



Landau-de Gennes Corrections to the Oseen-Frank Theory of Nematic Liquid Crystals

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Abstract

We study the asymptotic behavior of the minimisers of the Landau-de Gennes model for nematic liquid crystals in a two-dimensional domain in the regime of small elastic constant. At leading order in the elasticity constant, the minimum-energy configurations can be described by the simpler Oseen-Frank theory. Using a refined notion of Γ -development we recover Landau-de Gennes corrections to the Oseen-Frank energy. We provide an explicit characterisation of minimizing Q -tensors at this order in terms of optimal Oseen-Frank directors and observe the emerging biaxiality. We apply our results to distinguish between optimal configurations in the class of conformal director fields of fixed topological degree saturating the lower bound for the Oseen-Frank energy.

1. Introduction

Nematic liquid crystals are the simplest liquid crystalline phase as well as the most widely used in applications. Among the theoretical models for nematic liquid crystals, the most prevalent in the physics and mathematics literature are the Oseen-Frank [15] and Landau-de Gennes theories [12]. The Oseen-Frank theory is the simpler of the two, but fails to describe several characteristic features of nematic liquid crystals, including the isotropic-nematic phase transition, non-orientability of the director field, and the fine structure of defects. By incorporating additional degrees of freedom, the Landau-de Gennes theory accounts for these features, but is more difficult to solve and analyse.

The main focus of this paper is to establish a fine relation between the two theories, in the weak-elasticity regime and for two-dimensional domains. Employing a refined notion of Γ -development we obtain an approximate expression for Landau-de Gennes minimisers in terms of Oseen-Frank minimisers accurate to energies through the first two orders in the elasticity constant. The results are applied to a

family of boundary conditions of fixed topological degree which saturate a lower bound on the leading-order Oseen-Frank energy. For these boundary conditions, we provide explicit solutions in terms of the Green's function for the Laplacian on the domain, and show that the degeneracy in the Oseen-Frank energy is lifted at the next order. Below we introduce both theories and discuss the mathematical status of their relationship together with the results of this paper.

1.1. Landau-de Gennes and Oseen-Frank theories of liquid crystals

In the Oseen-Frank theory, the liquid crystalline material is assumed to be in the nematic phase. Its configuration in a domain $\Omega \subset \mathbb{R}^d$, $d = 2$ or $d = 3$, is described by a unit-vector field $n : \Omega \rightarrow \mathbb{S}^2$, called the *director field*, which represents the mean orientation of the rod-like constituents of the material and characterises its optical properties. In the absence of external fields, the director field is taken to be a minimiser of the Oseen-Frank energy

$$\mathcal{E}_{OF}[n] = \int_{\Omega} K_1 |\nabla \cdot n|^2 + K_2 |n \cdot (\nabla \times n)|^2 + K_3 |n \times (\nabla \times n)|^2, \quad (1.1)$$

subject to Dirichlet boundary conditions $n|_{\partial\Omega} = n_b$, where the K_j 's are material-dependent constants. For mathematical analysis, the one-constant approximation, $K_1 = K_2 = K_3$, is often adopted, according to which the Oseen-Frank energy reduces to the Dirichlet energy, with harmonic maps as critical points.

One shortcoming of this description is that in certain domains, the director field n is more appropriately represented by an $\mathbb{R}P^2$ -valued map, stemming from the fact that orientations n and $-n$ are physically indistinguishable. In simply-connected domains, a continuous $\mathbb{R}P^2$ -valued map n can be lifted to a continuous \mathbb{S}^2 -valued map, in which case we say that n is *orientable*. However, in non-simply-connected domains, this may not hold, in which case we say that n is *non-orientable*; see [3] for further discussion, where the notion of orientability is extended to $n \in W^{1,p}(\Omega, \mathbb{R}P^2)$.

Another difficulty is the description of defect patterns. These are singularities in the director field, which correspond physically to sharp changes in orientational ordering on a microscopic length scale. It is well known that boundary conditions can force the director field to have singularities. This occurs, for example, when Ω is a three-dimensional domain with boundary homeomorphic to \mathbb{S}^2 and the boundary map $n_b : \partial\Omega \rightarrow \mathbb{S}^2$ has nonzero degree. In this case, in spite of the singularity, the infimum Oseen-Frank energy is finite. The difficulty is more acute when the boundary data $n_b : \partial\Omega \rightarrow \mathbb{R}P^2$ is non-orientable. In this case, the Oseen-Frank energy is necessarily infinite.

The Landau-de Gennes theory resolves these difficulties by introducing additional degrees of freedom. The liquid crystalline material is described by a tensor field $Q : \Omega \rightarrow \mathcal{S}_0$ taking values in the five-dimensional space of 3×3 real symmetric traceless matrices, or Q -tensors, denoted

$$\mathcal{S}_0 = \{Q \in \mathbb{R}^{3 \times 3} : Q = Q^t, \text{ tr } Q = 0\}, \quad (1.2)$$

where Q^t and $\text{tr } Q$ denote the transpose and trace of Q respectively. The Q -tensor originates from a microscopic description; it represents the second (and lowest-order nontrivial) moments of a probability distribution on the space of single-particle orientations, \mathbb{S}^2 , given that orientations n and $-n$ are equally likely [12].

The Q -tensor field is taken to be a minimiser of an energy comprised of elastic and bulk terms,

$$\mathcal{F}[Q] = \frac{L}{2} \int_{\Omega} |\nabla Q|^2 + \int_{\Omega} f_{bulk}(Q), \quad Q \in H^1(\Omega, \mathcal{S}_0), \quad (1.3)$$

where L , the elastic constant, is a material parameter. For f_{bulk} smooth and sufficiently regular boundary conditions, standard results from the calculus of variations imply that \mathcal{F} has a smooth minimiser; singularities are absent in the Landau-de Gennes theory. The bulk potential is required to be invariant under rotations $Q \mapsto RQR^t$, $R \in \text{SO}(3)$, and is usually taken to be of the form introduced by de Gennes,

$$f_{bulk}(Q) = \frac{A}{2} \text{tr } Q^2 - \frac{B}{3} \text{tr } Q^3 + \frac{C}{4} (\text{tr } Q^2)^2. \quad (1.4)$$

¹Here A , B , and C , are material parameters, possibly temperature-dependent, with $C > 0$. From now on we will assume without loss of generality that the coefficients L , A , B , and C , are non-dimensional; see, for example, [16] and the appendix of [29] for suitable non-dimensionalisations. We will focus on the generic case $B \neq 0$ but also discuss some aspects of the case $B = 0$.

In the class of spatially homogeneous Q -tensors the equilibrium configurations correspond to the minimisers of f_{bulk} . For $A > 0$, the zero Q -tensor is a local minimiser, and becomes a global minimiser for A sufficiently large. The zero Q -tensor corresponds to the isotropic, or orientationally disordered, phase. For $A < 0$, the minimisers of f_{bulk} are, generically, a two-dimensional manifold within the larger class of *uniaxial* Q -tensors, that is Q -tensors with a doubly degenerate eigenvalue.

By identifying n , the normalised eigenvector orthogonal to the degenerate eigenspace, as the director, uniaxial Q -tensors correspond to the nematic phase as described within the Oseen-Frank theory. With A regarded as temperature-dependent, the Landau-de Gennes theory is seen to encompass the observed isotropic-nematic phase transition.

The sign of the degenerate eigenvalue of a uniaxial Q -tensor coincides with the sign of B , and distinguishes two qualitatively different phases. In terms of the probabilistic interpretation of the Q -tensor, a positive value of the degenerate eigenvalue corresponds to an ensemble of orientations predominantly orthogonal to the director n ; this is the *oblate uniaxial* phase. A negative value corresponds to an ensemble of orientations predominantly parallel to n ; this is the *prolate uniaxial* phase, which describes typical nematic liquid crystals. Since our focus is on the

¹ More general bulk potentials $g(\text{tr } Q^2, \text{tr } Q^3)$ have been studied in the literature; see, for example, [2, 14]. We expect the results presented here to apply more generally to bulk potentials with a unique minimiser (modulo rotations) which is nondegenerate and uniaxial.

nematic phase, we take $A = -a^2 < 0$, $B = -b^2 < 0$ and $C = c^2 > 0$. The set of minimisers of f_{bulk} , which we call the *limit manifold*, is given by

$$\mathcal{S}_* := \{Q \in \mathcal{S}_0; Q = s_+ (n \otimes n - \frac{1}{3}I), n \in \mathbb{S}^2\}, \tag{1.5}$$

where

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \tag{1.6}$$

The limit manifold is homeomorphic to the real projective plane $\mathbb{R}P^2$. In the non-generic case $b^2 = 0$ we have that the limit manifold is given by

$$\mathcal{S}_0^* := \{Q \in \mathcal{S}_0; |Q|^2 = (2/3)s_+^2 = a^2/c^2\}, \tag{1.7}$$

which is homeomorphic to \mathbb{S}^4 .

The minimum of the bulk energy is given by

$$f_* := f_{bulk}(\mathcal{S}_*) = -\frac{a^2}{3}s_+^2 - \frac{2b^2}{27}s_+^3 + \frac{c^2}{9}s_+^4. \tag{1.8}$$

It is convenient to replace f_{bulk} by

$$\tilde{f}_{bulk} = f_{bulk} - f_*, \tag{1.9}$$

so that $\tilde{f}_{bulk}(Q) \geq 0$ with $\tilde{f}_{bulk}(Q) = 0$ if and only if $Q \in \mathcal{S}_*$.

1.2. State of the art

The Landau-de Gennes theory is usually applied to a system in which the elastic constant L can be treated as a small parameter. This is the case when the size of the domain is much larger than a characteristic microscopic length scale (see, for example, [16] and the appendix of [29]). With such systems in mind, we write $L = \varepsilon^2 \ll 1$ and rescale the energy (1.3) to obtain

$$\mathcal{E}_\varepsilon[Q] = \int_\Omega \frac{1}{2}|\nabla Q|^2 + \frac{1}{\varepsilon^2}\tilde{f}_{bulk}(Q), \quad Q \in H^1(\Omega, \mathcal{S}_0), \tag{1.10}$$

so that deviation from the limit manifold is penalised. We restrict to differentiable boundary conditions taking values in the limit manifold,

$$Q_b = Q|_{\partial\Omega} \in C^1(\partial\Omega, \mathcal{S}_*); \tag{1.11}$$

indeed, boundary conditions violating this restriction induce a boundary layer of width ε . We say that the boundary conditions are *orientable* if

$$Q_b = s_+ (n_b \otimes n_b - \frac{1}{3}I), \quad \text{where } n_b \in C^1(\partial\Omega, \mathbb{S}^2). \tag{1.12}$$

It is in the small- ε regime that the relationship between the Landau-de Gennes and Oseen-Frank theories emerges. For orientable boundary conditions, if we formally take $\varepsilon = 0$, the Landau-de Gennes energy (1.10) becomes

$$\mathcal{E}_0[Q] = \begin{cases} \frac{1}{2} \int_{\Omega} |\nabla Q|^2 & \text{if } Q \in H^1(\Omega, \mathcal{S}_*), \\ +\infty & \text{otherwise.} \end{cases} \quad (1.13)$$

Provided the domain is simply-connected, given $Q \in H^1(\Omega, \mathcal{S}_*)$, there exists $n \in H^1(\Omega, \mathbb{S}^2)$ such that $Q(x) = s_+(n(x) \otimes n(x) - \frac{1}{3}I)$. In this case, the limiting energy $\mathcal{E}_0[Q]$ can be expressed in terms of the director field as

$$\mathcal{E}_{OF}[n] = s_+^2 \int_{\Omega} |\nabla n(x)|^2, \quad (1.14)$$

which is, up to a multiplicative constant, the one-constant Oseen-Frank energy.

There has been much recent work in the mathematics literature analysing the relationship between the two theories in the limit $\varepsilon \rightarrow 0$. For three-dimensional domains with orientable boundary conditions, it was shown in [28] that global minimisers $Q_\varepsilon \in H^1(\Omega, \mathcal{S}_0)$ of \mathcal{E}_ε converge to global minimisers $Q_0 = s_+(n_0 \otimes n_0 - \frac{1}{3}I) \in H^1(\Omega, \mathcal{S}_*)$ of \mathcal{E}_0 . Moreover, outside a finite set of point singularities of the one-constant Oseen-Frank director n_0 , the convergence holds in strong norms on compact sets. These results were extended in [8] to the case of non-orientable boundary conditions; the principal new features are (i) the Landau-de Gennes energy is logarithmically divergent in ε , (ii) the singular set contains one-dimensional curves as well as isolated points, and (iii) the limit map Q_0 is described by an $\mathbb{R}P^2$ -valued harmonic map rather than an \mathbb{S}^2 -valued harmonic map. Results for two-dimensional domains with more general boundary conditions and assumptions on the behaviour of the energy are given in [4, 7, 17].

Given the leading-order behaviour of the Landau-de Gennes minimisers away from singularities, one can pursue two distinct directions. The first concerns the behaviour of a minimiser Q_ε near the singular set, where deviations from Q_0 are no longer small. This amounts to analysing the profiles of point and line defects, an active area of research [4, 7–11, 13, 17, 19, 21–24, 26].

The second concerns the structure of deviations $Q_\varepsilon - Q_0$ away from the singular set. Formal asymptotics suggest that $Q_\varepsilon \sim Q_0 + \varepsilon^2 P_\varepsilon$, where P_ε is $O(\varepsilon^0)$. This question was addressed in [29] for three-dimensional domains with orientable boundary conditions. Subject to rather restrictive conditions on Q_0 (which in particular exclude defects), it was shown that P_ε approaches a limiting map $P_0 \in C_{\text{loc}}^\infty(\Omega, \mathcal{S}_0) \cap H^s(\Omega, \mathcal{S}_0)$ for any $0 < s < 1/2$. Moreover, P_0 splits naturally into a sum $P_0^\perp + P_0^\top$, where P_0^\top takes values in the two-dimensional tangent space $T_{Q_0}\mathcal{S}_*$ of \mathcal{S}_* at Q_0 , and P_0^\perp takes values in the three-dimensional orthogonal complement of $T_{Q_0}\mathcal{S}_*$. The transverse component P_0^\perp is given by an explicit expression involving Q_0 and its derivatives, while P_0^\top is shown to satisfy a linear inhomogeneous PDE.

1.3. Contributions of present work

Our results also pertain to corrections to Q_ε away from the singular set, and complement those of [29]. Specifically, we consider simply-connected two-dimensional domains with orientable boundary conditions (1.12) for which the boundary director n_b is planar, that is, $n_b \cdot e_3 = 0$. By identifying the boundary $\partial\Omega$ with \mathbb{S}^1 , we may regard a planar boundary director n_b as a map from \mathbb{S}^1 to itself, which therefore may be assigned an integer-valued degree, m . We consider the case of nonzero degree. We use energy-based methods to derive an explicit formula for the transverse component of the first-order correction. While we obtain only bounds for the tangential component, and not the linear PDE that it satisfies, we are able to relax the restrictive assumptions on Q_0 in [29]. Also, the Γ -convergence argument is much simpler than the PDE analysis of [29], and has potential further application to dynamics in terms of a corrected Oseen-Frank energy for the gradient flow.

