sqrt{1+|\nabla\phi|^2}}\right) = -KH = \left[|\nabla\mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\times\mathbf{n} + t^2|\mathbf{n}|^2\right]^{\pm} \tag{5.16}$$

where H *is the mean scalar curvature of the set* $\overline{S}_{\mathbf{n}} \cap A$*.*

Local Minimisers

One final aspect of bounded variation problems to introduce in this section which we have not covered up to this point, is the notion of local minimisers. It is more difficult to define local minimisers for bounded variation problems because the discontinuity set needs to be varied simultaneously with the elastic energy. We follow the definition from [5, Definition 6.6].

Definition 5.9 (Local minimiser)**.** $\mathbf{n} \in \mathcal{A}$ *is a local minimiser of* I *if*

$$I(\mathbf{n}) \leqslant I(\mathbf{m})$$

whenever $\mathbf{m} \in \mathcal{A}$ *and* $\{\mathbf{n} \neq \mathbf{m}\} \subset\subset \Omega_\epsilon$*.*

This definition is local in the sense that, loosely speaking, the candidate needs only to be a minimiser amongst admissible functions with the same boundary values. We cannot use the notions of strong and weak local minimisers as we could for Sobolev spaces because it would result in absurd predictions. For example any function $\mathbf{n} \in SBV(\Omega, \mathbb{S}^2)$ with $\nabla\mathbf{n} = 0$ and any number of jumps of fixed magnitude would be a strong local minimiser of the nematic problem in the sense of Chapter 1.

Remark 5.10. *It should be noted that if we set up a bounded variation problem where we wish to apply boundary conditions around the entirety of the boundary then* $\overline{\Omega} \subset \Omega_\epsilon$*. In this situation there is no difference between a local minimiser and a global minimiser.*

5.5 Lavrentiev Phenomena for Nematic Problems

The natural step to take once we have the Euler-Lagrange equations established is to find solutions with a non-trivial jump set. Clearly any $\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right)$ which satisfies the classical Euler-Lagrange equation also satisfies those in the previous section. In this section we will examine two problems associated with the nematic energy

$$I(\mathbf{n}) = \int_\Omega |\nabla\mathbf{n}|^2\, dx + K\mathcal{H}^{d-1}(S_{\mathbf{n}}). \tag{5.17}$$

For the first we will look for minimisers of (5.17) when the domain is a unit ball in two or more dimensions with radial boundary conditions. We will show that by removing a small core of isotropic liquid crystal we can lower the energy and prove a Lavrentiev gap phenomenon between Sobolev and SBV functions. In the second we set the problem in a cuboid with constant boundary conditions on the top and bottom faces which are perpendicular to each other. In this situation we can show another Lavrentiev gap phenomenon by finding a global minimiser in both the Sobolev and SBV spaces.

Theorem 5.11. *Consider the energy functional I as given in* (5.17)*. Let $d \geqslant 2$, if $\Omega = \left\{ x \in \mathbb{R}^d \,\middle|\, |x| < 1 \right\}$ and the sets of admissible functions are given by*

$$\mathcal{A} := \left\{ \mathbf{n} \in SBV^2\left(\Omega, \mathbb{S}^{d-1} \cup \{0\}\right) \,\middle|\, \mathbf{n}(x) = x \text{ on } \partial\Omega \right\},$$

and

$$\mathcal{B} := \left\{ \mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^{d-1}\right) \,\middle|\, \mathbf{n}(x) = x \text{ on } \partial\Omega \right\}.$$

Then if $K > 1$,

$$\inf_{\mathbf{n}\in\mathcal{A}} I(\mathbf{n}) < \inf_{\mathbf{n}\in\mathcal{B}} I(\mathbf{n}). \tag{5.18}$$

Proof

The infimum over the admissible set $\mathcal{B}$ has been extensively studied and Lin [60], among others, showed that when $d \geqslant 3$, $\mathbf{n}(x) = \frac{x}{|x|}$ is a global minimiser of I with an energy of $\frac{d-1}{d-2}S_{d-1}$, where S_{d-1} is the surface area of the sphere $\mathbb{S}^{d-1}$. In the case $d = 2$, $\mathcal{B}$ is empty so we consider the infimum from (5.18) to be infinite. To prove the statement we merely need to find a function $\mathbf{n} \in \mathcal{A}$ such that $I(\mathbf{n}) < \frac{d-1}{d-2}S_{d-1}$. However we will go further and find a solution of the Euler-Lagrange equation with this property. Let $\alpha \in (0, 1)$ and consider the function

$$\mathbf{n}_\alpha(x) = \begin{cases} \frac{x}{|x|} & |x| > \alpha \\ \\ 0 & |x| < \alpha. \end{cases}$$

It is clear that $\mathbf{n}_\alpha \in \mathcal{A}$ and $S_{\mathbf{n}_\alpha} = \{\, |x| = \alpha \,\}$. This set (up to a rotation) can easily be locally written as the graph of the C^2 function

$$\phi(x) = \sqrt{\alpha^2 - \sum_{i=0}^{d-1} x_i^2}.$$

Then when we substitute this into (5.16) we find

$$\begin{aligned} -K\mathrm{div}\left(\frac{\nabla\phi}{\sqrt{1+|\nabla\phi|^2}}\right) &= -K\mathrm{div}\left(-\frac{x}{\alpha}\right) \\ &= \frac{(d-1)K}{\alpha} \\ &= K\alpha\left[|\nabla\mathbf{n}_\alpha|^2\right]^{\pm}. \end{aligned}$$

Therefore the Euler-Lagrange equation is satisfied when $\alpha = \frac{1}{K}$ in every dimension $d \geqslant 2$. The associated energy of this state is given by

$$\begin{aligned} I\left(\mathbf{n}_{\frac{1}{K}}\right) &= \int_{\frac{1}{K}<|x|<1} \frac{(d-1)}{|x|^2}\, dV + K\left[K^{-(d-1)} S_{d-1}\right] \\ &= \begin{cases} \frac{d-1}{d-2} S_{d-1} - \frac{S_{d-1}}{(d-2)K^{d-2}} & d \geqslant 3 \\ \\ 2\pi\left[1 + \log K\right] & d = 2 \end{cases} \\ &= \begin{cases} \inf_{\mathbf{m}\in\mathcal{B}} I(\mathbf{m}) - \frac{S_{d-1}}{(d-2)K^{d-2}} & d \geqslant 3 \\ \\ 2\pi\left[1 + \log K\right] & d = 2. \end{cases} \end{aligned}$$

This proves the Lavrentiev gap phenomenon and we have also found a strong candidate for the minimiser of the bounded variation problem: $\mathbf{n}_{\frac{1}{K}}$.

□

For our second example we study a nematic liquid crystal problem, similar to the homeotropic problem from Theorem 3.1, in our new SBV setting. We look to minimise

$$I(\mathbf{n}) = \int_\Omega |\nabla \mathbf{n}|^2\, dx + K\mathcal{H}^{d-1}(S_{\mathbf{n}}) \tag{5.19}$$

where $\Omega = (-L_1, L_1) \times (-L_2, L_2) \times (0, d)$ and the set of admissible functions is given by

$$\mathcal{A} := \left\{ \mathbf{n} \in SBV^2\left(\Omega, \mathbb{S}^2 \cup \{0\}\right) \,\middle|\, \mathbf{n}|_{z=0} = \mathbf{e}_1,\ \mathbf{n}|_{z=d} = \mathbf{e}_3 \right\}. \tag{5.20}$$

For the next two results we need to utilise a result about the one-dimensional restrictions for SBV functions (See [5, Remark 3.104] or [20, Section 1]).