Most importantly, the variational analysis brings to light a physically significant difference between the energies associated with the transverse and tangential components of P_0 . The transverse component, which affects the bulk potential, contributes to the Landau-de Gennes energy at $O(\varepsilon^2)$, while the tangential component, which affects only the elastic energy, contributes at higher order. This observation suggests that the transverse component P_0^\perp assumes the same form for a wide class of Q -tensor models in which the Oseen-Frank theory provides the leading-order description. Insofar as the Landau-de Gennes model is necessarily approximate, this suggests that the transverse component of the Q -tensor, while small, is robust under perturbations; an additional $O(\varepsilon^\delta)$ contribution to the energy produces an $O(\varepsilon^\delta)$ correction to P_0^\perp . The tangential component lacks this robustness; an $O(\varepsilon^\delta)$ perturbation typically produces an $O(\varepsilon^{-2+\delta})$ deviation in P_0^\top (cf. Remark 2.7).

The additional information contained in the transverse component P_0^\perp is manifested through the resolution (cf. Remark 2.4)

$$P_0^\perp = c_0 Q_0 + c_1(p_0 \otimes p_0 - q_0 \otimes q_0) + c_2(p_0 \otimes q_0 + q_0 \otimes p_0), \quad (1.15)$$

where p_0, q_0 constitute an orthonormal basis for the plane perpendicular to the director n_0 , and $Q_0 = s_+(n_0 \otimes n_0 - \frac{1}{3}I)$. The c_0 -term preserves the eigenvalue degeneracy in Q_0 , and can be regarded as a correction to s_+ . The c_1 - and c_2 -terms produce a qualitative change in the Q -tensor; they break the eigenvalue degeneracy and thereby introduce *biaxiality*. The difference between the two negative eigenvalues of Q_ε can be regarded as a measure of biaxiality, and is given to leading order by $\varepsilon^2(c_1^2 + c_2^2)^{1/2}$, while the orientation of the associated eigenvectors in the plane orthogonal to n_0 is determined by c_2/c_1 . It has previously been established that a critical point of the Landau-de Gennes energy is either everywhere uniaxial or else almost everywhere biaxial [27, 28]. The results presented here make this statement quantitative.

Our principal application is to a special class of planar boundary conditions. A standard argument establishes the lower bound $2\pi|m|$ for the Dirichlet energy of an \mathbb{S}^2 -valued harmonic map n with degree- m planar boundary conditions. The lower bound is achieved for a special family of boundary conditions, which are parameterised by $|m|$ arbitrarily located escape points $(a_1, \dots, a_{|m|}) \in \Omega^{|m|}$ where

the director field is vertical, that is, $n(a_j) = \pm e_3$. The director field n is conformal with $n \cdot e_3$ sign-definite. Conformal director fields may be expressed explicitly in terms of the Green's function for the Laplacian on Ω . The associated textures are seen to be similar to the well-known Schlieren patterns observed in liquid crystal films (see Figure 1).

The degeneracy in the Oseen-Frank energy among these special boundary conditions is lifted by the first-order correction from the Landau-de Gennes energy. The expression for the first-order correction simplifies in the conformal case, and is proportional to the integral of $|\nabla Q_0|^4$. Regarded as a potential on $\Omega^{|m|}$, the first-order energy favours escape points moving to the boundary. This is illustrated in the case of the two-disk, for which closed-form expressions are obtained.

For the special case $b^2 = 0$ (as well as more general bulk potentials depending only on $\text{tr } Q^2$), our results can be extended to non-orientable boundary conditions. In this case, the minimising set of f_{bulk} is larger than \mathcal{S}_* ; it contains all Q -tensors with specified trace norm, and may be identified with \mathbb{S}^4 . For finite ε , the Landau-de Gennes energy is equivalent to a Ginzburg-Landau functional on \mathbb{R}^5 -valued maps, which in the $\varepsilon \rightarrow 0$ limit becomes the Dirichlet energy for \mathbb{S}^4 -valued maps. For both orientable and non-orientable planar boundary conditions, there is a unique minimising \mathbb{S}^4 -valued harmonic map (in the orientable case, it is distinct from the \mathcal{S}_* -valued minimisers of (2.3)), and the first-order correction can be expressed in terms of it. The Γ -convergence argument is simpler than in the $b^2 > 0$ case.

1.4. Outline

The remainder of the paper is organised as follows. In Section 2 we state and discuss our main results on the Landau-de Gennes corrections to the Oseen-Frank energy for the non-degenerate case $b^2 \neq 0$. The proof of the Γ -development result (cf. Theorem 2.1) is given in Section 3. In Section 4, we state and prove Theorem 4.1, which deals with the degenerate case $b^2 = 0$ and allows for non-orientable boundary conditions. Finally, in Section 5, we apply our results to distinguish between optimal configurations in the class of conformal director fields of fixed topological degree that saturate a lower bound on the Oseen-Frank energy.

2. Statement of Main Results

We are interested in studying the minimisers of the Landau-de Gennes energy \mathcal{E}_ε in the physically relevant regime $\varepsilon \ll 1$ for the generic case $b^2 > 0$. Throughout we assume that the domain $\Omega \subseteq \mathbb{R}^2$ is bounded and simply connected with C^1 -boundary. We consider orientable planar boundary conditions with director $n_b \in C^1(\partial\Omega, \mathbb{S}^2)$, so that $n_b \cdot e_3 = 0$; results for non-orientable planar boundary conditions in the special case $b^2 = 0$ are presented in Section 4.

Identifying the space of unit vectors orthogonal to e_3 with \mathbb{S}^1 , and likewise identifying the domain boundary $\partial\Omega$ with \mathbb{S}^1 , we may regard n_b as a map from \mathbb{S}^1 to itself, which may be assigned an integer-valued degree. Given n_b of nonvanishing

degree, we denote by \mathcal{U} the class of admissible Q -tensor fields

$$\mathcal{U} := \left\{ Q \in H^1(\Omega, \mathcal{S}_0), Q|_{\partial\Omega} = Q_b \right\}, \quad Q_b := s_+ (n_b \otimes n_b - \frac{1}{3}I). \tag{2.1}$$

We consider the minimisation problem (cf. (1.10))

$$\min_{Q \in \mathcal{U}} \mathcal{E}_\varepsilon[Q] = \min_{Q \in \mathcal{U}} \int_\Omega \frac{1}{2} |\nabla Q|^2 + \frac{1}{\varepsilon^2} \tilde{f}_{bulk}(Q). \tag{2.2}$$

As a first step, we need to understand the behaviour of Problem (2.2) in the limit $\varepsilon \rightarrow 0$. Using methods of Γ -convergence we obtain the following result, whose proof is standard and therefore omitted:

Proposition 2.1. *As $\varepsilon \rightarrow 0$, the following statements hold:*

- (i) *For any family $\{Q_\varepsilon\}_{\varepsilon>0} \subset \mathcal{U}$ such that $\mathcal{E}_\varepsilon[Q_\varepsilon] \leq C$ we have, possibly on a subsequence, $Q_\varepsilon \rightharpoonup Q$ weakly in $H^1(\Omega, \mathcal{S}_0)$ for some $Q \in H^1(\Omega, \mathcal{S}_*)$, where \mathcal{S}_* is the limit manifold defined by (1.5).*
- (ii) *The family $(\mathcal{E}_\varepsilon)_{\varepsilon>0}$ Γ -converges to \mathcal{E}_0 in the weak topology of $H^1(\Omega, \mathcal{S}_0)$, where*

$$\mathcal{E}_0[Q] = \begin{cases} \frac{1}{2} \int_\Omega |\nabla Q|^2 & \text{if } Q \in H^1(\Omega, \mathcal{S}_*) \cap \mathcal{U}, \\ +\infty & \text{otherwise.} \end{cases} \tag{2.3}$$

- (iii) *The minimisers $\{Q_\varepsilon^*\}_{\varepsilon>0}$ of the problem (2.2) converge strongly in $H^1(\Omega, \mathcal{S}_0)$ to the minimisers of the following harmonic map problem:*

$$\min_{Q \in \mathcal{U}_*} \mathcal{E}_0[Q], \tag{2.4}$$

with $\mathcal{U}_* \equiv H^1(\Omega, \mathcal{S}_*) \cap \mathcal{U}$.

Remark 2.1. In [31] (see also [25]), it is shown that Problem (2.4) has precisely two solutions,

$$Q_0^\pm = s_+ (n_0^\pm \otimes n_0^\pm - \frac{1}{3}I), \tag{2.5}$$

where $n_0^\pm \cdot e_3 = 0$ on $\partial\Omega$, and $n_0^+ \cdot e_3 > 0$ (resp $n_0^- \cdot e_3 < 0$) in Ω . The vector field n_0^\pm is a smooth harmonic map with values in \mathbb{S}^2 (see, for instance [18]) and solves the following minimisation problem:

$$\min \left\{ \int_\Omega |\nabla n|^2 : n \in H^1(\Omega, \mathbb{S}^2), n = n_b \text{ on } \partial\Omega \right\}. \tag{2.6}$$

From now on, we set $n_0 := n_0^\pm$ and $Q_0 := Q_0^\pm$, meaning that all the results we state hold for both n_0^+ and n_0^- .

2.1. A refined formulation of asymptotic Γ -expansion

The next step in understanding the link between the Landau-de Gennes and Oseen-Frank theories is the asymptotic expansion of the Landau-de Gennes energy \mathcal{E}_ε . Using the approach of Γ -expansion we can obtain a correction to the Oseen-Frank energy and quantify the difference between the two theories. Specifically, with $n_0 := n_0^\pm \in C^\infty(\Omega, \mathbb{S}^2) \cap C^1(\bar{\Omega}, \mathbb{S}^2)$ minimising (2.6), we define the *renormalised relative energy*

$$\mathcal{G}_\varepsilon[Q] := \frac{1}{\varepsilon^2} (\mathcal{E}_\varepsilon[Q] - \mathcal{E}_0[Q_0]), \quad Q \in H^1(\Omega, \mathcal{S}_0), \tag{2.7}$$

and proceed to investigate the behaviour of minimisers of \mathcal{G}_ε in \mathcal{U} . Before stating our main result about \mathcal{G}_ε , a few comments are in order.

The notion of Γ -expansion was introduced by Anzellotti and Baldo in [1]. Their framework permits to derive selection criteria for minimisers when the leading order Γ -limit manifests degeneracies in the energy landscape. However, our leading order Γ -limit \mathcal{E}_0 is not subject to this phenomenon as it admits just the two minimisers (2.5). This implies that the second-order Γ -limit will be infinite at every point but Q_0^\pm . No matter which (reasonable) topology is considered, the energy will blow up on families that do not converge to Q_0^\pm . In order to gain finer details on the convergence behaviour of the minimising sequences, a slightly different approach must be used. We proceed as follows:

- First, we observe that fairly extended arguments, that are nevertheless straightforward given the existing literature (see, for instance, [5,21,28,29]), allow to show that if $\{Q_\varepsilon^*\}_{\varepsilon>0}$ is a family of *minimisers* of \mathcal{E}_ε , there exists an $\varepsilon_0 > 0$ such that

$$\sup_{0<\varepsilon<\varepsilon_0} \|Q_\varepsilon^*\|_{W^{1,\infty}(\Omega, \mathcal{S}_0)} < \infty, \tag{2.8}$$

and, possibly for a subsequence, $Q_\varepsilon^* \rightarrow Q_0^\pm$ strongly in $H^1(\Omega, \mathcal{S}_0)$ with Q_0^\pm one of the two minimisers of problem (2.4).

- Next, we use (2.8) to deduce fine properties of the minimisers. We consider all possible families $\{Q_\varepsilon\}_{\varepsilon>0}$ that behave in a similar way to minimising families (see Definition 2.1 for the precise formulation), and we provide a description of the limiting energy capable of distinguishing different sequences. Then, the second-order Γ -limit follows as a particular instance of our analysis.

The previous considerations motivate the following terminology:

Definition 2.1. We say that a family $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ is *almost-minimising* whenever $\{Q_\varepsilon\}_{\varepsilon>0}$ satisfies the uniform bound (2.8), and $\mathcal{G}_\varepsilon[Q_\varepsilon] \leq C$ for some constant $C > 0$ independent of ε .

2.2. Main result: the case $b^2 > 0$.

Our main result provides detailed information about the expansion of the energy \mathcal{E}_ε and is stated in the next Theorem 2.1. Before stating it we need to introduce some basic definitions, notation and terminology that will be used throughout.

The set of Q -tensors, \mathcal{S}_0 , is a five-dimensional linear space, with inner product $Q : P = \text{tr}(QP)$. The norm induced by the inner product is denoted by $|Q| := (\text{tr } Q^2)^{\frac{1}{2}}$. It will be convenient to introduce the following orthonormal basis for \mathcal{S}_0 :

$$\begin{aligned} F_1 &= \frac{1}{\sqrt{2}}(e_1 \otimes e_1 - e_2 \otimes e_2), \\ F_2 &= \frac{1}{\sqrt{2}}(e_1 \otimes e_2 + e_2 \otimes e_1), \\ F_3 &= \sqrt{\frac{3}{2}}\left(e_3 \otimes e_3 - \frac{1}{3}I\right), \\ F_4 &= \frac{1}{\sqrt{2}}(e_1 \otimes e_3 + e_3 \otimes e_1), \\ F_5 &= \frac{1}{\sqrt{2}}(e_3 \otimes e_2 + e_2 \otimes e_3), \end{aligned} \tag{2.9}$$

with e_1, e_2, e_3 standard basis of \mathbb{R}^3 . A tensor $Q \in \mathcal{S}_0$ is called *biaxial* if all its eigenvalues are distinct. We say that Q is *uniaxial* if it has a doubly degenerate eigenvalue $-\lambda/3$. In this case, it can be represented uniquely as

$$Q = \lambda \left(n \otimes n - \frac{1}{3}I \right), \tag{2.10}$$

where $n \in \mathbb{S}^2$ is called the *director* and $\frac{2}{3}\lambda \in \mathbb{R}$ is the (unique) non-degenerate eigenvalue of Q . More specifically, Q is *prolate uniaxial* if $\lambda > 0$ and *oblate uniaxial* if $\lambda < 0$. Finally, $Q \in \mathcal{S}_0$ is *isotropic* if it has a triply degenerate eigenvalue, in which case $Q = 0$. If the largest (necessarily positive) eigenvalue of $Q \in \mathcal{S}_0$ is nondegenerate, it is called the *principal eigenvalue*, and the associated normalised eigenvector is called the *principal eigenvector*. The remaining two eigenvalues of Q (which may be degenerate) and the associated orthonormal eigenvectors are called the *subprincipal eigenvalues* and *subprincipal eigenvectors*.

We introduce a parameterised family of rotations in $\text{SO}(3)$. For any $n \in \mathbb{S}^2 \setminus \{-e_3\}$, we define

$$R_n = I + [e_3 \times n]_\times + \frac{[e_3 \times n]_\times^2}{1 + n \cdot e_3}, \tag{2.11}$$

where, for every $\omega \in \mathbb{R}^3$, the symbol $[\omega]_\times$ denotes the antisymmetric matrix that maps $v \in \mathbb{R}^3$ to $\omega \times v$. It is easy to check that $R_n \in \text{SO}(3)$ and that $R_n e_3 = n$. Indeed, R_n may be uniquely characterised as the rotation about an axis orthogonal to e_3 by an angle $0 \leq \theta < \pi$ that maps e_3 into n . Note that, when $n \neq e_3$ the axis of rotation is $e_3 \times n$, and the angle of rotation is $\cos^{-1}(n \cdot e_3)$.

Remark 2.2. Given a bounded domain $\Omega \subset \mathbb{R}^2$, we note the following: for any $1 \leq p \leq \infty$, if $n \in W^{1,p}(\Omega, \mathbb{S}^2)$ and $1 + n \cdot e_3$ is bounded away from 0, then $R_n \in W^{1,p}(\Omega, \text{SO}(3))$.

In what follows, to shorten notation, we set $Q[n] := s_+ (n \otimes n - \frac{1}{3}I)$ for any $n \in \mathbb{S}^2$. Also, we set

$$V_\rho := \sum_{j=1}^3 \rho_j F_j, \quad \nabla n_0 \otimes \nabla n_0 := \sum_{i=1}^2 \partial_i n_0 \otimes \partial_i n_0. \quad (2.12)$$

Here, $\rho \in \mathbb{R}^3$, and the F_j are the first three elements of the basis (2.9). Note that any V_ρ has e_3 as eigenvector.

Theorem 2.1. *As $\varepsilon \rightarrow 0$, the following assertions hold:*

- (i) *For any family $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ such that $\mathcal{G}_\varepsilon[Q_\varepsilon] \leq C$ we have, possibly on a subsequence, $Q_\varepsilon \rightarrow Q_0^\pm := s_+ (n_0^\pm \otimes n_0^\pm - \frac{1}{3}I)$ strongly in $H^1(\Omega, \mathcal{S}_0)$, where Q_0^\pm is one of the two minimisers of problem (2.4).*
- (ii) *If $\{Q_\varepsilon\}_{\varepsilon>0}$ is almost-minimising then, possibly on a subsequence, $Q_\varepsilon \rightarrow Q_0 = Q[n_0]$ in $H^1(\Omega, \mathcal{S}_0)$ and there exists a family of principal eigenvectors of Q_ε , denoted as $n_\varepsilon \in W^{1,\infty}(\Omega, \mathbb{S}^2)$, and a vector-valued function $\rho \in L^2(\Omega, \mathbb{R}^3)$, such that*

$$\|n_\varepsilon - n_0\|_{H_0^1(\Omega, \mathbb{R}^3)} \leq C\varepsilon \quad (2.13)$$

and

$$P_\varepsilon^\perp := \frac{1}{\varepsilon^2} (Q_\varepsilon - Q[n_\varepsilon]) \rightharpoonup R_{n_0} V_\rho R_{n_0}^t \text{ weakly in } L^2(\Omega, \mathcal{S}_0), \quad (2.14)$$

where $R_{n_0} \in W^{1,\infty}(\Omega, \text{SO}(3))$ is the field of rotation matrices given by (2.11).

- (iii) *Let $\{Q_\varepsilon\}_{\varepsilon>0}$ be an almost-minimising family such that $Q_\varepsilon \rightarrow Q_0$ in $H^1(\Omega, \mathcal{S}_0)$. For any family of principal eigenvectors $n_\varepsilon \in W^{1,\infty}(\Omega, \mathbb{S}^2)$ satisfying (2.13), and any $P_\varepsilon^\perp \in H_0^1(\Omega, \mathcal{S}_0)$ satisfying (2.14) we have*

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] \geq \mathcal{H}_0[n_0, \rho] := \int_\Omega \frac{1}{2} B_0 \rho \cdot \rho + b_0 \cdot \rho. \quad (2.15)$$

Here, $B_0 = \text{diag}(\mu, \mu, \nu)$ with $\mu = b^2 s_+$, $\nu = \frac{1}{3} b^2 s_+ + 2a^2$, and $b_0 \in L^\infty(\Omega, \mathbb{R}^3)$ is defined by

$$\begin{aligned} b_0 \cdot e_j &:= -2s_+ (\nabla n_0 \otimes \nabla n_0) : (R_{n_0} F_j R_{n_0}^t), \quad j = 1, 2, \\ b_0 \cdot e_3 &:= \sqrt{6} s_+ |\nabla n_0|^2. \end{aligned} \quad (2.16)$$

Also, for every $\rho \in L^2(\Omega, \mathbb{R}^3)$ there exists a recovery almost-minimising family $Q_\varepsilon = Q[n_\varepsilon] + \varepsilon^2 P_\varepsilon^\perp$ satisfying (2.13), (2.14) for which $\lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] = \mathcal{H}_0[n_0, \rho]$.

(iv) *The unique minimiser of $\mathcal{H}_0[n_0, \cdot]$ is given by $\rho_0 := -B_0^{-1} b_0$. The corresponding minimum value of the energy is given by*

$$\mathcal{H}_0[n_0, \rho_0] = -s_+^2 \int_{\Omega} \frac{2}{\mu} |\nabla n_0 \otimes \nabla n_0|^2 + \left(\frac{3}{\nu} - \frac{1}{\mu}\right) |\nabla n_0|^4. \tag{2.17}$$

In particular, in the topology induced by (2.13) and (2.14), the family of energies $\{\mathcal{G}_\varepsilon\}_{\varepsilon>0}$ Γ -converges to \mathcal{G}_0 , where

$$\mathcal{G}_0[Q] = \begin{cases} \mathcal{H}_0[n_0, \rho_0] & \text{if } Q = Q_0, \\ +\infty & \text{otherwise.} \end{cases} \tag{2.18}$$

Moreover, if $Q_\varepsilon^ \rightarrow Q_0$ in $H^1(\Omega, \mathcal{S}_0)$ is a family of minimisers of $\{\mathcal{E}_\varepsilon\}_{\varepsilon>0}$ with principal eigenvectors $n_\varepsilon^* \in W^{1,\infty}(\Omega, \mathbb{S}^2)$, then $\mathcal{G}_\varepsilon[Q_\varepsilon^*] \rightarrow \mathcal{H}_0[n_0, \rho_0]$, and we have*

$$\frac{1}{\varepsilon} (n_\varepsilon^* - n_0) \rightarrow 0 \text{ strongly in } H_0^1(\Omega, \mathbb{S}^2), \tag{2.19}$$

$$\frac{1}{\varepsilon^2} (Q_\varepsilon^* - Q[n_\varepsilon^*]) \rightarrow P_0^\perp := R_{n_0} V_{\rho_0} R_{n_0}^T \text{ strongly in } L^2(\Omega, \mathcal{S}_0). \tag{2.20}$$

The proof of Theorem 2.1 is given in Section 3. Key components include a quadratic lower bound on the variation of the \mathbb{S}^2 -valued Dirichlet energy at n_0 (Lemma 3.2) and a Q -tensor decomposition (Lemma 3.1) into a sum of two terms with a common eigenbasis, one taking values on the limit manifold, and the other taking values transverse to it. The fact that almost-minimisers Q_ε have uniformly bounded finite $W^{1,\infty}$ -norm is used to bound \mathcal{G}_ε from below (in fact, finite $W^{1,4}$ -norm would suffice).

Remark 2.3. We note that P_0^\perp in (2.20) does not vanish on the boundary, so that higher-order corrections to the minimiser Q_ε^* contain a boundary layer.

Remark 2.4. The expression for P_0^\perp can be written as (cf. (1.15))

$$P_0^\perp = c_0 Q_0 + c_1 (p_0 \otimes p_0 - q_0 \otimes q_0) + c_2 (p_0 \otimes q_0 + p_0 \otimes q_0), \tag{2.21}$$

where $p_0 = R_{n_0} e_1$ and $q_0 = R_{n_0} e_2$ (so that n_0, p_0 and q_0 constitute an orthonormal frame), and

$$c_0 = -\frac{2\sqrt{6}}{\nu} |\nabla n_0|^2, \tag{2.22}$$

$$c_1 = \frac{\sqrt{2}s_+}{\mu} (|\nabla n_0 \cdot p_0|^2 - |\nabla n_0 \cdot q_0|^2), \tag{2.23}$$

$$c_2 = \frac{2\sqrt{2}s_+}{\mu} (\nabla n_0 \cdot p_0) \cdot (\nabla n_0 \cdot q_0). \tag{2.24}$$

The coefficients c_1 and c_2 describe biaxiality;

the quantity $\varepsilon^2(c_1^2 + c_2^2)$ is the square of the difference of the two subprincipal eigenvalues of the minimiser Q_ε^* , to leading order in ε .

The coefficient c_0 describes an $O(\varepsilon^2)$ correction to the principal eigenvalue of Q_ε^* .

Remark 2.5. The energy $\mathcal{H}_0[n_0, \rho]$ distinguishes between various almost-minimising families $\{Q_\varepsilon\}$ and gives a non-trivial energy landscape. The Γ -limit \mathcal{H}_0 provides a starting point for an asymptotic analysis of Q -tensor dynamics under gradient flow. The fact that \mathcal{H}_0 depends only on ρ indicates that the director dynamics is much slower than that of displacements transverse to the limit manifold. Specifically, for an initial condition with $o(\varepsilon)$ -displacements from the optimal director and $O(\varepsilon^2)$ -displacements from the limit manifold, the time scale for director dynamics is nevertheless longer.

Remark 2.6. It is easy to generalise Theorem 2.1 to boundary conditions where $n_b \cdot e_3 \geq 0$ (or $n_b \cdot e_3 \leq 0$). Moreover, if $n_b \cdot e_3$ is strictly positive (or strictly negative) at some point $x_0 \in \partial\Omega$ then it is not necessary to assume that n_b has nonzero degree (indeed, the degree might not be well defined in this case).

Remark 2.7. An informal argument suggests that Theorem 2.1 may extend to more general Q -tensor energy densities of the form $|\nabla Q|^2 + \varepsilon^{-2}f(Q) + \varepsilon^\delta g(Q, \nabla Q)$, where f is any bulk potential minimised by prolate uniaxial Q -tensors of fixed norm, and g represents an additional contribution to the energy. In order that the generalised model reduce to the (one-constant) Oseen-Frank description away from defects, we require that $\delta > 0$. Under suitable conditions on g , we expect the transverse component P_0^\perp to be unaffected by this additional contribution, and Theorem 2.1 still to hold but with a rate of convergence of $\|n_\varepsilon - n_0\|_{H^1} \rightarrow 0$ possibly depending on δ . The key point is that P_0^\perp should still be given by (2.20), with μ and ν the nonvanishing eigenvalues of the Hessian of f at its minimum.

The argument may be illustrated by a finite-dimensional proxy for the Landau-de Gennes energy, in which the tensor field Q is replaced by just two quantities: x , a proxy for the director displacement $n - n_0$, where n is the principal eigenvector of Q ; and y , a proxy for the transverse component, $Q - Q[n]$. The proxy energy is given by

$$\mathcal{E}_\varepsilon(x, y) = \left(\frac{1}{2}px^2 + qxy + \frac{1}{2}ry^2 + by \right) + \frac{\mu}{2\varepsilon^2}y^2 + \varepsilon^\delta g(x, y), \quad (2.25)$$

where $p, \delta, \mu > 0$. The term $(\frac{1}{2}px^2 + qxy + \frac{1}{2}ry^2 + by)$ corresponds to the elastic energy expanded about its minimum – hence the absence of a term linear in x and the requirement that $p > 0$. The term $\frac{1}{2}\mu y^2/\varepsilon^2$ corresponds to the bulk potential expanded about its minimum; the absence of terms in x^2 and xy reflects the rotational invariance of the bulk potential. To leading order in ε , the minimiser $(x_\varepsilon^*, y_\varepsilon^*)$ is given by

$$x_\varepsilon^* = -\frac{\varepsilon^\delta}{r} \frac{\partial}{\partial y} g(0, 0) + \frac{\varepsilon^2}{\mu r} b, \quad y_\varepsilon^* = \varepsilon^2 \frac{b}{\mu}. \quad (2.26)$$

Thus, the “transverse component” y_ε^* is independent of g , while the “director displacement” x_ε^* is driven by g , at least for $\delta < 2$.

3. Γ -Expansion: Proof of Theorem 2.1

3.1. Proof of (i): equi-coercivity of the energy functionals (compactness)

Here we prove statement (i) of Theorem 2.1. Consider a family $\{Q_\varepsilon\}_{\varepsilon>0} \subset \mathcal{U}$ such that $\mathcal{G}_\varepsilon[Q_\varepsilon] \leq C$ for some constant $C > 0$. It is clear that

$$\mathcal{E}_\varepsilon[Q_\varepsilon] = \int_\Omega \frac{1}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon^2} \tilde{f}_{bulk}(Q_\varepsilon) \leq C\varepsilon^2 + \mathcal{E}_0[Q_0]. \tag{3.1}$$

In particular, $\{\mathcal{E}_\varepsilon[Q_\varepsilon]\}_{\varepsilon>0}$ is bounded for ε sufficiently small. Since $\tilde{f}_{bulk} \geq 0$, there exist a (not relabeled) subfamily $\{Q_\varepsilon\}_{\varepsilon>0} \subset \mathcal{U}$, and a tensor field $Q_* \in H^1(\Omega, \mathcal{S}_0)$, such that

$$Q_\varepsilon \rightharpoonup Q_* \text{ in } H^1(\Omega, \mathcal{S}_0), \quad \tilde{f}_{bulk}(Q_\varepsilon) \rightarrow 0 \text{ almost everywhere in } \Omega. \tag{3.2}$$

From the above, $Q_* \in H^1(\Omega, \mathcal{S}_*)$ and $Q_\varepsilon \rightarrow Q_*$ strongly in $L^2(\Omega, \mathcal{S}_0)$. By the lower semicontinuity of the norm and the bound (3.1) we obtain

$$\begin{aligned} \int_\Omega |\nabla Q_*|^2 &\leq \liminf_{\varepsilon \rightarrow 0} \int_\Omega |\nabla Q_\varepsilon|^2 \leq \lim_{\varepsilon \rightarrow 0} (C\varepsilon^2 + \mathcal{E}_0[Q_0]) = \mathcal{E}_0[Q_0] \\ &= \int_\Omega |\nabla Q_0|^2, \end{aligned} \tag{3.3}$$

with $Q_0 \in \operatorname{argmin}_{Q \in \mathcal{U}} \mathcal{E}_0[Q]$. Therefore,

$$Q_* \in \operatorname{argmin}_{Q \in \mathcal{U}} \mathcal{E}_0[Q] \quad \text{and} \quad \|\nabla Q_\varepsilon\|_{L^2} \rightarrow \|\nabla Q_*\|_{L^2} = \|\nabla Q_0\|_{L^2}. \tag{3.4}$$

Combining this information with (3.2) we conclude that $Q_\varepsilon \rightarrow Q_*$ strongly in $H^1(\Omega, \mathcal{S}_0)$. Eventually, by Remark 2.1, $Q_* = s_+(n_0^\pm \otimes n_0^\pm - \frac{1}{3}I)$ where n_0^\pm is one of the two minimisers of problem (2.6).