Theorem 5.12. *Let $U \subset \mathbb{R}^d$ be an open set, $\zeta \in \mathbb{S}^{d-1}$. Define $A := \left\{x \in \mathbb{R}^d \,|\, x \cdot \zeta = 0\right\}$. If $\mathbf{n} \in SBV\left(U, \mathbb{R}^k\right)$, then for $\mathcal{H}^{d-1}$ almost every $x \in A$*

$$\mathbf{m}(t) := \mathbf{n}(x + t\zeta) \in SBV\left(U_{x\zeta}, \mathbb{R}^k\right),$$

where $U_{x\zeta} := \{\, t \in \mathbb{R} \,|\, x + t\zeta \in U \,\}$. Furthermore $S_{\mathbf{m}} = (S_{\mathbf{n}})_{x\zeta}$.

Theorem 5.13. *If $K > \frac{\pi^2}{4d}$ then the unique global minimiser of* (5.19) *over* (5.20) *is given by*

$$\mathbf{n}^* = \begin{pmatrix} \cos\left(\frac{\pi z}{2d}\right) \\ 0 \\ \sin\left(\frac{\pi z}{2d}\right) \end{pmatrix}.$$

If $K < \frac{\pi^2}{4d}$ then the global minimisers are given by the one parameter family

$$\mathbf{n}'_\alpha = \begin{cases} \mathbf{e}_1 & z \in (0, \alpha) \\ \\ \mathbf{e}_3 & z \in (\alpha, 1), \end{cases}$$

for $\alpha \in [0, d]$. In the critical case both $\mathbf{n}'_\alpha$ and $\mathbf{n}^*$ are global minimisers.

Proof

We take an arbitrary $\mathbf{n} \in \mathcal{A}$. Then we define the set

$$\Gamma(S_{\mathbf{n}}) = \{\,(x,y)\,|\,(x,y,z) \in S_{\mathbf{n}} \text{ for some } z\,\}.$$

This is the projection of $S_{\mathbf{n}}$ onto the (x,y)-plane. Then we have the following inequality

$$I(\mathbf{n}) \geqslant \int_{\Gamma(S_{\mathbf{n}})^c} \int_0^d |\nabla \mathbf{n}|^2 \, dz\, dx\, dy + K\mathcal{H}^2(\Gamma(S_{\mathbf{n}})), \tag{5.21}$$

where $\Gamma(S_{\mathbf{n}})^c = (-L_1, L_1) \times (-L_2, L_2) \setminus \Gamma(S_{\mathbf{n}})$. From (5.21) we can use our knowledge from previous work to deduce a further inequality. By Theorem 5.12 it is clear that for $\mathcal{H}^2$ almost every $(x,y) \in \Gamma(S_{\mathbf{n}})$, that $\mathbf{m}(\cdot) := \mathbf{n}(x,y,\cdot) \in SBV^2\left((-\epsilon, d+\epsilon), \mathbb{S}^2 \cup \{0\}\right)$. However we know that $S_{\mathbf{m}} = \emptyset$. Therefore

$$\mathbf{n}(x,y,\cdot) \in W^{1,2}\left((0,d), \mathbb{S}^2\right), \;\; \mathbf{n}(x,y,0) = \mathbf{e}_1, \;\; \mathbf{n}(x,y,d) = \mathbf{e}_3. \tag{5.22}$$

We have already shown in Chapter 2 that any function satisfying the conditions in (5.22) also satisfies

$$\int_0^d |\nabla \mathbf{n}(x,y,z)|^2 \, dz \geqslant \frac{\pi^2}{4d}.$$

By applying this reasoning to equation (5.21) we get

$$I(\mathbf{n}) \geqslant \frac{\pi^2}{4d}\mathcal{H}^2(\Gamma(S_{\mathbf{n}})^c) + K\mathcal{H}^2(\Gamma(S_{\mathbf{n}})). \tag{5.23}$$

Now we split the proof into the three cases. First we suppose that $K > \frac{\pi^2}{4d}$. Then have the following inequality

$$I(\mathbf{n}) \geqslant \frac{\pi^2}{4d}(4L_1L_2), \tag{5.24}$$

with a necessary condition for equality being

$$\mathcal{H}^2(\Gamma(S_{\mathbf{n}})) = 0. \tag{5.25}$$

Suppose that $\mathbf{n}$ satisfies (5.25) and achieves equality in (5.24). These two assumptions allow us to immediately deduce

$$\int_0^1 |\nabla \mathbf{n}|^2 \, dx \geqslant \frac{\pi^2}{4d},$$

for $\mathcal{H}^2$ almost every, $(x,y) \in (-L_1, L_1) \times (-L_2, L_2)$. Hence

$$I(\mathbf{n}) \geqslant \frac{\pi^2 L_1 L_2}{d} + K\mathcal{H}^2(S_{\mathbf{n}}) \geqslant \frac{\pi^2 L_1 L_2}{d},$$

with equality only if $\mathcal{H}^2(S_{\mathbf{n}}) = 0$. Therefore equality can only be achieved if and only if $\mathbf{n} = \mathbf{n}^*$, the unique minimum over Sobolev functions. The second case where $K < \frac{\pi^2}{4d}$ is a very similar one. We have the inequality (from (5.23)) that

$$I(\mathbf{n}) \geqslant K(4L_1L_2), \tag{5.26}$$

with a necessary condition for equality being

$$\mathcal{H}^2(\Gamma(S_{\mathbf{n}})^c) = 0. \tag{5.27}$$

As before, if we suppose that $\mathbf{n}$ satisfies (5.27), then we deduce that equality in (5.26) implies

$$I(\mathbf{n}) = \int_\Omega |\nabla \mathbf{n}|^2 \, dx + K\mathcal{H}^2\left(S_{\mathbf{n}}\right) \geqslant \int_\Omega |\nabla \mathbf{n}|^2 \, dx + K\mathcal{H}^2\left(\Gamma(S_{\mathbf{n}})\right) \geqslant 4KL_1L_2$$

which has equality when $\nabla \mathbf{n} = 0$ and $\mathcal{H}^2(S_{\mathbf{n}}) = \mathcal{H}^2(\Gamma(S_{\mathbf{n}})) = 4L_1L_2$. These relations only hold when

$$S_{\mathbf{n}} = \{\, (x, y, z) \,|\, z = \alpha \,\}.$$

Hence $\mathbf{n} = \mathbf{n}'_\alpha$ for some $\alpha \in [0, d]$. The critical case $K = \frac{\pi^2}{4d}$, immediately follows from (5.23).

□

5.6 Cholesteric Problem

We are now in a position to return to our central cholesteric problem in three dimensions and tread some new ground in our bounded variation framework. Recall that when the problem was set in a Sobolev space we were able to prove that the minimiser among functions of z only was the global minimum of the whole problem if t was sufficiently small (Theorem 2.18). However we were not able to deduce any conclusive result when t was large. In contrast to these difficulties, in the new setting we can demonstrate that if the cholesteric twist is small and the constant K is large, the minimum of the variational problem is the smooth one variable minimiser from Theorem 2.18. Whereas if the cholesteric twist is large enough, the minimiser of the problem cannot be a function of a single variable. We consider the functional

$$I(\mathbf{n}) = \int_\Omega |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{n}|^2 \, dx + K\mathcal{H}^2(S_{\mathbf{n}}), \tag{5.28}$$

over the following set of admissible functions

$$\mathcal{A} := \left\{ \mathbf{n} \in SBV^2\left(\Omega, \mathbb{S}^2 \cup \{0\}\right) \,\middle|\, \mathbf{n}|_{z=0} = \mathbf{e}_1,\ \mathbf{n}|_{z=d} = \mathbf{e}_3,\ \mathbf{n}|_{x=-L_1} = \mathbf{n}|_{x=L_1},\ \mathbf{n}|_{y=-L_2} = \mathbf{n}|_{y=L_2} \right\}. \tag{5.29}$$

We have reintroduced periodicity to the problem to ensure that we can directly compare the predictions of the classical Sobolev space model and our new discontinuous director field model. We did not need to include periodicity in x and y for our admissible functions when studying the nematic problem because it yielded a stronger result. If a function of z is a global minimum without periodicity then it certainly will be with it.