3.2. Proof of (ii): parameterisation of almost-minimising families and convergence estimates

Here we prove statement (ii) of Theorem 2.1. In agreement with Remark 2.1, and to fix the ideas, we set $n_0 := n_0^+$ and $Q_0 := Q_0^+ = s_+(n_0 \otimes n_0 - \frac{1}{3}I)$. Also, to shorten notation, we set $Q[n] := s_+(n \otimes n - \frac{1}{3}I)$ for any $n \in \mathbb{S}^2$, and $V_\rho := \sum_{j=1}^3 \rho_j F_j$ for any vector $\rho \in \mathbb{R}^3$, where F_j are the first three elements of the basis (2.9).

We show that any almost-minimising family $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ admits a parameterisation in terms of two families of vector fields:

- the family $\{n_\varepsilon\}_{\varepsilon>0} \subseteq W^{1,\infty}(\Omega, \mathbb{S}^2)$ of principal normalised eigenvectors of $\{Q_\varepsilon\}_{\varepsilon>0}$;
- the family of vector fields $\{\rho_\varepsilon\}_{\varepsilon>0} \subseteq W_0^{1,\infty}(\Omega, \mathbb{R}^3)$ that characterises the displacement between Q_ε and the limit manifold \mathcal{S}_* defined by (1.5).

The parameterisation facilitates the fine control of the energy difference $\mathcal{E}_\varepsilon[Q_\varepsilon] - \mathcal{E}_0[Q_0]$; contributions to $\mathcal{E}_\varepsilon[Q_\varepsilon]$ from ρ_ε are controlled by the bulk potential, which takes its minimum on the limit manifold, while contributions from n_ε are controlled by the elastic energy, using Lemma 3.2 below. This separation is necessitated by the fact that, by rotational invariance, the second variation $\nabla^{(2)} f_{\text{bulk}}$ of the bulk potential on \mathcal{S}_* is only positive semidefinite, not positive definite. To linear order, variations in n_ε are tangent to \mathcal{S}_* and lie in the null space of $\nabla^{(2)} f_{\text{bulk}}$, while variations in ρ_ε are normal to \mathcal{S}_* and lie in the subspace on which $\nabla^{(2)} f_{\text{bulk}}$ is positive definite.

Lemma 3.1. *Let $\Omega \subset \mathbb{R}^2$ be a bounded and simply-connected domain and $n \in C^1(\bar{\Omega}, \mathbb{S}^2)$.*

Suppose that $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ is uniformly bounded in $W^{1,\infty}(\Omega, \mathcal{S}_0)$, and

$$Q_\varepsilon \rightarrow Q[n] := s_+ (n \otimes n - \frac{1}{3}I) \quad \text{strongly in } H^1(\Omega, \mathcal{S}_0).$$

Then, for ε sufficiently small, the following hold:

(i) *There exists a principal eigenvector $n_\varepsilon \in W^{1,\infty}(\Omega, \mathbb{S}^2)$ of Q_ε such that for any $1 \leq p < \infty$,*

$$n_\varepsilon \rightarrow n \text{ in } W^{1,p}(\Omega, \mathbb{S}^2), \text{ as well as in } C(\bar{\Omega}, \mathbb{S}^2). \quad (3.5)$$

(ii) *There exists a vector-valued function $\rho_\varepsilon \in W_0^{1,\infty}(\Omega, \mathbb{R}^3)$ such that*

$$Q_\varepsilon = Q[n_\varepsilon] + \varepsilon^2 P_\varepsilon^\perp, \quad P_\varepsilon^\perp := R_{n_\varepsilon} V_{\rho_\varepsilon} R_{n_\varepsilon}^t. \quad (3.6)$$

Here, R_{n_ε} is the rotation given by (2.11). Moreover, we have, for any $1 \leq p < \infty$,

$$R_{n_\varepsilon} \rightarrow R_{n_0} \text{ in } W^{1,p}(\Omega, \text{SO}(3)), \quad \varepsilon^2 \rho_\varepsilon \rightarrow 0 \text{ in } W_0^{1,p}(\Omega, \mathbb{R}^3). \quad (3.7)$$

as well as, respectively, in $C(\bar{\Omega}, \text{SO}(3))$ and in $C(\bar{\Omega}, \mathbb{R}^3)$.

Proof. Since $Q_\varepsilon \rightarrow Q[n]$ in $H^1(\Omega, \mathcal{S}_0)$ with Q_ε uniformly bounded in $W^{1,\infty}(\Omega, \mathcal{S}_0)$, by interpolation it is clear that $Q_\varepsilon \rightarrow Q[n]$ in $W^{1,p}(\Omega, \mathcal{S}_0)$ for every $1 \leq p < \infty$, as well as in $C(\bar{\Omega}, \mathcal{S}_0)$.

(i) The tensor field $Q[n]$ has everywhere a principal eigenvalue equal to $2s_+/3$. It follows that for ε sufficiently small, Q_ε has everywhere a principal eigenvalue λ_ε with principal eigenvector n_ε uniquely determined up to a sign. The fact that λ_ε is nondegenerate implies that the projector $n_\varepsilon \otimes n_\varepsilon$ can be expressed as a smooth function of Q_ε (see for instance [30]). Thereby, $Q[n_\varepsilon] \in W^{1,\infty}(\Omega, \mathcal{S}_0)$ and $Q[n_\varepsilon] \rightarrow Q[n]$ in $H^1(\Omega, \mathcal{S}_0)$, as well as uniformly. In particular, $n_\varepsilon \cdot n \neq 0$ for ε sufficiently small. We may then choose the sign of n_ε so that $n_\varepsilon \cdot n$ is everywhere positive. For this choice, $n_\varepsilon \in W^{1,\infty}(\Omega, \mathbb{S}^2)$ and $n_\varepsilon \rightarrow n$ in $W^{1,p}(\Omega, \mathbb{S}^2)$, $1 \leq p < \infty$, as well as in $C(\bar{\Omega}, \mathbb{S}^2)$.

(ii) Consider the quantity $U_\varepsilon := \varepsilon^{-2} R_{n_\varepsilon}^t (Q_\varepsilon - Q[n_\varepsilon]) R_{n_\varepsilon}$. As n_ε is an eigenvector of Q_ε and of $n_\varepsilon \otimes n_\varepsilon$, it follows that e_3 is an eigenvector of U_ε . The unit vector e_3

is an eigenvector of $Q \in \mathcal{S}_0$ if, and only if, Q is a linear combination of F_1, F_2 and F_3 . Therefore $U_\varepsilon = V_{\rho_\varepsilon}$ with $\rho_\varepsilon \cdot e_j := U_\varepsilon : F_j$. Setting

$$P_\varepsilon^\perp = R_{n_\varepsilon} V_{\rho_\varepsilon} R_{n_\varepsilon}^t, \tag{3.8}$$

we establish (3.6). Next, we prove that $\rho_\varepsilon \in W_0^{1,p}(\Omega, \mathbb{R}^3)$. It is clear from the assumptions on Q_ε that $\rho_\varepsilon \in W^{1,\infty}(\Omega, \mathbb{R}^3)$. Now, $Q_\varepsilon \in \mathcal{W}$ implies $Q_\varepsilon|_{\partial\Omega} = Q[n]|_{\partial\Omega}$; also, since n_ε is the principal eigenvector of Q_ε , $n_\varepsilon|_{\partial\Omega} = n|_{\partial\Omega}$; overall, $\rho_\varepsilon|_{\partial\Omega} = 0$.

Finally, since Q_ε and R_{n_ε} approach $Q[n]$ and R_n with respect to their $W^{1,p}$ -norms, as well as uniformly, it follows from (3.6) that $\varepsilon^2 \rho_\varepsilon \rightarrow 0$ in $W_0^{1,p}(\Omega, \mathbb{R}^3)$ as well as uniformly. \square

3.2.1. Strong minimality of \mathbb{S}^2 -valued harmonic maps We will require a lower bound on the Dirichlet energy of \mathbb{S}^2 -valued maps sufficiently close to a minimising harmonic map. The following is based on results from [21], and is of independent interest; for completeness we give an account here. Let $n_b \in C^1(\partial\Omega, \mathbb{S}^2)$ denote planar boundary conditions of nonzero degree, and let

$$\mathcal{N}_0 := \left\{ n \in H^1(\Omega, \mathbb{S}^2) : n|_{\partial\Omega} = n_b \right\}.$$

Lemma 3.2. *Let $\{n_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{N}_0$ and suppose $n_\varepsilon \rightarrow n_0$ in $H_0^1(\Omega, \mathbb{S}^2)$, where we denote by $n_0 \in \mathcal{N}_0$ a minimiser of the Dirichlet energy. There exists $\alpha > 0$ such that for all sufficiently small ε ,*

$$\int_\Omega |\nabla n_\varepsilon|^2 - |\nabla n_0|^2 \geq \alpha^2 \|n_\varepsilon - n_0\|_{H_0^1(\Omega, \mathbb{R}^3)}^2. \tag{3.9}$$

Proof. We first note that as $-\Delta n_0 = |\nabla n_0|^2 n_0$ and $|n_\varepsilon| = |n_0| = 1$ in Ω , one has

$$\int_\Omega |\nabla n_\varepsilon|^2 - |\nabla n_0|^2 = \int_\Omega |\nabla(n_\varepsilon - n_0)|^2 - |\nabla n_0|^2 |n_\varepsilon - n_0|^2. \tag{3.10}$$

Now, we consider the second-order variation of the unconstrained Dirichlet energy, namely, the functional $\mathcal{W} : H_0^1(\Omega, \mathbb{R}^3) \rightarrow \mathbb{R}$ defined by

$$\mathcal{W}[v] := \int_\Omega |\nabla v|^2 - |\nabla n_0|^2 |v|^2. \tag{3.11}$$

We will reason as in [25] to show that $\mathcal{W}[n_\varepsilon - n_0] \geq 0$ and then use an argument inspired by one in [21] to obtain the coercivity of this functional, which together with (3.10) will establish the result (3.9).

Since n_0 is a harmonic map, we have

$$-\Delta(n_0 \cdot e_3) = |\nabla n_0|^2 (n_0 \cdot e_3). \tag{3.12}$$

Also, due to Remark 2.1, without loss of generality, we may assume that $n_0 \cdot e_3 > 0$ in Ω . This means that any $\varphi \in C_c^\infty(\Omega, \mathbb{R}^3)$ can be written in the form $\varphi = (n_0 \cdot e_3)w$

for some $w \in H_0^1(\Omega, \mathbb{R}^3) \cap L^\infty(\Omega, \mathbb{R}^3)$; just set $w := (n_0 \cdot e_3)^{-1}\varphi$. Then, using (3.12) and an integration by parts, we get

$$\mathscr{W}[\varphi] = \int_{\Omega} (n_0 \cdot e_3)^2 |\nabla w|^2 \geq 0. \tag{3.13}$$

The last inequality shows in particular that

$$\mathscr{W}[v] = 0 \quad \text{if, and only if,} \quad \exists \gamma \in \mathbb{R}^3 : v = (n_0 \cdot e_3)\gamma \quad \text{in } \Omega. \tag{3.14}$$

Next, consider the following constrained minimisation problem:

$$\lambda_1 := \inf_{v \in H_0^1(\Omega, \mathbb{R}^3)} \left\{ \mathscr{W}[v] : \|v\|_{L^2(\Omega)} = 1, -|v| \leq 2v \cdot n_0 \leq 0 \text{ in } \Omega \right\}. \tag{3.15}$$

Standard arguments show that λ_1 is achieved by some $v_* \in H_0^1(\Omega, \mathbb{R}^3)$ with $\|v_*\|_{L^2(\Omega)}^2 = 1$. We claim that $\lambda_1 > 0$. Indeed, assume for contradiction that $\lambda_1 = \mathscr{W}(v_*) = 0$. Then, from (3.14), we get $v_* = (n_0 \cdot e_3)\gamma$ for some fixed $\gamma \in \mathbb{R}^3$, so that the constraint $v_* \cdot n_0 \leq 0$ reads as

$$\gamma \cdot n_0 \leq 0. \tag{3.16}$$

On the other hand, the boundary data n_b has nonzero degree, and therefore for any $e \in \mathbb{S}^1 \times \{0\} \subset \mathbb{S}^2$, there exists a sequence $(x_j)_{j \in \mathbb{N}}$ in Ω such that $x_j \rightarrow x_b \in \partial\Omega$ and $n_0(x_j) \rightarrow e$. Hence, from (3.16), $\gamma \cdot e \leq 0$ for every $e \in \mathbb{S}^1 \times \{0\}$. Taking this into account as well as the fact that $(n_0 \cdot e_3) > 0$ in Ω , we must have $\gamma = -re_3$ for some positive r . But then, the condition $-|v| \leq 2v \cdot n_0$ implies that $0 < n_0 \cdot e_3 \leq \frac{1}{2}$ in Ω , and this cannot happen because, otherwise, since n_0 is continuous, we would contradict the assumption that $n_0|_{\partial\Omega} = n_b$ has nonzero degree. Thus, we obtain

$$\int_{\Omega} |\nabla v|^2 - |\nabla n_0|^2 |v|^2 \geq \lambda_1 \int_{\Omega} |v|^2, \tag{3.17}$$

with $\lambda_1 > 0$, provided $v \in H_0^1(\Omega, \mathbb{R}^3)$ satisfies the inequality constraint $-|v| \leq 2v \cdot n_0 \leq 0$. This implies that

$$\int_{\Omega} |\nabla v|^2 - |\nabla n_0|^2 |v|^2 \geq \beta \int_{\Omega} |\nabla n_0|^2 |v|^2 \tag{3.18}$$

where $\beta = \lambda_1 / \|\nabla n_0\|_{L^\infty(\Omega)}^2 > 0$ (we recall that n_0 is smooth), and thereby

$$\frac{1}{1 + \beta} \int_{\Omega} |\nabla v|^2 \geq \int_{\Omega} |\nabla n_0|^2 |v|^2. \tag{3.19}$$

Substituting the preceding into (3.11), we get that

$$\mathscr{W}[v] \geq \frac{\beta}{1 + \beta} \int_{\Omega} |\nabla v|^2. \tag{3.20}$$

The claimed relation (3.9) follows on setting, $\alpha^2 := \frac{\beta}{1 + \beta}$, $v := n_\varepsilon - n_0$, and noting that the inequality constraint is satisfied for all sufficiently small ε . \square

3.2.2. Convergence estimates The expression (2.7) of the energy \mathcal{G}_ε reads, in extended form, as

$$\mathcal{G}_\varepsilon[Q_\varepsilon] = \frac{1}{2\varepsilon^2} \int_\Omega |\nabla Q_\varepsilon|^2 - |\nabla Q_0|^2 + \frac{1}{\varepsilon^4} \int_\Omega \tilde{f}_{bulk}(Q_\varepsilon). \tag{3.21}$$

We consider separately the difference in the Dirichlet and bulk potential energies of Q_ε and Q_0 . We first focus on the bulk energy and derive an equivalent expression of the bulk potential in terms of a suitable quadratic form. Precisely, let $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ be an almost-minimising family. According to Lemma 3.1, there exist $n_\varepsilon \in W^{1,\infty}(\Omega, \mathbb{S}^2)$, $\rho_\varepsilon \in W_0^{1,\infty}(\Omega, \mathbb{R}^3)$, such that

$$Q_\varepsilon = Q[n_\varepsilon] + \varepsilon^2 P_\varepsilon^\perp, \quad P_\varepsilon^\perp := R_{n_\varepsilon} V_{\rho_\varepsilon} R_{n_\varepsilon}^t. \tag{3.22}$$

Hence, $Q_\varepsilon = R_{n_\varepsilon} (V_+ + \varepsilon^2 V_{\rho_\varepsilon}) R_{n_\varepsilon}^t$, with $V_+ := s_+ (e_3 \otimes e_3 - \frac{1}{3}I) \in \mathcal{S}_*$. From the rotational invariance of \tilde{f}_{bulk} it follows that $\tilde{f}_{bulk}(Q_\varepsilon) = \tilde{f}_{bulk}(V_+ + \varepsilon^2 V_{\rho_\varepsilon})$. A straightforward calculation yields

$$\tilde{f}_{bulk}(Q_\varepsilon) = \frac{\varepsilon^4}{2} B_\varepsilon \rho_\varepsilon \cdot \rho_\varepsilon, \tag{3.23}$$

where $B_\varepsilon := B_0 + \varepsilon^2(\rho_\varepsilon \cdot e_3)B_1 + \varepsilon^4|\rho_\varepsilon|^2 B_2$, with $B_0 = \text{diag}(\mu, \mu, \nu)$ given by (2.15), and

$$B_1 = \sqrt{\frac{8}{3}}s_+c^2I + \sqrt{\frac{2}{3}}b^2 \text{diag}(1, 1, \frac{1}{3}), \quad B_2 = \frac{c^2}{2}I. \tag{3.24}$$

We note that μ and ν are the coefficients of the second variation of \tilde{f}_{bulk} about its minimum due to biaxial and uniaxial perturbations respectively. Moreover, from Lemma 3.1, it follows that $B_\varepsilon \rightarrow B_0$ uniformly. Since $B_0 = \text{diag}(\mu, \mu, \nu)$ is positive definite, it follows that B_ε is positive definite for sufficiently small ε .

Next, we plug the representation of Q_ε given by (3.22) into the Dirichlet part of \mathcal{G}_ε (cf. (3.21)), and we expand the energy. In doing this, we note that P_ε^\perp is in $H_0^1(\Omega, \mathcal{S}_0)$ because n_ε and n_0 coincide on $\partial\Omega$. After a simple calculation we obtain the identity

$$\begin{aligned} \frac{1}{2} \int_\Omega |\nabla Q_\varepsilon|^2 - |\nabla Q_0|^2 &= s_+^2 \int_\Omega |\nabla n_\varepsilon|^2 - |\nabla n_0|^2 \\ &\quad + s_+ \varepsilon^2 \int_\Omega \nabla(n_\varepsilon \otimes n_\varepsilon) : \nabla P_\varepsilon^\perp + \frac{\varepsilon^4}{2} \int_\Omega |\nabla P_\varepsilon^\perp|^2, \end{aligned} \tag{3.25}$$

Next, recalling that $P_\varepsilon^\perp = R_{n_\varepsilon} V_{\rho_\varepsilon} R_{n_\varepsilon}^t$ is symmetric, we get

$$\frac{1}{2} \int_\Omega \nabla(n_\varepsilon \otimes n_\varepsilon) : \nabla P_\varepsilon^\perp = \sum_{i=1}^2 \int_\Omega \partial_i n_\varepsilon \otimes n_\varepsilon : \partial_i P \tag{3.26}$$

$$= \sum_{i=1}^2 \int_\Omega [\partial_i (P_\varepsilon^\perp n_\varepsilon) - P_\varepsilon^\perp \partial_i n_\varepsilon] \cdot \partial_i n_\varepsilon \tag{3.27}$$

$$= - \int_{\Omega} \nabla n_{\varepsilon} \otimes \nabla n_{\varepsilon} : P_{\varepsilon}^{\perp} + \sqrt{2/3} \int_{\Omega} (\rho_{\varepsilon} \cdot e_3) |\nabla n_{\varepsilon}|^2, \tag{3.28}$$

the last equality being a consequence of the fact that n_{ε} is an eigenvector of P_{ε}^{\perp} , and of the constraint $|n_{\varepsilon}| = 1$. Eventually, introducing the vector-valued function $b_{\varepsilon} \in L^{\infty}(\Omega, \mathbb{R}^3)$ defined by

$$b_{\varepsilon} \cdot e_j := -2s_+ \nabla n_{\varepsilon} \otimes \nabla n_{\varepsilon} : R_{n_{\varepsilon}} F_j R_{n_{\varepsilon}}^T, \quad j = 1, 2, \tag{3.29}$$

$$b_{\varepsilon} \cdot e_3 := \sqrt{6} s_+ |\nabla n_{\varepsilon}|^2, \tag{3.30}$$

we get $-s_+ \Delta(n_{\varepsilon} \otimes n_{\varepsilon}) : P_{\varepsilon}^{\perp} = b_{\varepsilon} \cdot \rho_{\varepsilon}$. Overall, the energy $\mathcal{G}_{\varepsilon}$ can be decomposed in the form

$$\mathcal{G}_{\varepsilon}[Q_{\varepsilon}] = \frac{s_+^2}{\varepsilon^2} \left(\|\nabla n_{\varepsilon}\|_{L^2}^2 - \|\nabla n_0\|_{L^2}^2 \right) + \mathcal{H}_{\varepsilon}[n_{\varepsilon}, \rho_{\varepsilon}] + \frac{1}{2} \varepsilon^2 \|\nabla P_{\varepsilon}^{\perp}\|_{L^2}^2, \tag{3.31}$$

with

$$\mathcal{H}_{\varepsilon}[n_{\varepsilon}, \rho_{\varepsilon}] := \int_{\Omega} \frac{1}{2} B_{\varepsilon} \rho_{\varepsilon} \cdot \rho_{\varepsilon} + b_{\varepsilon} \cdot \rho_{\varepsilon}. \tag{3.32}$$

Combining the above representation (3.31) with Lemma 3.2, we obtain

$$\begin{aligned} \mathcal{G}_{\varepsilon}[Q_{\varepsilon}] &\geq \frac{1}{\varepsilon^2} \alpha^2 s_+^2 \|n_{\varepsilon} - n_0\|_{H_0^1}^2 + \mathcal{H}_{\varepsilon}[n_{\varepsilon}, \rho_{\varepsilon}] + \frac{1}{2} \varepsilon^2 \|\nabla P_{\varepsilon}^{\perp}\|_{L^2}^2 \\ &\geq \frac{1}{\varepsilon^2} \alpha^2 s_+^2 \|n_{\varepsilon} - n_0\|_{H_0^1}^2 + \beta \|\rho_{\varepsilon}\|_{L^2}^2 - \gamma \|b_{\varepsilon}\|_{L^2}^2 + \frac{1}{2} \varepsilon^2 \|\nabla P_{\varepsilon}^{\perp}\|_{L^2}^2, \end{aligned} \tag{3.33}$$

for some $\beta, \gamma > 0$ independent of ε . Next, Lemma 3.1, assures that $\|b_{\varepsilon}\|_{L^2}$ is bounded independently of ε and, therefore, the bound $\mathcal{G}_{\varepsilon}[Q_{\varepsilon}] \leq C$ implies that $\|n_{\varepsilon} - n_0\|_{H_0^1} \leq C\varepsilon$, that is, (2.13). On the other hand, Lemma 3.1 also assures that $\|\rho_{\varepsilon}\|_{L^2}$ is bounded independently of ε , so there exists $\rho \in L^2(\Omega, \mathbb{R}^3)$ such that

$$\rho_{\varepsilon} \rightharpoonup \rho \text{ weakly in } L^2(\Omega, \mathbb{R}^3). \tag{3.34}$$

This, used in (3.22), implies (2.14). This concludes the proof of part (ii) of Theorem 2.1.

3.3. Proof of (iii): lower bound and the existence of recovery sequences

We note that (3.33) holds for any almost-minimising family $Q_{\varepsilon} = Q[n_{\varepsilon}] + \varepsilon^2 P_{\varepsilon}^{\perp}$ having n_{ε} for principal eigenvectors. After that, taking into account that B_0 is positive definite, by standard lower semicontinuity arguments we get

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{G}_{\varepsilon}[Q_{\varepsilon}] \geq \liminf_{\varepsilon \rightarrow 0} \mathcal{H}_{\varepsilon}[n_{\varepsilon}, \rho_{\varepsilon}] \geq \mathcal{H}[n_0, \rho] = \int_{\Omega} \frac{1}{2} B_0 \rho \cdot \rho + b_0 \cdot \rho, \tag{3.35}$$

where B_0 and b_0 are given by (2.15).

To proceed, we observe that since Ω is a Lipschitz domain, it admits a family of Hopf cutoff functions [20], that is, compactly supported smooth functions $\chi_\varepsilon \in C_0^\infty(\Omega)$ such that, for any sufficiently small $\varepsilon > 0$, we have: $\chi_\varepsilon(x) = 1$ if $d(x, \partial\Omega) \geq \varepsilon$, $\chi_\varepsilon \rightarrow 1$ strongly in $L^2(\Omega)$, and $\|\nabla\chi_\varepsilon\|_{L^\infty(\Omega)} \leq C\varepsilon^{-1}$ for some positive constant $C > 0$ independent of ε . Then we define, for any $\rho \in L^2(\Omega, \mathbb{R}^3)$,

$$Q_\varepsilon = Q_0 + \varepsilon^2 P_\varepsilon^\perp, \quad P_\varepsilon^\perp = R_{n_0} V_{\rho_\varepsilon} R_{n_0}^t, \tag{3.36}$$

where $\rho_\varepsilon = \chi_\varepsilon \zeta_\varepsilon$, $\zeta_\varepsilon \in C^\infty(\Omega, \mathbb{R}^3)$ is such that $\zeta_\varepsilon \rightarrow \rho$ in $L^2(\Omega, \mathbb{R}^3)$, and $\|\nabla\zeta_\varepsilon\|_{L^2(\Omega)}^2 \leq C\varepsilon^{-1}$. The convergence relations (2.13), (2.14) are trivially satisfied because for any $\varepsilon > 0$ the director n_ε is the principal eigenvector of Q_ε . In particular, a direct computation yields

$$\lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] = \lim_{\varepsilon \rightarrow 0} \left(\int_\Omega \frac{1}{2} (B_\varepsilon \rho \cdot \rho + b_\varepsilon \cdot \rho) \chi_\varepsilon + \frac{\varepsilon^2}{2} \int_\Omega |\nabla P_\varepsilon^\perp|^2 \right). \tag{3.37}$$

Denoting by $\Omega_\varepsilon := \{x \in \Omega : d(x, \partial\Omega) < \varepsilon\}$ the tubular neighbourhood of $\partial\Omega$ of radius ε , we obtain for ε sufficiently small, the existence of a positive constant C_0 depending only on n_0 such that

$$\frac{\varepsilon^2}{2} \int_\Omega |\nabla P_\varepsilon^\perp|^2 \leq C_0 \left(\varepsilon^2 \int_{\Omega_\varepsilon} |\zeta_\varepsilon \nabla \chi_\varepsilon|^2 + \varepsilon^2 \int_\Omega |\chi_\varepsilon \nabla \zeta_\varepsilon|^2 + |\chi_\varepsilon \zeta_\varepsilon|^2 \right) \rightarrow 0. \tag{3.38}$$

Combining the previous estimate with (3.37), and recalling the definition of B_ε and ζ_ε , we infer that

$$\lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] = \mathcal{H}_0[n_0, \rho]. \tag{3.39}$$

This establishes (iii) of Theorem 2.1.