Theorem 5.14. *There exists constants $t^*, K^* > 0$ such that if $t < t^*$ and $K > K^*$, then the unique global minimum of* (5.28) *over* (5.29) *is the smooth function* $\mathbf{n}(z)$ *defined in* (2.45).

Proof

During this proof, C will represent any arbitrary positive constant. As such its value may not be constant during calculations. Let $\mathbf{n}$ be the smooth minimiser defined by (2.45) and let $\mathbf{m} \in \mathcal{A}$ be arbitrary. The main work of the proof is to show that

$$I(\mathbf{m}) - I(\mathbf{n}) \geqslant \int_\Omega |\nabla \mathbf{m} - \nabla \mathbf{n}|^2 + 2t\,(\mathbf{n} - \mathbf{m}) \cdot \nabla \times (\mathbf{n} - \mathbf{m}) - \lambda |\mathbf{n} - \mathbf{m}|^2 + (\lambda + t^2)\left[|\mathbf{m}|^2 - 1\right] dx \\ - C(1+t)\mathcal{H}^2\left(S_{\mathbf{m}}\right) + K\mathcal{H}^2\left(S_{\mathbf{m}}\right), \tag{5.30}$$

where $\lambda := |\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \times \mathbf{n}$. We start with a simple rearrangement

$$\begin{aligned} I(\mathbf{m}) - I(\mathbf{n}) &= \int_\Omega |\nabla \mathbf{m}|^2 - |\nabla \mathbf{n}|^2 + 2t\mathbf{m} \cdot \nabla \times \mathbf{m} - 2t\mathbf{n} \cdot \nabla \times \mathbf{n} + t^2|\mathbf{m}|^2 - t^2\, dx + K\mathcal{H}^2(S_{\mathbf{m}}) \\ &= \int_\Omega |\nabla \mathbf{m} - \nabla \mathbf{n}|^2 + 2t(\mathbf{m} - \mathbf{n}) \cdot \nabla \times (\mathbf{m} - \mathbf{n}) - \lambda |\mathbf{n} - \mathbf{m}|^2 + (\lambda + t^2)\left[|\mathbf{m}|^2 - 1\right] dx \\ &\quad + 2\int_\Omega \nabla \mathbf{n} : \nabla \mathbf{m} + t(\mathbf{n} \cdot \nabla \times \mathbf{m} + \mathbf{m} \cdot \nabla \times \mathbf{n}) - \lambda \mathbf{m} \cdot \mathbf{n}\, dx + K\mathcal{H}^2\left(S_{\mathbf{m}}\right). \end{aligned} \tag{5.31}$$

Clearly to show (5.30), we need to prove that the final integral term in the above equation can be estimated by $C(1+t)\mathcal{H}^2\left(S_{\mathbf{m}}\right)$. This is possible because it is almost the weak form of the Euler-Lagrange equation which is satisfied by $\mathbf{n}$. We know that

$$\Delta \mathbf{n} - 2t\nabla \times \mathbf{n} + \lambda \mathbf{n} = 0.$$

Hence by multiplying by $\mathbf{m}$ and integrating we get

$$\int_\Omega \mathbf{m} \cdot (\Delta \mathbf{n} - 2t\nabla \times \mathbf{n} + \lambda \mathbf{n})\; dx = 0.$$

Integration by parts is a little different in SBV because we have the discontinuity set to deal with. However a generalised Gauss-Green formula still holds.

Theorem 5.15. *[7, Thm 10.2.1] If $U \subset \mathbb{R}^d$ is an open set (with Lipschitz boundary), $f \in SBV(U, \mathbb{R})$, and $\phi \in C^1\left(\overline{U}, \mathbb{R}^3\right)$ then*

$$\int_U \phi \cdot \nabla f\, dx + \int_{S_f \cap U} (f^+ - f^-)\phi \cdot \boldsymbol{\nu}\, d\mathcal{H}^{d-1} = \int_U \phi \cdot Df = -\int_U f \operatorname{div} \phi\, dx + \int_{\partial U} f\phi \cdot \boldsymbol{\nu}\, d\mathcal{H}^{d-1}.$$

By applying the above equation to each term of $\mathbf{m}$ separately we get

$$\int_\Omega \nabla \mathbf{m} \cdot \nabla \mathbf{n}\, dx = -\int_\Omega \mathbf{m} \cdot \Delta \mathbf{n}\, dx + \int_{\partial\Omega} \mathbf{m} \cdot (\nabla \mathbf{n} \cdot \boldsymbol{\nu})\, d\mathcal{H}^2 - \sum_i \int_{S_{\mathbf{m}_i}} (\mathbf{m}_i^+ - \mathbf{m}_i^-) \nabla \mathbf{n} \cdot \boldsymbol{\nu}\, d\mathcal{H}^2. \tag{5.32}$$

The term around the boundary can be shown to be zero using our knowledge of $\mathbf{n}$ and the boundary conditions for $\mathbf{m}$. On the lateral faces we simply have that $\nabla \mathbf{n} \cdot \boldsymbol{\nu} = 0$ and on the top and bottom faces we have that

$$\mathbf{m} \cdot (\nabla \mathbf{n} \cdot \boldsymbol{\nu})|_{z=0} = -\mathbf{n}_1'(0) = \theta' \sin(\theta)\cos(tz) - t\cos(\theta)\sin(tz)\Big|_{z=0} = 0$$

and

$$\mathbf{m} \cdot (\nabla \mathbf{n} \cdot \boldsymbol{\nu})|_{z=d} = \mathbf{n}_3'(d) = \theta' \cos(\theta)\Big|_{z=d} = 0.$$

Furthermore the integral over the jump set in (5.32) can easily be estimated by

$$\left| \sum_i \int_{S_{\mathbf{m}_i}} (\mathbf{m}_i^+ - \mathbf{m}_i^-) \nabla \mathbf{n} \cdot \boldsymbol{\nu} \, d\mathcal{H}^2 \right| \leqslant C \|\mathbf{n}\|_{1,\infty} \mathcal{H}^2(S_{\mathbf{m}}) = C\mathcal{H}^2(S_{\mathbf{m}}).$$

The $\|\mathbf{n}\|_{1,\infty}$ can be absorbed into the arbitrary constant because for any fixed $T > 0$, there exists some $D > 0$ such that $\|\mathbf{n}\|_{1,\infty} < D$ for all $t < T$. Hence

$$\left| \int_\Omega \mathbf{m} \cdot \Delta \mathbf{n} + \nabla \mathbf{m} : \nabla \mathbf{n} \, dx \right| \leqslant C\mathcal{H}^2(S_{\mathbf{m}}). \tag{5.33}$$

Using very similar logic we can also show that

$$\left| \int_\Omega \mathbf{n} \cdot \nabla \times \mathbf{m} - \mathbf{m} \cdot \nabla \times \mathbf{n} \, dx \right| \leqslant C\mathcal{H}^2(S_{\mathbf{m}}). \tag{5.34}$$