3.4. Proof of statement (iv): Γ -convergence and convergence estimates for the minimisers

The Γ -convergence of \mathcal{G}_ε to $\mathcal{H}_0[n_0, \rho_0]$, with $\rho_0 := -B_0^{-1} b_0$, is clear from the lower bound (3.35) and the upper bound (3.39). It remains to prove the convergence estimates for the minimisers. Let $\{Q_\varepsilon^*\}_{\varepsilon > 0} \subseteq W^{1,\infty}(\Omega, \mathcal{S}_0)$ be a family of minimisers of \mathcal{E}_ε . According to Lemma 3.1, Q_ε^* may be expressed in terms of its principal eigenvector, $n_\varepsilon^* \in W^{1,\infty}(\Omega, \mathbb{S}^2)$, and the vector-valued function $\rho_\varepsilon^* \in W_0^{1,\infty}(\Omega, \mathbb{R}^3)$. Precisely, we have

$$Q_\varepsilon^* = Q[n_\varepsilon^*] + \varepsilon^2 P_\varepsilon^{*\perp}, \quad P_\varepsilon^{*\perp} := R_{n_\varepsilon^*} V_{\rho_\varepsilon^*} R_{n_\varepsilon^*}^t, \tag{3.40}$$

with $\varepsilon^2 \rho_\varepsilon^* \rightarrow 0$ in $W_0^{1,p}(\Omega, \mathbb{R}^3)$. Since $\mathcal{E}_\varepsilon[Q_\varepsilon^*]$ is bounded, it follows from the same argument that led to (3.34), that, perhaps up to a subsequence, ρ_ε^* converges weakly in $L^2(\Omega, \mathbb{R}^3)$ to some ρ^* . In particular, we have

$$B_\varepsilon \rightarrow B_0 \quad \text{strongly in } L^2(\Omega, \mathbb{R}^{3 \times 3}), \tag{3.41}$$

$$\rho_\varepsilon^* \rightharpoonup \rho^* \text{ weakly in } L^2(\Omega, \mathbb{R}^3), \tag{3.42}$$

where $B_\varepsilon := B_0 + \varepsilon^2(\rho_\varepsilon^* \cdot e_3)B_1 + \varepsilon^4|\rho_\varepsilon^*|^2B_2$. Since B_0 is positive definite, by the lower semicontinuity of the norms and (3.31), we have that

$$\begin{aligned} \liminf_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon^*] &\geq \liminf_{\varepsilon \rightarrow 0} \mathcal{H}_\varepsilon[n_\varepsilon^*, \rho_\varepsilon^*] \geq \mathcal{H}_0[n_0, \rho^*] \\ &= \int_\Omega \frac{1}{2} B_0 \rho^* \cdot \rho^* + b_0 \cdot \rho^* \geq \mathcal{H}_0[n_0, \rho_0], \end{aligned} \tag{3.43}$$

with $\rho_0 := \operatorname{argmin}_{\sigma \in \mathbb{R}^3} (\frac{1}{2} B_0 \sigma \cdot \sigma + b_0 \cdot \sigma) = -B_0^{-1} b_0$, and b_0 given by (2.16). Also, by (iii), there exists an almost-minimising recovery family $\{Q_\varepsilon\}_{\varepsilon > 0} \subseteq \mathcal{U}$ such that $\lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] = \mathcal{H}_0[n_0, \rho_0]$. Since $\mathcal{E}_\varepsilon[Q_\varepsilon] \geq \mathcal{E}_\varepsilon[Q_\varepsilon^*]$, it follows that $\lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon^*] = \mathcal{H}_0[n_0, \rho_0]$ because

$$\mathcal{H}_0[n_0, \rho_0] = \lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] \geq \limsup_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon^*] \geq \liminf_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon^*] \geq \mathcal{H}_0[n_0, \rho_0]. \tag{3.44}$$

From (3.31) and the preceding, we deduce that

$$\begin{aligned} \mathcal{G}_\varepsilon[Q_\varepsilon^*] - \mathcal{H}_0[n_0, \rho_0] &= \frac{s_+^2}{\varepsilon^2} \left(\|\nabla n_\varepsilon^*\|_{L^2}^2 - \|\nabla n_0\|_{L^2}^2 \right) + \frac{1}{2} \varepsilon^2 \|\nabla P_\varepsilon^\perp\|_{L^2}^2 \\ &\quad + \mathcal{H}_\varepsilon[n_\varepsilon^*, \rho_\varepsilon^*] - \mathcal{H}_0[n_0, \rho_0]. \end{aligned} \tag{3.45}$$

On the other hand, since $\rho_0 = -B_0^{-1} b_0$, we have

$$\begin{aligned} \mathcal{H}_\varepsilon[n_\varepsilon^*, \rho_\varepsilon^*] - \mathcal{H}_0[n_0, \rho_0] &= \int_\Omega \frac{1}{2} B_\varepsilon \rho_\varepsilon^* \cdot \rho_\varepsilon^* + b_\varepsilon \cdot \rho_\varepsilon^* - \int_\Omega \frac{1}{2} B_0 \rho_0 \cdot \rho_0 + b_0 \cdot \rho_0 \\ &= \frac{1}{2} \int_\Omega B_0^{-1} b_0 \cdot b_0 - B_\varepsilon^{-1} b_\varepsilon^* \cdot b_\varepsilon^* \\ &\quad + \frac{1}{2} \int_\Omega B_\varepsilon (\rho_\varepsilon^* + B_\varepsilon^{-1} b_\varepsilon^*) \cdot (\rho_\varepsilon^* + B_\varepsilon^{-1} b_\varepsilon^*), \end{aligned}$$

with b_ε^* defined as in (3.29), (3.30). Since $n_\varepsilon \rightarrow n_0$ strongly in $W^{1,p}(\Omega, \mathbb{S}^2)$, it follows that $b_\varepsilon^* \rightarrow b_0$ strongly in $L^2(\Omega, \mathbb{R}^3)$. Hence,

$$\begin{aligned} 0 &\leq \frac{1}{2} \int_\Omega B_0 (\rho^* + B_0^{-1} b_0) \cdot (\rho_0 + B_0^{-1} b_0) \\ &\leq \liminf_{\varepsilon \rightarrow 0} (\mathcal{H}_\varepsilon[n_\varepsilon^*, \rho_\varepsilon^*] - \mathcal{H}_0[n_0, \rho_0]). \end{aligned}$$

Summarizing from the previous inequality and (3.45), we infer that

$$\begin{aligned} 0 &\geq \lim_{\varepsilon \rightarrow 0} (\mathcal{G}_\varepsilon[Q_\varepsilon^*] - \mathcal{H}_0[n_0, \rho_0]) \\ &\geq \lim_{\varepsilon \rightarrow 0} \left[\frac{s_+^2}{\varepsilon^2} \left(\|\nabla n_\varepsilon^*\|_{L^2}^2 - \|\nabla n_0\|_{L^2}^2 \right) + \frac{1}{2} \varepsilon^2 \|\nabla P_\varepsilon^\perp\|_{L^2}^2 \right] \\ &\quad + \frac{1}{2} \int_\Omega B_0 (\rho^* + B_0^{-1} b_0) \cdot (\rho_0 + B_0^{-1} b_0). \end{aligned}$$

As each term on the right-hand side is nonnegative, they separately vanish in the limit $\varepsilon \rightarrow 0$. In particular, $\rho^* = -B_0^{-1}b_0 = \rho_0$ and, by Lemma 3.2, $(n_\varepsilon^* - n_0)/\varepsilon \rightarrow 0$ in $H^1(\Omega, \mathbb{S}^2)$. This establishes the convergence estimates (2.19) and (2.20), and completes the proof of Theorem 2.1.

4. The Case $b^2 = 0$ and Non-orientable Boundary Conditions

Generally speaking, for non-orientable boundary conditions on a two-dimensional domain, the Landau-de Gennes energy $\mathcal{E}_\varepsilon[Q_\varepsilon]$ of a minimising sequence Q_ε diverges logarithmically as $\varepsilon \rightarrow 0$ (cf. [8]), and an analysis different from the one developed in this paper is required to describe the small- ε behaviour. However, in the special case $b^2 = 0$ in the Landau-de Gennes bulk potential, results similar to those of Section 2 can be established. The key point is that $b^2 = 0$ corresponds to a degeneracy in the bulk potential, which reduces to a function of $\text{tr } Q^2$ only:

$$\tilde{f}_{bulk} = \left(\frac{c}{4\varepsilon}\right)^2 \left(|Q|^2 - \frac{a^2}{c^2}\right)^2, \tag{4.1}$$

with four-dimensional limit manifold

$$\mathcal{S}_0^* := \{Q \in \mathcal{S}_0; |Q|^2 = (2/3)s_+^2 = a^2/c^2\} \tag{4.2}$$

homeomorphic to \mathbb{S}^4 , as opposed to $\mathbb{R}P^2$ in the generic case.

In addition to taking boundary conditions to lie in the degenerate limit manifold \mathcal{S}_0^* , we restrict them to be planar prolate uniaxial, in analogy with the $b^2 \neq 0$ case. This allows for a convenient generalisation of degree to non-orientable boundary conditions, as follows: let \mathcal{B}_Q denote the set of planar prolate uniaxial Q -tensors in \mathcal{S}_0^* , and $\mathcal{B}_D = \{n \in \mathbb{S}^2 \mid n \cdot e_3 = 0\}$ denote the set of planar directors. The parameterisation $n \mapsto Q = s_+(n \otimes n - \frac{1}{3}I)$ is a double covering of \mathcal{B}_Q by \mathcal{B}_D (since n and $-n$ parameterise the same Q -tensor). Since \mathcal{B}_D is homeomorphic to \mathbb{S}^1 , it follows that \mathcal{B}_Q is homeomorphic to the real projective line $\mathbb{S}^1/\mathbb{Z}_2$, which is also homeomorphic to \mathbb{S}^1 via the map

$$e^{i\theta} \in \mathbb{S}^1 \mapsto \{e^{i\theta/2}, e^{i(\pi+\theta/2)}\} \in \mathbb{S}^1/\mathbb{Z}_2. \tag{4.3}$$

Thus, boundary conditions $Q_b \in C^1(\partial\Omega, \mathcal{B}_Q)$ may be assigned an integer degree, $\text{deg } Q_b$. If $\text{deg } Q_b$ is even, say equal to $2m$, there exists a planar director $n_b \in C^1(\partial\Omega, \mathcal{B}_D)$ such that $\text{deg } n_b = m$; in this case, Q_b is orientable. In the non-orientable case, $\text{deg } Q_b = k$ is odd; any n_b which parameterises Q_b necessarily has a discontinuity in sign, so that $n_b \notin C^1(\partial\Omega, \mathcal{B}_D)$. In this case, one says that n_b has half-integer degree $k/2$.

Throughout this section we assume that Ω is a bounded, simply-connected domain with C^1 boundary. The following result can be shown in a manner similar to that of Proposition 2.1:

Theorem 4.1. *Let $Q_b \in C^1(\partial\Omega, \mathcal{B}_Q)$ and let $\mathcal{U} = \{Q \in H^1(\Omega, \mathcal{S}_0); Q|_{\partial\Omega} = Q_b\}$. Then, as $\varepsilon \rightarrow 0$, the following statements hold:*

- (i) Let $C > 0$. For any family $\{Q_\varepsilon\}_{\varepsilon>0} \subset \mathcal{U}$ such that $\mathcal{E}_\varepsilon[Q_\varepsilon] \leq C$ we have, possibly on a subfamily, $Q_\varepsilon \rightarrow Q$ weakly in $H^1(\Omega, \mathcal{S}_0)$ for some $Q \in H^1(\Omega, \mathcal{S}_0^*)$.
- (ii) The family of energies $(\mathcal{E}_\varepsilon)_{\varepsilon>0}$ Γ -converges to \mathcal{E}_0 in the weak topology of $H^1(\Omega, \mathcal{S}_0)$, where

$$\mathcal{E}_0[Q] = \begin{cases} \frac{1}{2} \int_\Omega |\nabla Q|^2 & \text{if } Q \in H^1(\Omega, \mathcal{S}_0^*) \cap \mathcal{U}, \\ +\infty & \text{otherwise,} \end{cases} \tag{4.4}$$

with \mathcal{S}_0^* the limit manifold defined by (4.2).

- (iii) The minimisers $\{Q_\varepsilon\}_{\varepsilon>0}$ of the problem (2.2) converge strongly in $H^1(\Omega, \mathcal{S}_0)$ to the minimisers of the following harmonic map problem

$$\min_{Q \in \mathcal{U}} \mathcal{E}_0[Q]. \tag{4.5}$$

Remark 4.1. Note that a planar uniaxial Q -tensor $Q = s_+(n \otimes n - \frac{1}{3}I)$ has the following expression in terms of the orthonormal basis (2.9):

$$Q = \sum_{j=1}^5 c_j F_j = \frac{s_+}{\sqrt{2}} \left((n_1^2 - n_2^2)F_1 + 2n_1n_2F_2 - \frac{1}{\sqrt{3}}F_3 \right), \tag{4.6}$$

where $n_i = n \cdot e_i, i = 1, 2$. Thus, c_4 and c_5 vanish, while c_3 is fixed and negative. It follows that every element $Q_b \in C^1(\partial\Omega, \mathcal{B}_Q)$ admits a representation of the form $Q_b = \sqrt{2/3}s_+ \sum_{j=1}^3 c_{bj} F_j$, for some vector field $c_b \in C^1(\partial\Omega, \mathbb{S}^2)$. After that, standard arguments based on the maximum principle show the existence of a unique minimiser of problem (4.5); it can be expressed as

$$Q_0 = \sqrt{2/3}s_+ (c_{01}F_1 + c_{02}F_2 + c_{03}F_3), \tag{4.7}$$

where $c_0 \in H^1(\Omega, \mathbb{S}^2)$ solves the following minimisation problem:

$$\min \left\{ \int_\Omega |\nabla c|^2 : c \in H^1(\Omega, \mathbb{S}^2), c = c_b \text{ on } \partial\Omega \right\}. \tag{4.8}$$

In particular, c_0 is an \mathbb{S}^2 -valued harmonic map, that is, $-\Delta c_0 = |\nabla c_0|^2 c_0$. We note that Q_0 is biaxial unless one of the following conditions holds: *i*) $c_0 \cdot e_3 = -1/\sqrt{3}$, in which case Q_0 is planar uniaxial; *ii*) $c_0 \cdot e_3 = -1$, in which case $Q_0 = -\sqrt{2/3}s_+ F_3$ is oblate uniaxial with director e_3 ; or *iii*) $c_0 \cdot e_3 = 1$, in which case $Q_0 = \sqrt{2/3}s_+ F_3$ is prolate uniaxial with director e_3 . In fact, the maximum principle implies that $c_0 \cdot e_3 < 0$, so that the last possibility is excluded.

We need to go to the next-order term in the Γ -asymptotic expansion of the energy \mathcal{E}_ε and define the renormalised relative energy as in (2.7),

$$\mathcal{G}_\varepsilon[Q] = \frac{1}{\varepsilon^2} (\mathcal{E}_\varepsilon[Q] - \mathcal{E}_0[Q_0]), \tag{4.9}$$

where Q_0 is the unique minimiser of the problem (4.5); in particular, Q_0 is a harmonic map. Information about the expansion of the energy \mathcal{E}_ε is given by the following result:

Theorem 4.2. *Let Q_0 be a minimiser of \mathcal{E}_0 over \mathcal{U} as in the problem (4.5). The following assertions hold:*

(i) *Let $C > 0$. For any family $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ such that $\mathcal{G}_\varepsilon[Q_\varepsilon] \leq C$, there exist $P \in H_0^1(\Omega, \mathcal{S}_0)$, pointwise orthogonal to Q_0 , and $\rho \in L^2(\Omega)$, for which, possibly on a subsequence,*

$$Q_\varepsilon \rightarrow Q_0 \quad \text{strongly in } H^1(\Omega, \mathcal{S}_0) \tag{4.10}$$

$$\frac{1}{\varepsilon^2}(Q_\varepsilon - Q_0) : Q_0 \rightharpoonup \rho \quad \text{weakly in } L^2(\Omega), \tag{4.11}$$

$$\frac{1}{\varepsilon}(Q_\varepsilon - Q_0) \rightharpoonup P \quad \text{weakly in } H_0^1(\Omega, \mathcal{S}_0) \text{ with } P : Q_0 = 0. \tag{4.12}$$

(ii) *For any $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ such that (4.10), (4.11), and (4.12) hold, we have*

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] \geq \mathcal{H}[P, \rho], \tag{4.13}$$

with

$$\mathcal{H}[P, \rho] := \frac{1}{2} \int_\Omega |\nabla P|^2 + \int_\Omega \frac{c^2}{a^2} |\nabla Q_0|^2 \rho + \frac{c^2}{4} \int_\Omega (|P|^2 + 2\rho)^2. \tag{4.14}$$

Also, for any $P \in H_0^1(\Omega, \mathcal{S}_0)$ pointwise orthogonal to Q_0 , and any $\rho \in L^2(\Omega)$, there exists a recovery family $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ such that (4.10), (4.11), (4.12) hold, and

$$\lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] = \mathcal{H}[P, \rho]. \tag{4.15}$$

(iii) *The family of energies $\{\mathcal{G}_\varepsilon\}_{\varepsilon>0}$ Γ -converges to \mathcal{G}_0 in $H^1(\Omega, \mathcal{S}_0)$, where*

$$\mathcal{G}_0[Q] = \begin{cases} -\frac{c^2}{4a^4} \int_\Omega |\nabla Q_0|^4 & \text{if } Q = Q_0, \\ +\infty & \text{otherwise.} \end{cases} \tag{4.16}$$

Moreover if $(Q_\varepsilon)_{\varepsilon>0}$ is a family of minimisers of \mathcal{E}_ε on \mathcal{U} then

$$\frac{1}{\varepsilon^2}(Q_\varepsilon - Q_0) : Q_0 \rightarrow \frac{1}{2a^2} |\nabla Q_0|^2 \quad \text{in } L^2(\Omega, \mathcal{S}_0), \tag{4.17}$$

$$\frac{1}{\varepsilon}(Q_\varepsilon - Q_0) \rightarrow 0 \quad \text{in } H^1(\Omega, \mathcal{S}_0). \tag{4.18}$$

Proof. (i) If Q_ε satisfies $\mathcal{G}_\varepsilon[Q_\varepsilon] \leq C$, by the same argument used in the proof of the Theorem 2.1, we get that necessarily $Q_\varepsilon \rightarrow Q_0$ strongly in $H^1(\Omega, \mathcal{S}_0)$. After that, let $(Q_\varepsilon)_{\varepsilon>0}$ be such that $Q_\varepsilon \rightarrow Q$ in $H^1(\Omega, \mathcal{S}_0)$. We set $P_\varepsilon := (Q_\varepsilon - Q_0)/\varepsilon^2$, so that $Q_\varepsilon = Q_0 + \varepsilon^2 P_\varepsilon$ with $P_\varepsilon \in H_0^1(\Omega, \mathcal{S}_0)$. Plugging the expression of Q_ε into the energy \mathcal{G}_ε , and taking into account that Q_0 is a harmonic map, we obtain

$\mathcal{G}_\varepsilon[Q_\varepsilon]$

$$= \frac{1}{2} \int_\Omega \varepsilon^2 |\nabla P_\varepsilon|^2 + \int_\Omega \nabla Q_0 : \nabla P_\varepsilon + \frac{c^2}{4} \int_\Omega (\varepsilon^2 |P_\varepsilon|^2 + 2Q_0 : P_\varepsilon)^2 \tag{4.19}$$

$$= \frac{1}{2} \int_\Omega \varepsilon^2 |\nabla P_\varepsilon|^2 + \int_\Omega \frac{c^2}{a^2} |\nabla Q_0|^2 (Q_0 : P_\varepsilon) + \frac{c^2}{4} \int_\Omega (\varepsilon^2 |P_\varepsilon|^2 + 2Q_0 : P_\varepsilon)^2, \tag{4.20}$$

and, after some further computation,

$$\begin{aligned} \mathcal{G}_\varepsilon[Q_\varepsilon] &= \int_\Omega \left(\frac{c}{2a^2} |\nabla Q_0|^2 + c(Q_0 : P_\varepsilon) + \frac{c}{2} \varepsilon^2 |P_\varepsilon|^2 \right)^2 - \frac{c^2}{4a^4} \int_\Omega |\nabla Q_0|^4 \\ &\quad + \frac{\varepsilon^2}{2} \int_\Omega |\nabla P_\varepsilon|^2 - \frac{c^2}{a^2} |\nabla Q_0|^2 |P_\varepsilon|^2. \end{aligned} \tag{4.21}$$

Using the decomposition trick (cf. Lemma A.1. in [23]) we claim that, for some $\alpha > 0$, the following estimate holds:

$$\int_\Omega |\nabla P_\varepsilon|^2 - \frac{c^2}{a^2} |\nabla Q_0|^2 |P_\varepsilon|^2 \geq \alpha \int_\Omega |\nabla P_\varepsilon|^2. \tag{4.22}$$

Indeed, we know that $q_3 = Q_0 : F_3$ solves $-\Delta q_3 = \frac{c^2}{a^2} |\nabla Q_0|^2 q_3$ and, by the maximum principle, $q_3 < 0$ in Ω because $\min_{\partial\Omega} q_3 < 0$. Thus, we can represent any second-order perturbation in the form $P_\varepsilon = q_3 U_\varepsilon$ with $U_\varepsilon := q_3^{-1} P_\varepsilon$. Arguing as in the proof of Lemma 3.2, we deduce the existence of a positive constant β such that

$$\begin{aligned} \int_\Omega |\nabla P_\varepsilon|^2 - \frac{c^2}{a^2} |\nabla Q_0|^2 |P_\varepsilon|^2 &= \int_\Omega |\nabla q_3 U_\varepsilon + q_3 \nabla U_\varepsilon|^2 + \Delta q_3 q_3 |U_\varepsilon|^2 \\ &= \int_\Omega |q_3|^2 |\nabla U_\varepsilon|^2 \geq \beta \int_\Omega \frac{c^2}{a^2} |\nabla Q_0|^2 |P_\varepsilon|^2. \end{aligned} \tag{4.23}$$

This, for $\alpha := \frac{\beta}{1+\beta}$, immediately implies the desired result (4.22).

Since $\mathcal{G}_\varepsilon(Q_\varepsilon) \leq C$, by (4.21) and (4.22), we obtain $\|\varepsilon P_\varepsilon\|_{H^1} \leq C$ and $\|P_\varepsilon : Q_0\|_{L^2} \leq C$. Thereby, the existence of $P \in H_0^1(\Omega, \mathcal{S}_0)$, $\rho \in L^2(\Omega)$ such that $Q_0 : P_\varepsilon \rightharpoonup \rho$ weakly in $L^2(\Omega)$, and $\varepsilon P_\varepsilon \rightharpoonup P$ weakly in $H_0^1(\Omega, \mathcal{S}_0)$. Therefore, also $P : Q_0 = 0$.

(ii) The lower bound (4.13) follows from (4.21) and the lower semicontinuity of the norms under weak convergence. Now, for any $P \in H_0^1(\Omega, \mathcal{S}_0)$ pointwise orthogonal to Q_0 , and any $\rho \in L^2(\Omega)$, we want to construct a recovery family $\{Q_\varepsilon\}_{\varepsilon>0} \subseteq \mathcal{U}$ such that (4.10), (4.11), (4.12) hold, and $\lim_{\varepsilon \rightarrow 0} \mathcal{G}_\varepsilon[Q_\varepsilon] = \mathcal{H}[P, \rho]$. To this end we recall the construction for the case $b \neq 0$ and define $\xi_\varepsilon = \chi_\varepsilon \zeta_\varepsilon$ with $\zeta_\varepsilon \in C^\infty(\Omega)$, $\zeta_\varepsilon \rightarrow \rho$ in L^2 , $\|\nabla \zeta_\varepsilon\|_{L^2}^2 \leq C\varepsilon^{-1}$ and χ_ε defined as in section 3.3. For any $P \in H_0^1(\Omega, \mathcal{S}_0)$ such that $P : Q_0 = 0$ we set, as a recovery family,

$$Q_\varepsilon := Q_0 + \varepsilon P + \frac{3}{2s_+^2} \varepsilon^2 \xi_\varepsilon Q_0. \tag{4.24}$$

Plugging this expression into (4.20) we infer

$$\begin{aligned} \mathcal{G}_\varepsilon(Q_\varepsilon) &= \frac{1}{2} \int_\Omega |\nabla(P + \varepsilon \xi_\varepsilon Q_0)|^2 \\ &+ \int_\Omega \frac{c^2}{a^2} |\nabla Q_0|^2 \xi_\varepsilon + \frac{c^2}{4} \int_\Omega \left(|P + \frac{3\varepsilon}{2s_+^2} \xi_\varepsilon Q_0|^2 + 2\xi_\varepsilon \right)^2. \end{aligned} \tag{4.25}$$

Finally, taking the limit as $\varepsilon \rightarrow 0$ we conclude.

(iii) It is clear that if $Q \neq Q_0$ we can take $Q_\varepsilon = Q$ to recover $\mathcal{G}_\varepsilon[Q_\varepsilon] \rightarrow \infty$. It is also clear that if Q_ε is a family of minimisers of \mathcal{E}_ε , then (i) holds. Minimising (4.16) with respect to P and ρ , we obtain $P = 0$ and $\rho = \frac{1}{2a^2} |\nabla Q_0|^2$. Moreover the minimal energy is

$$\min \mathcal{G}_0(\rho) = -\frac{c^2}{4a^4} \int_\Omega |\nabla Q_0|^4.$$

In order to obtain (4.17) and (4.18), we combine (4.20) with the results stated in (ii). \square

5. Applications to Conformal Director Fields

Our previous results provide refined information on minimisers of the Landau-de Gennes energy for any fixed planar boundary conditions of nonzero degree. In this section we apply Theorem 2.1 and Theorem 4.2 to two families of planar boundary conditions n_b of independent interest. In particular, we consider a class of boundary data for which Q_0 , the leading-order Landau-de Gennes minimiser, is, up to a normalisation factor, an \mathbb{S}^4 -valued harmonic map.

In both cases ($b = 0$ and $b \neq 0$), Q_0 is related to a conformal (and therefore harmonic) \mathbb{S}^2 -valued map. However, the relationship is different in the two cases. In the case $b^2 \neq 0$, Q_0 is given by $Q[n_0]$, where n_0 is a conformal director field. In the case $b^2 = 0$, Q_0 is given up to normalisation by $c_{01}F_1 + c_{02}F_2 + c_{03}F_3$, where $c_0 : \Omega \rightarrow \mathbb{S}^2$ is conformal. These conformal families are parameterised by the positions of interior *escape points*, where n_0 or c is vertical, that is, parallel to e_3 .

The above class of boundary conditions is interesting for several reasons. First, the leading-order Oseen-Frank energy saturates a topological lower bound, and is the same for all boundary conditions within the family. Therefore it is impossible to distinguish between minimal Q -tensor configurations generated by these boundary conditions using only the leading-order approximation. The first-order correction breaks this degeneracy, and provides a mechanism to describe how the Landau-de Gennes energy depends on the position of escape points (defined by the boundary conditions) for Q -tensor fields that are harmonic at leading order. Also, rather explicit results are available for both the leading- and next-order Landau-de Gennes minimiser in terms of the Green’s function of the Laplacian on Ω . Interestingly, for these special boundary conditions, the biaxial component of the next-order correction vanishes; biaxiality appears only at order higher than $O(\varepsilon^2)$. Results for the case $b^2 \neq 0$ are stated in Section 5.1, and proofs are given in Section 5.2. Results for the case $b^2 = 0$ are stated in Section 5.3.

5.1. Harmonic Q -tensors and conformal director fields-main results

We begin by establishing a connection between harmonic uniaxial Q -tensors and conformal director fields.

Definition 5.1. A director field $n \in H^1(\Omega, \mathbb{S}^2)$ is *conformal* if

$$\partial_2 n = \sigma n \times \partial_1 n, \quad (5.1)$$

with $\sigma \equiv 1$ or $\sigma \equiv -1$ in Ω .

If Ω is equipped with the Euclidean metric and \mathbb{S}^2 equipped with its standard Riemannian metric, then (5.1) is equivalent to the usual definition of conformal maps as isometries up to a scale factor; the sign σ determines whether n is orientation-preserving ($\sigma = 1$) or reversing ($\sigma = -1$).

Proposition 5.1. *If $n \in H^1(\Omega, \mathbb{S}^2)$ is conformal, then n is an \mathbb{S}^2 -valued harmonic map.*

The proof involves showing that n conformal implies that n is a weakly harmonic map. One then appeals to a result of Hel  n [18] that weakly harmonic maps over two-dimensional domains are real analytic.

A director field n may be identified with a complex-valued function w on Ω via stereographic projection between \mathbb{S}^2 and the extended complex plane \mathbb{C}^* , as follows:

$$w = \frac{n_1 + in_2}{1 + n_3}, \quad n = \frac{(2 \operatorname{Re} w, 2 \operatorname{Im} w, 1 - |w|^2)}{1 + |w|^2}. \quad (5.2)$$

Then n being conformal is equivalent to w being either meromorphic ($\sigma = 1$) or antimeromorphic ($\sigma = -1$).

We identify \mathbb{S}^4 with the space of Q -tensors of unit norm.

Definition 5.2. A Q -tensor field $Q \in H^1(\Omega, \mathbb{S}^4)$ is a (weakly) \mathbb{S}^4 -valued harmonic map if

$$\Delta Q = -|\nabla Q|^2 Q \text{ in } \mathcal{D}'(\Omega, \mathcal{S}_0). \quad (5.3)$$

As with director fields, if Q is a weakly harmonic map, it is real analytic [18].

Proposition 5.2. *Let $n \in H^1(\Omega, \mathbb{S}^2)$ and define $Q \in H^1(\Omega, \mathbb{S}^4)$ by*

$$Q = \sqrt{3/2} \left(n \otimes n - \frac{1}{3} I \right). \quad (5.4)$$

Then Q is an \mathbb{S}^4 -valued harmonic map if and only if n is conformal.

The proof is given in Section 5.2. Below, in a slight abuse of terminology we will say

Definition 5.3. A Q -tensor field $Q \in H^1(\Omega, \mathcal{S}_0)$ is *harmonic* if $|Q|$ is everywhere constant and $Q/|Q|$ is an \mathbb{S}^4 -valued harmonic map.

Next, we use the connection between harmonic uniaxial Q -tensors and conformal director fields to determine the planar boundary conditions of given degree that minimise the leading-order Landau-de Gennes energy. Given $a \in \Omega$, let $g_a \in C^\infty(\Omega)$ denote the solution of the Laplace equation

$$\Delta g_a = 0, \quad g_a|_{\partial\Omega}(x) = \log|x - a|. \tag{5.5}$$

Thus, $\log|x - a| - g_a$ is the Green’s function for the Laplacian on Ω with Dirichlet boundary conditions.