By substituting (5.34) and (5.33) into (5.31) we deduce that

$$I(\mathbf{m}) - I(\mathbf{n}) \geqslant \int_\Omega |\nabla \mathbf{v}|^2 + 2t\mathbf{v} \cdot \nabla \times \mathbf{v} - \lambda |\mathbf{v}|^2 + (\lambda + t^2) \left[|\mathbf{m}|^2 - 1 \right] dx + (K - C(1+t)) \mathcal{H}^2(S_{\mathbf{m}}), \tag{5.35}$$

where $\mathbf{v} := \mathbf{m} - \mathbf{n}$. If we define the set

$$\Gamma(S_{\mathbf{m}}) := \{ (x, y) \mid (x, y, z) \in S_{\mathbf{m}} \text{ for some } z \},$$

we can estimate the integral in (5.35) in the following way. We know from equation (3.21) that

$$|\nabla \mathbf{v}| + 2t\mathbf{v} \nabla \times \mathbf{v} + t^2 |\mathbf{v}|^2 \geqslant -t^2 |\mathbf{v}|^2.$$

We also know that $|\mathbf{v}| \leqslant 2$ and $|\lambda| \leqslant \frac{\pi^2}{4} + t^2$. Hence the integrand in (5.35) is bounded below by $-C(1 + t^2)$, therefore

$$\begin{aligned} I(\mathbf{m}) - I(\mathbf{n}) \geqslant & \int_{\Gamma(S_{\mathbf{n}})^c} \int_0^d |\nabla \mathbf{v}|^2 + 2t\mathbf{v} \cdot \nabla \times \mathbf{v} - \lambda |\mathbf{v}|^2 \, dz \, dx \, dy \\ & - C(1 + t^2) \mathcal{H}^2 \left(\Gamma(S_{\mathbf{m}}) \right) + (K - C(1 + t)) \mathcal{H}^2(S_{\mathbf{m}}). \end{aligned}$$

By the definition of $\Gamma(S_{\mathbf{m}})$ we know that for $\mathcal{H}^2$ almost every $(x, y) \in \Gamma(S_{\mathbf{m}})^c$, we have $\mathbf{v}(x, y, \cdot) \in W_0^{1,2}\left((0, 1), \mathbb{R}^3\right)$. Fortunately we have already studied this precise integral in Theorem 2.18 and reasoning from its proof can be applied in this situation. By following the argument in the proof of Theorem 2.18 from equation (2.52) to (2.54), we see that there exists some $t^* > 0$, such that if $t \in (0, t^*)$ then

$$I(\mathbf{m}) - I(\mathbf{n}) \geqslant \alpha \int_{\Gamma(S_{\mathbf{m}})^c} \int_0^d |\mathbf{m} - \mathbf{n}|^2 \, dz \, dx \, dy - C(1 + t^2) \mathcal{H}^2 \left(\Gamma(S_{\mathbf{m}}) \right) + (K - C(1 + t)) \mathcal{H}^2(S_{\mathbf{m}}).$$

Finally we note that $\mathcal{H}^2(\Gamma(S_{\mathbf{m}})) \leqslant \mathcal{H}^2(S_{\mathbf{m}})$ so that if K is sufficiently large then

$$I(\mathbf{m}) - I(\mathbf{n}) \geqslant \alpha \int_{\Gamma(S_{\mathbf{m}})^c} \int_0^d |\mathbf{m} - \mathbf{n}|^2 \, dz \, dx \, dy + \beta \mathcal{H}^2(S_{\mathbf{m}}) \geqslant 0. \tag{5.36}$$

To demonstrate uniqueness we note that for equality to hold in (5.36), we would require that $\mathcal{H}^2(S_{\mathbf{m}}) = 0$ so that $\mathbf{m} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right)$. But we already know that if $t < t^*$ then $\mathbf{n}$ is the unique global minimum amongst such functions, hence it is the unique global minimum here as well.

□

Proposition 5.16. *Let $K > 0$. Then there exists some $\bar{t} > 0$ such that if $t > \bar{t}$, there exists a state $\mathbf{n} \in \mathcal{A}$ such that*

$$I(\mathbf{n}) < 0,$$

whereas any $\mathbf{m} = \mathbf{m}(z) \in \mathcal{A}$ satisfies $I(\mathbf{m}) \geqslant 0$.

Proof

The state that we construct will not satisfy the boundary conditions anywhere on the horizontal faces. This will result in an energy penalty of $8KL_1L_2$. In the bulk we will piece together a periodic array of double twist cylinders (which were introduced in Chapter 3), all lying perpendicular to the (x, z)-plane, in a hexagonal close packing system. This method is the most efficient way of close packing circles and would cover just over 90% of the plane if the pattern was repeated indefinitely. The double twist cylinders that we use in this construction have a radius of $\frac{\pi}{2t}$.

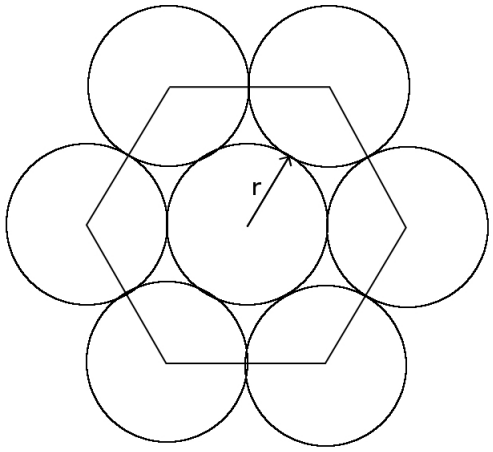


Figure 5.1: Hexagonal Packing: Volume fraction occupied = $\frac{3\pi r^2}{6\sqrt{3}r^2} = 0.907$

Importantly with the domain having width $2L_1$ and height d, the number of cylinders used in the pattern, N_{cyl} has the following upper and lower bounds:

$$\lfloor 4L_1 t\pi^{-1} \rfloor \lfloor dt(2\pi)^{-1} \rfloor \leqslant N_{cyl} \leqslant \lfloor 8L_1 dt^2\pi^{-3} \rfloor,$$

where $\lfloor x \rfloor$ denotes the integer part of a real number. In other words, if t is sufficiently large then there exist constants A_1, A_2, independent of t, such that

$$A_1 t^2 \leqslant N_{cyl} \leqslant A_2 t^2.$$

Around each of the cylinders we assign a discontinuity and in between the cylinders we simply set $\mathbf{n}$ to be zero. Now we estimate the energy of this state by looking at the elastic and jump parts separately. With the upper bound on the number of cylinders we know that

$$\mathcal{H}^2(S_{\mathbf{n}}) \leqslant 8L_1L_2 + (2L_2)\left(2\pi\left(\frac{\pi}{2t}\right)\right)A_2t^2 \leqslant A + Bt,$$

for some $A, B > 0$. It is a short calculation from (3.24) to show that the integral of the elastic energy over each cylinder is $-\alpha < 0$. Therefore using the lower bound for N_{cyl} we get

$$\begin{aligned}\int_\Omega w(\mathbf{n}, \nabla\mathbf{n})\,dx &= \int_{Cylinders} w(\mathbf{n}, \nabla\mathbf{n})\,dx + \int_{\Omega\setminus Cylinders} w(\mathbf{n}, \nabla\mathbf{n})\,dx \\ &= \int_{Cylinders} w(\mathbf{n}, \nabla\mathbf{n})\,dx \\ &\leqslant -\alpha A_1t^2.\end{aligned} \tag{5.37}$$

Hence

$$I(\mathbf{n}) \leqslant -\alpha A_1t^2 + K(A + Bt).$$

This means that if t is sufficiently large then

$$I(\mathbf{n}) < 0.$$

Whereas any function of $\mathbf{m} = \mathbf{m}(z) \in \mathcal{A}$, satisfies $w(\mathbf{m}, \nabla\mathbf{m}) \geqslant 0$ and hence $I(\mathbf{m}) \geqslant 0$.

□

Combining the previous two results together allows us to draw an interesting conclusion if the constant K for our model is suitably large. For long cholesteric pitch the minimiser is the smooth minimiser which we already know and for short cholesteric pitch any minimiser must depend on more than a single variable.

Corollary 5.17. *There exists some $\bar{t} > 0$ such that if $t > \bar{t}$ and $\mathbf{n} = \mathbf{n}(z) \in \mathcal{A}$ then $\mathbf{n}$ is not a local minimiser of I.*

Proof

Take some $\mathbf{n} = \mathbf{n}(z) \in \mathcal{A}$. We remind ourselves that the domain in which our problem is set is the extended domain Ω_ϵ, therefore for some $\delta << 1$ we define

$$A_\delta := (-L_1 + \delta, L_1 - \delta) \times (-L_2 + \delta, L_2 - \delta) \times (0, 1)\,,$$

so that $A_\delta \subset\subset \Omega_\epsilon$. Take some $\mathbf{m} \in \mathcal{A}$ such that $\mathbf{m} = \mathbf{n}$ on $\Omega \setminus \overline{A_\delta}$. Inside the set $A_\delta \cap \Omega$ we define $\mathbf{m}$ to be the array of double twist cylinders as shown in Figure 5.1. Then from (5.37) we know that the elastic energy of this configuration has an upper bound of $-\alpha A_1t^2$ (provided δ is sufficiently small). Hence

$$\begin{aligned}\int_{A_\delta} w(\mathbf{m}, \nabla\mathbf{m})\,dx + K\mathcal{H}^2\left(S_{\mathbf{m}} \cap \overline{A_\delta}\right) &\leqslant -\alpha A_1t^2 + K\mathcal{H}^2\left(S_{\mathbf{m}} \cap \overline{A_\delta}\right) \\ &\leqslant -\alpha A_1t^2 + K(At + B),\end{aligned}$$

where the constants are independent of $\mathbf{n}$ and t. Therefore if t is sufficiently large we get

$$\int_{A_\delta} w(\mathbf{m}, \nabla \mathbf{m})\, dx + K\mathcal{H}^2\left(S_{\mathbf{m}} \cap \overline{A_\delta}\right) < 0 \leqslant \int_{A_\delta} w(\mathbf{n}, \nabla \mathbf{n})\, dx + K\mathcal{H}^2\left(S_{\mathbf{n}} \cap \overline{A_\delta}\right)$$

and $\{\mathbf{n} \neq \mathbf{m}\} \subset A_\delta \subset\subset \Omega_\epsilon$ so that $I(\mathbf{m}) < I(\mathbf{n})$. Hence $\mathbf{n}$ is not a local minimiser of I.

□

These final cholesteric results are particularly interesting because they prove the necessary existence of multidimensional cholesteric patterns. We know that a minimiser of the problem must exist and it cannot be any function of one variable and furthermore any function of one variable cannot even be a local minimiser.

5.7 Smectic liquid crystals

Thus far in this thesis, we have focused our attention entirely on cholesteric and nematic liquid crystals. However in this chapter we have been exploring the possibility of using order parameters which are discontinuous across surfaces and such models seem to have possible applications to smectic liquid crystals as well. This final short section represents joint work between myself and John Ball and has been accepted for publication as part of a conference proceedings [10].

In the introduction we briefly defined smectic liquid crystals: they have a positional ordering so that the molecules arrange themselves in liquid-like layers. However there are multiple types of smectic liquid crystals. In smectic A, the molecules prefer to align parallel to the layer normal, whereas smectic C liquid crystal molecules prefer to make some fixed angle α with the layer normal. In a series of recent papers [54, 66, 67, 96, 97], the work of Lacaze and her collaborators appear to show the existence of surface discontinuities for 8CB smectic A liquid crystal. The experiments involve thin films of liquid crystals whose thicknesses varied from 50nm - 2μm. This is a much thicker situation than that which was considered in the molecular simulations in [79]. The thin film of smectic liquid crystal lies on a substrate and the upper surface of the film is open to the air. An interface with air naturally imposes homeotropic boundary conditions and the substrate is treated to induce a planar anchoring. These frustrated boundary conditions produce defect structures such as the one shown in Figure 5.2.

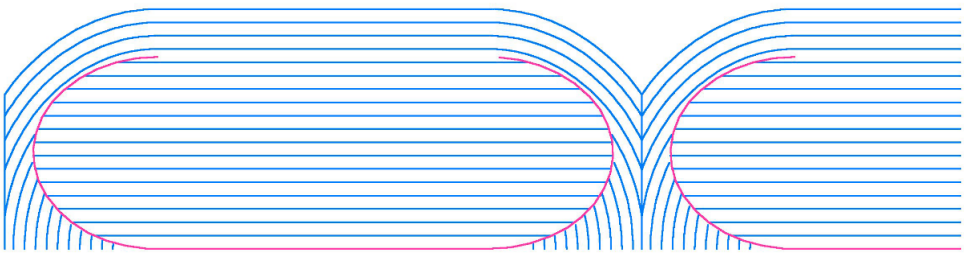


Figure 5.2: Smectic layers in 8CB thin film [67] (courtesy Emmanuelle Lacaze)

These flattened hemi-cylinders separated by vertical walls repeat periodically and importantly are not generally observed for thicker films. In other words these surface discontinuities occur

in much more frustrated liquid crystal systems. This is qualitatively similar to the nematic order reconstruction result in Theorem 5.13 where we showed that the global minimiser is smooth above a critical thickness and is discontinuous across a surface below the critical thickness. In terms of the mathematical modelling of smectic liquid crystals, the literature is very divided on any general form of a free energy density to describe the system. There are a number of proposed theories (see for example [21, 53, 61] [88, Chapter 6]) which use a complex order parameter $\Psi(x) = r(x)e^{i\phi(x)}$. With this choice, the molecular density is given by

$$\rho_0 + \rho(x) = \rho_0 + \mathrm{Re}\Psi(x) = \rho_0 + r(x)\cos(\phi(x))$$

where ρ_0 is the average density of the system. Thus ρ represents the variance from this average due to the smectic layers and $\nabla\phi$ gives the normal to the layers. However this gives rise to some of the same issues that we have already studied in the Oseen-Frank theory. The function ρ is independent of changing ϕ to $-\phi$ whereas the layer normal, $\nabla\phi$, is not. Pevnyi, Selinger & Sluckin [78] made the similar point that because of this problem, the complex order parameter cannot be chosen to be single valued for index $\pm\frac{1}{2}$ defects. As a result they proposed a model to remedy this problem and for our existence result we will follow their reasoning. They proposed an energy density in which the variables are $\mathbf{n}\otimes\mathbf{n}$ for the director and the density variation ρ. The line-field representation for the director clearly eliminates any problems with the head-to-tail symmetry. We however, consider a modified version of their functional as follows. Suppose $\Omega \subset \mathbb{R}^3$ is a bounded Lipschitz domain, then we look to minimise

$$I(\mathbf{Q},\rho) = \int_\Omega \psi_E(\mathbf{Q},\nabla\mathbf{Q}) + K\left|D^2\rho + \frac{q^2}{3s}(3\mathbf{Q}+s\mathbf{1})\rho\right|^2 + f(\rho)\,dx + k\int_{S_\mathbf{Q}} |\mathbf{Q}_+ - \mathbf{Q}_-|^\alpha \; d\mathcal{H}^2 \tag{5.38}$$

over

$$\mathcal{A} := \left\{ \mathbf{Q}\in SBV\left(\Omega,\mathbb{R}^{3\times3}\right),\ \rho\in W^{2,2}(\Omega,\mathbb{R}) \;\middle|\; \mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right),\ |\mathbf{n}| = 1,\ \mathbf{Q}|_{\partial\Omega} \cong \overline{\mathbf{Q}} \right\}. \tag{5.39}$$

where $\overline{\mathbf{Q}} \in C^\infty\left(\mathbb{R}^3,\mathbb{R}^{3\times3}\right)$. The function $f(x)$ is defined to be $\frac{ax^2}{2} + \frac{bx^3}{3} + \frac{cx^4}{4}$ and the constants satisfy $c, K, k, q > 0$, $\alpha \in (0,1)$, and $a, b, s \in \mathbb{R}$.

Remark 5.18. *By $\mathbf{Q}|_{\partial\Omega} \cong \overline{\mathbf{Q}}$ we mean that there is some open set U which contains Ω such that $\mathbf{Q} = \overline{\mathbf{Q}}$ on $U \setminus \Omega$. As in the nematic and cholesteric problems, the discontinuity set of $\mathbf{Q}$ may intersect $\partial\Omega$.*

Theorem 5.19. *Suppose that*

- *$\psi_E(\mathbf{Q},\cdot)$ is a convex function for any $\mathbf{Q}$.*
- *$\psi_E(\mathbf{Q},\mathbf{H}) \geqslant C|\mathbf{H}|^p + D$ for constants $C > 0$, $D \in \mathbb{R}$, and $p > 1$.*

Then the minimisation problem given by (5.38) *and* (5.39) *has a minimiser.*

Proof

Since the integrand is bounded below we can take a minimising sequence $\left(\mathbf{Q}^j, \rho^j\right) \subset \mathcal{A}$. By doing so we clearly find that

$$\sup_j \int_\Omega |\nabla \mathbf{Q}^j|^p \, dx + \int_{S_\mathbf{Q}} \left|\mathbf{Q}_+^j - \mathbf{Q}_-^j\right|^\alpha \, d\mathcal{H}^2 < \infty. \tag{5.40}$$

Therefore by utilising the closure and compactness theorems ([5, Theorem 4.7] and [4, Theorem 2.1]) for each component of $\mathbf{Q}$ we deduce that there exists some $\mathbf{Q} \in SBV\left(\Omega, \mathbb{R}^{3\times 3}\right)$ such that for some subsequence, $\mathbf{Q}^j \overset{*}{\rightharpoonup} \mathbf{Q}$ in SBV and $\nabla \mathbf{Q}^j \rightharpoonup \nabla \mathbf{Q}$ in L^1. As for the density term, analogously to (5.40), we know that

$$\sup_j \int_\Omega |D^2 \rho^j|^2 + \rho^{j2} \, dx < \infty. \tag{5.41}$$

Now we need to show that (5.41) implies a suitable bound on $\nabla \rho^j$. We will show that there exists some $C > 0$ such that

$$\int_\Omega |\nabla f|^2 \, dx \leqslant C \left(\int_\Omega |D^2 f|^2 + f^2 \, dx \right) \tag{5.42}$$

for every $f \in W^{2,2}(\Omega, \mathbb{R})$. Suppose for a contradiction that this were not the case. Then there exists some $\left(f^j\right) \subset W^{2,2}(\Omega)$ such that $\|\nabla f^j\|_2 = 1$ and

$$\int_\Omega |D^2 f^j|^2 + f^{j2} \, dx \leqslant \frac{1}{j}. \tag{5.43}$$

The sequence is therefore bounded in $W^{2,2}$ and the estimate (5.43) implies that it has a weakly convergent subsequence with zero as its limit. This is incompatible with $\|\nabla f^j\|_2 = 1$ for each j. This means that (5.42) holds. Hence $\left(\rho^j\right)$ is bounded in $W^{2,2}$ and we can find some $\rho \in W^{2,2}(\Omega, \mathbb{R})$ such that, for some subsequence, $\rho^j \rightharpoonup \rho$ in $W^{2,2}$. This completes the compactness part of the proof and to conclude we just need to show lower semicontinuity of our functional given these weak convergences. The convexity with respect to $\nabla \mathbf{Q}$ means that we can simply apply Ioffe's Theorem [5, Theorem 5.8] to get

$$\liminf_{j\to\infty} \int_\Omega \psi_E \left(\mathbf{Q}^j, \nabla \mathbf{Q}^j\right) dx \geqslant \int_\Omega \psi_E \left(\mathbf{Q}, \nabla \mathbf{Q}\right) dx.$$

Equally, we know that the jump term satisfies weak* lower semicontinuity because it is jointly convex (See [5, Example 5.23 (a)] and [5, Theorem 5.20], or for a separate proof see [36, Theorem 2.1]). Hence

$$\liminf_{j\to\infty} \int_{S_{\mathbf{Q}^j}} \left|\mathbf{Q}_+^j - \mathbf{Q}_-^j\right|^\alpha \, d\mathcal{H}^2 \geqslant \int_{S_\mathbf{Q}} |\mathbf{Q}_+ - \mathbf{Q}_-|^\alpha \, d\mathcal{H}^2.$$

For the cross term we note that $\rho^j \to \rho$, $\mathbf{Q}^j \to \mathbf{Q}$, and $D^2\rho^j \rightharpoonup D^2\rho$ in L^2. Then we can use the facts that $\|\mathbf{Q}^j\|_\infty \leqslant \frac{4|s|}{3}$ and $\|\rho\|_\infty < \infty$ to deduce that $\rho^j \mathbf{Q}^j \to \rho \mathbf{Q}$ in L^2 and

$$\rho^j (3\mathbf{Q}^j + sId) : D^2\rho^j \rightharpoonup \rho(3\mathbf{Q} + sId) : D^2\rho \text{ in } L^2.$$

Hence

$$\begin{aligned}
&\liminf_{j\to\infty} \int_\Omega \left| D^2\rho^j - \frac{q^2}{3s}\left(3\mathbf{Q}^j + sId\right)\rho^j \right|^2 dx \\
&= \liminf_{j\to\infty} \int_\Omega \left|D^2\rho^j\right|^2 - \frac{2q^2}{3s}\rho^j\left(3\mathbf{Q}^j + sId\right) : D^2\rho^j + q^4\rho^{j4}\, dx \\
&\geqslant \int_\Omega |D^2\rho|^2 - \frac{2q^2}{3s}\rho\,(3\mathbf{Q} + sId) : D^2\rho^j + q^4\rho^4\, dx.
\end{aligned}$$

Therefore we have used compactness and lower-semicontinuity to find a pair $(\mathbf{Q}, \rho)$ such that $I(\mathbf{Q}, \rho) = \inf_{\mathcal{A}} I(\mathbf{Q}', \rho')$. Finally we note that the L^2 convergence of $\mathbf{Q}^j$ (so a subsequence converges almost everywhere) together with the compactness of the unit sphere ensures that $\mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}I\right)$ and $\mathbf{Q}|_{\partial\Omega} \cong \overline{\mathbf{Q}}$ in our extended domain sense. Therefore $(\mathbf{Q}, \rho) \in \mathcal{A}$ and we have completed the proof.

□

The mathematical modelling of smectics is not as far advanced as that of the modelling of cholesteric and nematic liquid crystals. However many modelling issues overlap between all three types of liquid crystal. What this brief foray into smectics illustrates, is that our proposed idea of using order parameters with SBV regularity, gives us well posed problems and tackles the orientability issues which plague liquid crystals. However it is clear that a great deal more work would need to be done to verify whether this changes the predictions of the existing smectic models.

Conclusions

For this thesis we were initially motivated by the various patterns which form in cholesteric liquid crystals under certain conditions. There are many different kinds of stable structures which can occur from cholesteric fingers to blue phase lattices to the more recently discovered torons [22, 77, 84]. While these structures are reasonably well understood at a local level, to the best of our knowledge they have never been shown to arise analytically from a rigorous variational problem. Using the Oseen-Frank free energy and director fields $\mathbf{n} \in W^{1,2}\left(\Omega, \mathbb{S}^2\right)$, we were able to find the minimisers over functions of one variable. We could prove that these one variable minimisers were the unique global minimisers for both the nematic and cholesteric problem if the cholesteric pitch was suitably long. For short cholesteric pitch we used the local minimiser results we developed from Chapter 1, together with some numerical data, to indicate that the one variable functions are still local minimisers. Hence using the classical Oseen-Frank theory, we were unable to prove the existence of multi-variable minimisers.

It has long been known that any director theory has the inherent flaw that it does not respect the head to tail symmetry exhibited by many commonly used liquid crystal molecules. The matrix order parameter involved in the Landau-de Gennes theory has no such problem which is a distinct advantage. The desire to bring this advantage over to a director theory was the motivation for Chapter 4. The core results from that chapter were the lifting results to determine a regularity for the director field $\mathbf{n}$ given a line field $\mathbf{n}\otimes\mathbf{n}$. Lifting results

have been studied by a number of authors for director fields in both Sobolev and BV spaces [13, 28]. However, unlike their results, we were able to show that if the domain was not simply connected then in general the vector field must have a different regularity to the line field. This led us to the results showing equivalence between the uniaxial Landau-de Gennes theory and Ericksen's theory, provided that the director field is a special function of bounded variation.

Ultimately this indicated to us that perhaps the flaw in the Oseen-Frank theory could be rectified by considering special bounded variation functions as we have done in this chapter. The suggestion of studying nematic liquid crystals with functions of bounded variation is not completely new [5, 23]. However we are not aware of any specific nematic liquid crystal problem being studied beyond the existence of a minimiser. Furthermore studying cholesterics with functions of bounded variation appears to be a completely new idea which has not been explored before. As a result, in this chapter we were able to show with relatively straightforward analysis, that multi-variable minimisers must exist for short cholesteric pitch. We did so by constructing a state which consists of an array of double-twist cylinders and a large discontinuity set. As our model in this chapter is formally based upon the Landau-de Gennes model, our cholesteric results suggest that in the high chirality limit, the structure predicted by the Landau-de Gennes theory, may be very complex with rapid changes in $\mathbf{Q}$ near surfaces where $\mathbf{Q}$ is biaxial. In the nematic case, Theorem 5.13 predicts the existence of a jump across a suitably thin cell which is qualitatively in agreement with the eigenvalue exchange predicted in the molecular simulations of Zannoni [79]. These are early indicators that show this idea deserves some serious attention; it is predicting behaviour which previously could only be explained with a matrix order parameter. We believe that this particular area of study could yield many more interesting results and predictions. However we have only just scratched the surface of these notions and those more well versed than I in functions of bounded variation could make good progress in using the intuitive simplicity of a director model to really further our theoretical understanding of liquid crystals.

Appendix A

MATLAB code

```
function planar_method(N,t,steps_x,steps_z,W)

% In this program we investigate the second variation of the functional by
% writing it as a function of w'(0) then using the fact that w'(0) is
% perpendicular to the candidate minimiser to find its general form.

% N - number of modes
% t - cholesteric twist
% steps_x - number of steps in x
% steps_z - number of steps in z
% W - HALF of the width of the domain:
% x \in [-W,W]

% Initial conditions and setting up the problem.

% CHOICES
timestep_z=1/steps_z;
timestep_x=2*W/steps_x;
L=W;
% CHOICES

format long

% Type saving constants
M=2*N+4*N^2;
n=1+steps_z;
m=1+steps_x;
% Type saving constants

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%% SET UP SECTION %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Firstly solving the ODE to determine theta

    % ODE function
    function ode = myode(k,y)
    ode=[y(2);t*t*cos(y(1))*sin(y(1))];
    end

    % Boundary condition function
    function res=boundary_condition(y0,y1)
    res=[y0(1);y1(1)-pi/2];
    end
```

```
% Solving the ode
sol=bvpinit(linspace(0,1,n),[0,1]);
options=odeset('RelTol',1e-13);
mysol = bvp4c(@myode,@boundary_condition,sol,options);
Theta = deval(mysol,linspace(0,1,n));


% Setting up our candidate minimiser n (and its derivatives)

% Declaration
n1=zeros(n,1);
n13=zeros(n,1);
n2=zeros(n,1);
n23=zeros(n,1);
n3=zeros(n,1);
n33=zeros(n,1);

% Initialisation
% NOTE ni(1) corresponds to z=0 ni(n) corresponds to z=1
for i=1:n
    n1(i) = cos(Theta(1,i))*cos(t*(i-1)*timestep_z);
    n2(i) = cos(Theta(1,i))*sin(t*(i-1)*timestep_z);
    n3(i) = sin(Theta(1,i));

    n13(i) = -Theta(2,i)*sin(Theta(1,i))*cos(t*(i-1)*timestep_z)...
             -t*cos(Theta(1,i))*sin(t*(i-1)*timestep_z);
    n23(i) = -Theta(2,i)*sin(Theta(1,i))*sin(t*(i-1)*timestep_z)...
             +t*cos(Theta(1,i))*cos(t*(i-1)*timestep_z);
    n33(i) = Theta(2,i)*cos(Theta(1,i));
end

% n and derivatives now set up in a series of vectors


% Now we create our Fourier series f,g and their derivatives
% We will store them in U1 U2
% Derivatives in x: U11 U21
% Derivatives in z: U13 U23

% The information will be stored in an array of vectors. The ith component
% of the (j,k) vector represents the numerical coefficient of the fourier
% coefficient a_i at the mesh position (j,k)

% This cell A represents the set of basis vectors
A=cell(M,1);

for i=1:M
    A{i}=zeros(M,1);
    A{i}(i)=1;
end

% Declaring the cells which we will fill with vectors with dimensions
% (M,1) of zeros

U1=cell(n,m); U2=cell(n,m);

U11=cell(n,m); U13=cell(n,m);

U21=cell(n,m); U23=cell(n,m);

for i=1:n
```

```
    for j=1:m
        U1{i,j}=zeros(M,1); U2{i,j}=zeros(M,1);

        U11{i,j}=zeros(M,1); U13{i,j}=zeros(M,1);

        U21{i,j}=zeros(M,1); U23{i,j}=zeros(M,1);
    end
end

% End of initialization

% Filling up U1, U2, U11, U21, U13, U23
%

for i=1:n
    for j=1:m

        tempx=-W+(j-1)*timestep_x;
        tempz=(i-1)*timestep_z;

        for k=1:N
            U1{i,j}(k) = (L^(-0.5))*sin(k*pi*tempz);
            U2{i,j}(N+k) = (L^(-0.5))*sin(k*pi*tempz);

            U13{i,j}(k) = (L^(-0.5))*k*pi*cos(k*pi*tempz);
            U23{i,j}(N+k) = (L^(-0.5))*k*pi*cos(k*pi*tempz);
        end

        for k=1:N
            for l=1:N
                U1{i,j}(2*N+N*(k-1)+l) = sin(k*pi*tempz)...
                    *cos(l*pi*tempx/L)*((2/L)^(0.5));
                U1{i,j}(2*N+N^2+N*(k-1)+l) = sin(k*pi*tempz)...
                    *sin(l*pi*tempx/L)*((2/L)^(0.5));

                U2{i,j}(2*N+2*N^2+N*(k-1)+l) = +sin(k*pi*tempz)...
                    *cos(l*pi*tempx/L)*((2/L)^(0.5));
                U2{i,j}(2*N+3*N^2+N*(k-1)+l) = +sin(k*pi*tempz)...
                    *sin(l*pi*tempx/L)*((2/L)^(0.5));

                U11{i,j}(2*N+N*(k-1)+l) = -sin(k*pi*tempz)*l*pi...
                    *(1/L)*sin(l*pi*tempx/L)*((2/L)^(0.5));
                U11{i,j}(2*N+N^2+N*(k-1)+l) = +sin(k*pi*tempz)...
                    *l*pi*(1/L)*cos(l*pi*tempx/L)*((2/L)^(0.5));

                U21{i,j}(2*N+2*N^2+N*(k-1)+l) = -sin(k*pi*tempz)...
                    *l*pi*(1/L)*sin(l*pi*tempx/L)*((2/L)^(0.5));
                U21{i,j}(2*N+3*N^2+N*(k-1)+l) = +sin(k*pi*tempz)...
                    *l*pi*(1/L)*cos(l*pi*tempx/L)*((2/L)^(0.5));

                U13{i,j}(2*N+N*(k-1)+l) = k*pi*cos(k*pi*tempz)...
                    *cos(l*pi*tempx/L)*((2/L)^(0.5));
                U13{i,j}(2*N+N^2+N*(k-1)+l) = +k*pi*cos(k*pi*tempz)...
                    *sin(l*pi*tempx/L)*((2/L)^(0.5));

                U23{i,j}(2*N+2*N^2+N*(k-1)+l) = +k*pi*cos(k*pi*tempz)...
                    *cos(l*pi*tempx/L)*((2/L)^(0.5));
                U23{i,j}(2*N+3*N^2+N*(k-1)+l) = +k*pi*cos(k*pi*tempz)...
                    *sin(l*pi*tempx/L)*((2/L)^(0.5));
            end
        end
```

```
    end
end

clearvars tempx tempz

% END of U creation

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%% END OF SETUP SECTION %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%% START OF CALCULATION SECTION %%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


% Forming the all important matrix MAT1 which we use to calculate the
% numerical integral of the second variation
% (This is where most of the computing time is spent!)

% By performing a careful calculation we find that in terms of the fourier
% series f and g, the second variation integrand can be written as

% |\nabla f|^2 + |\nabla g|^2 + f^2(-t^2-lambda)
% +g^2(theta'^2 - t^2 sin^2(theta) -lambda) + 2tg(f_{,1})cos(theta)cos(phi)
% -2tg(g_{,1})cos(theta)cos(phi)

% Where
% lambda = |\nabla n|^2 + 2t n \cdot\nabla n
lambda = zeros(n,1);

for i=1:n
    lambda(i) = n13(i)*n13(i)+n23(i)*n23(i)+n33(i)*n33(i)...
                +2*t*(-n1(i)*n23(i)+n2(i)*n13(i));
end

% We save |\nabla f|^2 + |\nabla g|^2 terms until last because they have a
% special form and so can be done more simply

% Terms involving 'f'
Cell1=cell(n,m);

for i=1:n
    for j=1:m
        Cell1{i,j} = U1{i,j}*(-t*t-lambda(i));
        Cell1{i,j} = Cell1{i,j}+U21{i,j}...
            *(-2*t*cos(t*(i-1)*timestep_z)*cos(Theta(1,i)));
    end
end


% Terms involving 'g'
Cell2=cell(n,m);

for i=1:n
    for j=1:m
        Cell2{i,j} = U2{i,j}*(Theta(2,i)*Theta(2,i)...
            -t*t*sin(Theta(1,i))*sin(Theta(1,i))-lambda(i));
        Cell2{i,j} = Cell2{i,j}+U11{i,j}...
            *(2*t*cos(t*(i-1)*timestep_z)*cos(Theta(1,i)));
    end
```

```
end



% This section performs a two dimensional trapezium rule to numerically
% calculate the value of the integral of the terms we have included so far.

% The value MAT1_ij represents the coefficient of the a_ia_j term where
% the a_i are the Fourier coefficients.

MAT1=zeros(M,M);

A1 = U1;
B1 = Cell1;
A2 = U2;
B2 = Cell2;

% Shortening the timestep variables
t_z=timestep_z;
t_x=timestep_x;


% Main portion of the cell
for i=2:n-1
    for j=2:m-1

        MAT1=MAT1+(t_x*t_z)*(A1{i,j}*(B1{i,j}.')+A2{i,j}*(B2{i,j}.'));

    end
end

% Sides of the cell
for i=2:n-1

    MAT1=MAT1+0.5*(t_x*t_z)*(A1{i,1}*(B1{i,1}.')+A2{i,1}*(B2{i,1}.'));
    MAT1=MAT1+0.5*(t_x*t_z)*(A1{i,m}*(B1{i,m}.')+A2{i,m}*(B2{i,m}.'));

end

for j=2:m-1

    MAT1=MAT1+0.5*(t_x*t_z)*(A1{1,j}*(B1{1,j}.')+A2{1,j}*(B2{1,j}.'));
    MAT1=MAT1+0.5*(t_x*t_z)*(A1{n,j}*(B1{n,j}.')+A2{n,j}*(B2{n,j}.'));

end

% Corners of the cell
MAT1=MAT1+0.25*(t_x*t_z)*(A1{1,1}*(B1{1,1}.')+A2{1,1}*(B2{1,1}.'));
MAT1=MAT1+0.25*(t_x*t_z)*(A1{n,1}*(B1{n,1}.')+A2{n,1}*(B2{n,1}.'));
MAT1=MAT1+0.25*(t_x*t_z)*(A1{1,m}*(B1{1,m}.')+A2{1,m}*(B2{1,m}.'));
MAT1=MAT1+0.25*(t_x*t_z)*(A1{n,m}*(B1{n,m}.')+A2{n,m}*(B2{n,m}.'));


% Halving the off diagonal terms to get the correct output in the final
% calculation

MAT1=0.5*(MAT1+(MAT1'));


% As we have a nice form for the terms involving just the derivatives:
% U11*U11 + U13*U13 + U31*U31 + U33*U33
% we can calculate their integrals explicitly since they are Fourier
```

```
% series.

% We store the outcome in the matrix MAT2
MAT2 = zeros(M,M);

% This nice form of the derivative terms ensures that there are only
% entries on the diagonal since fourier terms form an orthogonal basis
for i=1:N

    MAT2(i,i) = (i^2)*(pi^2);
    MAT2(N+i,N+i) = (i^2)*(pi^2);

    for j=1:N

        MAT2(2*N+N*(i-1)+j,2*N+N*(i-1)+j) =...
            (i^2)*(pi^2)+(j^2)*(pi^2)/(L^2);

        MAT2(2*N+N^2+N*(i-1)+j,2*N+N^2+N*(i-1)+j) =...
            (i^2)*(pi^2)+(j^2)*(pi^2)/(L^2);

        MAT2(2*N+2*N^2+N*(i-1)+j,2*N+2*N^2+N*(i-1)+j) =...
            (i^2)*(pi^2)+(j^2)*(pi^2)/(L^2);

        MAT2(2*N+3*N^2+N*(i-1)+j,2*N+3*N^2+N*(i-1)+j) =...
            (i^2)*(pi^2)+(j^2)*(pi^2)/(L^2);

    end
end

MAT1 = MAT1 + MAT2;
% END OF MATRIX CREATION



% Now we find the minimum eigenvalue of MAT1 to prove the positivity of the
% second variation.

Vals = eig(MAT1);

answer = 100000;

% Finding the smallest of the eigenvalues
for i=1:M
    if(Vals(i)<answer)
        answer = Vals(i);
    end
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%% END OF CALCULATION SECTION %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%



%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%% PRINTING RESULTS AND END %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


% Printing out the results
disp('************************************************')
fprintf('\nNumber of modes : %d\n',N)
```

```
fprintf('No of steps in z: %d\n',steps_z)
fprintf('No of steps in x: %d\n',steps_x)
fprintf('t : %d\n',t)
fprintf('Domain width : %d\n\n',L);
fprintf('Min e-value =')
disp(answer)
fprintf('\n')
disp('************************************************')
fprintf('\n')
end
```

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