In what follows, it will be convenient to regard Ω as a subset of \mathbb{C} rather than \mathbb{R}^2 ; expressions such as $1/(x - a)$ for $x, a \in \Omega$ should be understood in this context. Since Ω is simply connected, g_a has a harmonic conjugate, which is determined up to an additive constant. Let h_a denote a harmonic conjugate of g_a . Then $g_a + ih_a$ is holomorphic on Ω . Let $m \in \mathbb{Z}$ and $\mathbf{a} = (a_{(1)}, \dots, a_{(|m|)}) \in \Omega^{|m|}$ denote an $|m|$ -tuple of points in Ω , not necessarily distinct. We define

$$w_{0;\mathbf{a}} := e^{i\alpha} \left[\prod_{j=1}^{|m|} \frac{x - a_{(j)}}{\exp(g_{a_{(j)}} + ih_{a_{(j)}})} \right]^{\text{sgn } m} \tag{5.6}$$

for some $\alpha \in \mathbb{R}$.

Theorem 5.1. *Let $n_b \in C^1(\partial\Omega, \mathbb{S}^1)$ be a planar boundary director field of degree $m \neq 0$, and let $Q_b = s_+(n_b \otimes n_b - \frac{1}{3}I)$. The following assertions hold:*

(i) *For $Q \in H^1(\Omega, \mathcal{S}_0)$ with $Q|_{\partial\Omega} = Q_b$, we have that*

$$\mathcal{E}_0[Q] \geq 2s_+^2\pi|m|, \tag{5.7}$$

with equality if, and only if, $Q = s_+(n_0 \otimes n_0 - \frac{1}{3}I)$ with n_0 conformal and $n_0 \cdot e_3$ sign-definite (that is, $n_0 \cdot e_3$ is either strictly positive or strictly negative).

(ii) *The director field n_0 is conformal with $n_0 \cdot e_3$ sign-definite if, and only if, its stereographic projection (5.2) is given by $w_{0;\mathbf{a}}$ or by $1/\overline{w_{0;\mathbf{a}}}$ for some $\mathbf{a} \in \Omega^{|m|}$ (the two alternatives for n_0 are related by reflection in e_3). The planar boundary conditions satisfied by n_0 are given by*

$$n_{b;\mathbf{a}} = \cos \phi_{\mathbf{a}} e_1 + \sin \phi_{\mathbf{a}} e_2, \quad \text{where } \phi_{\mathbf{a}} = \arg w_{0;\mathbf{a}}. \tag{5.8}$$

The points \mathbf{a} are precisely the escape points where $n_0 = e_3$ (if n has stereographic projection $w_{0;\mathbf{a}}$) or $n_0 = -e_3$ (if n has stereographic projection $1/\overline{w_{0;\mathbf{a}}}$).

Thus, amongst degree- m planar boundary conditions, the leading-order Landau-de Gennes energy achieves its minimum, namely $2\pi|m|s_+^2$, for the $2|m|$ -dimensional family $n_{b;\mathbf{a}}$, and is independent of the positions \mathbf{a} of the escape points. The proof of Theorem 5.1 is given in Section 5.2.

Given $\mathbf{a} \in \Omega^{|m|}$, let $Q_{\mathbf{a}}^*$ denote a minimiser of the Landau-de Gennes energy subject to boundary conditions (1.12) with boundary director $n_{b;\mathbf{a}}$ given by (5.8).

From Proposition 2.1 and Theorem 5.1, we have that $Q_{\varepsilon; \mathbf{a}}^* \rightarrow Q[n_{0; \mathbf{a}}]$ as $\varepsilon \rightarrow 0$. From Theorems 2.1 and 5.1, we have that

$$\begin{aligned} \frac{1}{s_+^2} \mathcal{E}_\varepsilon[Q_{\varepsilon; \mathbf{a}}] &= 2\pi|m| + \varepsilon^2 W_{LdG}(\mathbf{a}) + o(\varepsilon^2), \quad \text{where } W_{LdG}(\mathbf{a}) \\ &= -\frac{3}{\nu} \|\nabla n_{0; \mathbf{a}}\|_{L^4}^4. \end{aligned} \quad (5.9)$$

The above energy expression provides a tool to distinguish between various conformal configurations using locations of escape points. Let us examine how the first-order energy, $W_{LdG}(\mathbf{a})$, depends on \mathbf{a} . Since the L^2 -norm of $\nabla n_{0; \mathbf{a}}$ is fixed (its square is equal to $2\pi|m|$), it follows that $W_{LdG}(\mathbf{a})$ decreases as $\nabla n_{0; \mathbf{a}}$ becomes more concentrated. Concentration occurs as the escape points move towards the boundary, since $n_{0; \mathbf{a}} = \pm e_3$ at escape points while $n_{0; \mathbf{a}} \cdot e_3 = 0$ at the boundary.

One can show that as the distance $\delta := \min_j \text{dist}(a_{(j)}, \partial\Omega)$ goes to zero, $W_{LdG}(\mathbf{a})$ diverges as δ^{-2} . This is compatible with Theorem 2.1, which concerns the behaviour of the energy as $\varepsilon \rightarrow 0$ for fixed boundary conditions. To analyse the energy for $\varepsilon, \delta \rightarrow 0$ simultaneously, one would need to go to higher order in the Γ -expansion and include a boundary-layer analysis.

In the case of the two-disk $\Omega = D^2$, g_a and h_a are given by

$$g_a(x) + ih_a(x) = \frac{1}{1 - ax}. \quad (5.10)$$

In this case, if $\mathbf{a} = 0$, that is, if the escape points coincide at the origin, then the conformal boundary condition n_b is *m-radial* [22, 26], and

$$n_b = \cos(m\varphi + \alpha) e_1 + \sin(m\varphi + \alpha) e_2, \quad (5.11)$$

where φ is the polar angle coordinate on \mathbb{R}^2 and α is a constant.

Remark 5.1. Let Q_ε^* denote a Landau-de Gennes minimiser with conformal leading-order Oseen-Frank director n_0 . It follows from (2.21)–(2.24) and Definition 5.1 that $Q_\varepsilon^* - Q[n_\varepsilon^*]$ is proportional to $Q[n_\varepsilon^*]$ to leading order; that is, the induced biaxiality in Q_ε^* does not appear at $O(\varepsilon^2)$ but at higher order.

Let us indicate a generalisation of Theorem 5.1. The space of director fields $n \in H^1(\Omega, \mathbb{S}^2)$ satisfying planar boundary conditions can be partitioned into homotopy classes (r, s) labeled by a pair of integers. For n differentiable, r and s correspond respectively to a signed count of the preimages of regular values of n in the northern and southern hemispheres of \mathbb{S}^2 , with the sign given by the sign of the determinant of the Jacobian at the preimage. The director field with stereographic projection $w_{0; \mathbf{a}}$ belongs to the class $(m, 0)$ for $m > 0$ and to $(0, -m)$ for $m < 0$. Its reflection in e_3 , which has stereographic projection $1/\bar{w}_{0; \mathbf{a}}$, belongs to the class $(-m, 0)$ for $m > 0$ and to $(0, m)$ for $m < 0$. For a general class (r, s) , the degree of the planar boundary conditions is given by $m = r - s$. It is straightforward to show (for C^1 -boundary conditions) that for n in the class (r, s) , the one-constant Oseen-Frank energy $\mathcal{E}_{OF}(n)$ is bounded below by $2\pi s_+^2(|r| + |s|)$ - this generalises the first assertion in Theorem 5.1.

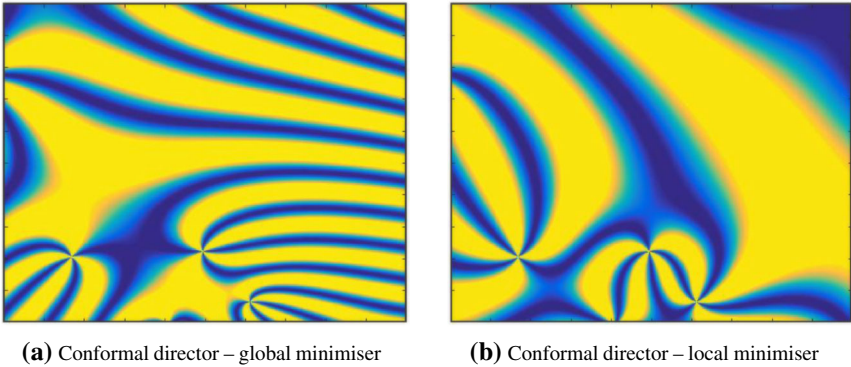


Fig. 1. Schlieren textures in conformal director fields. The colour scale corresponds to the quantity $[n_1 n_2 / (n_1^2 + n_2^2)]^2$, where $n_j := n \cdot e_j$; this quantity is proportional to the intensity of light passing through a nematic film with director $n(x, y)$ placed between polarisers with polarisation axes e_1 and e_2 . Random conformal director fields were constructed from (a) Eq. (5.6) and (b) Eq. (5.12) by setting $g = h = 0$, corresponding to an infinite planar domain, with escape points chosen at random in a large region of the plane, one portion of which is shown in the figures. In (a), the director is equal to $+e_3$ at all escape points, while in (b), the director is randomly taken to be $+e_3$ or $-e_3$ at escape points. Note that in (b), contours (lines of constant hue) can join pairs of escape points, but not in (a). This can be understood in terms of the analytic representations (5.6) and (5.12). Contour lines correspond to lines on which $\arg w$ is fixed, which are also lines of steepest descent of $|w|$. Escape points with $n = e_3$ or $n = -e_3$ correspond respectively to zeros or poles of w . A zero and a pole of w can be joined by a line of steepest descent, but two zeros of w cannot, nor can two poles

The second assertion may be generalised as follows: for r and s non-negative, conformal directors in the homotopy class (r, s) that saturate the lower bound are given by

$$w_{0,\mathbf{b},\mathbf{c}}(x) = e^{i\alpha} \prod_{j=1}^{|\mathbf{r}|} \frac{x - b_{(j)}}{\exp(g_{b_{(j)}} + ih_{b_{(j)}})} \prod_{k=1}^{|\mathbf{s}|} \frac{\exp(g_{c_{(k)}} + ih_{c_{(k)}})}{x - c_{(k)}}, \quad (5.12)$$

where \mathbf{b} and \mathbf{c} are respectively $|\mathbf{r}|$ - and $|\mathbf{s}|$ -tuples of points in Ω . The $b_{(j)}$'s are the points where $n_0 = e_3$, and the $c_{(k)}$'s are the points where $n_0 = -e_3$. For r (resp. s) negative, the first (resp. second) product in (5.12) is replaced by its complex conjugate. These are local minimizers of the Dirichlet energy with respect to their boundary conditions (they are global minimisers for $r = 0$ or $s = 0$). Director fields corresponding to (5.6) and (5.12) are shown in Figure 1.

5.2. Applications to conformal director fields: proofs

Proof of Proposition 5.1. Note that n conformal implies that $\partial_2 n = \sigma n \times \partial_1 n$ and $\partial_1 n = -\sigma n \times \partial_2 n$. Therefore, for $\phi \in \mathcal{D}(\Omega, \mathbb{R}^3)$, we have that

$$\int_{\Omega} \Delta n \cdot \phi = \sigma \int_{\Omega} (\partial_1 \phi \times n) \cdot \partial_2 n - (\partial_2 \phi \times n) \cdot \partial_1 n$$

$$= \sigma \int_{\Omega} (\partial_1(\phi \times n) - \phi \times \partial_1 n) \cdot \partial_2 n - (\partial_2(\phi \times n) - \phi \times \partial_2 n) \cdot \partial_1 n. \quad (5.13)$$

We note that $m := \phi \times n \in H_0^1(\Omega, \mathbb{R}^3)$, so that

$$\int_{\Omega} \partial_1 m \cdot \partial_2 n - \partial_2 m \cdot \partial_1 n = 0. \quad (5.14)$$

From (5.13) and (5.14),

$$\int_{\Omega} \Delta n \cdot \phi = 2\sigma \int_{\Omega} (\phi \times \partial_2 n) \cdot \partial_1 n = -2\sigma \int_{\Omega} (\partial_1 n \times \partial_2 n) \cdot \phi. \quad (5.15)$$

The fact that n is conformal implies that $\partial_1 n \times \partial_2 n = \frac{1}{2}\sigma|\nabla n|^2 n$, from which it follows that n is a weakly harmonic map, that is, $\Delta n = -|\nabla n|^2 n$. From the regularity result of Hélein [18], it follows that n is real analytic. \square

Proof of Proposition 5.2. First, suppose that $n \in H^1(\Omega, \mathbb{S}^2)$ is conformal. From Proposition 5.1, we have that n is a real analytic \mathbb{S}^2 -valued harmonic map. Let

$$Q = \sqrt{3/2} (n \otimes n - \frac{1}{3}I) \in C^\infty(\Omega, \mathbb{S}^4). \quad (5.16)$$

Using the harmonic map equation for n , we have that

$$\Delta Q = \sqrt{3/2} (\Delta n \otimes n + 2\nabla n \otimes \nabla n + n \otimes \Delta n) \quad (5.17)$$

$$= -\sqrt{6} (|\nabla n|^2 n \otimes n - \nabla n \otimes \nabla n). \quad (5.18)$$

Also, n conformal implies that $\partial_1 n \cdot \partial_2 n = 0$ and $|\partial_1 n| = |\partial_2 n|$. Therefore, if $\lambda := |\nabla n|/\sqrt{2} \neq 0$, then the three unit-vectors $\lambda^{-1}\partial_1 n$, $\lambda^{-1}\partial_2 n$ and n constitute an orthonormal frame. It follows that

$$\nabla n \otimes \nabla n = \frac{1}{2}|\nabla n|^2(I - n \otimes n). \quad (5.19)$$

Substituting (5.19) into (5.18), we get that

$$\Delta Q = -3\sqrt{3/2}|\nabla n|^2 (n \otimes n - \frac{1}{3}I) = -3|\nabla n|^2 Q = -|\nabla Q|^2 Q, \quad (5.20)$$

as $|\nabla Q|^2 = 3|\nabla n|^2$. Thus, Q is an \mathbb{S}^4 -valued harmonic map.

Next, let $Q \in H^1(\Omega, \mathbb{S}^4)$ be given by (5.16) with $n \in H^1(\Omega, \mathbb{S}^2)$, and suppose Q is an \mathbb{S}^4 -valued harmonic map. Then Q is real analytic [18], which implies that n is real analytic. From the harmonic map equation for Q , we get that

$$\Delta n \otimes n + 2\nabla n \otimes \nabla n + n \otimes \Delta n = -3|\nabla n|^2 (n \otimes n - \frac{1}{3}I). \quad (5.21)$$

Applying both sides of the preceding equation to n and using the identities $\partial_i n \cdot n = 0$, $i = 1, 2$ and $\Delta n \cdot n = -|\nabla n|^2$, which follow from $|n| = 1$, we get that n is a harmonic map, that is, $\Delta n = -|\nabla n|^2 n$. Substitution of this relation into (5.21) yields

$$2\nabla n \otimes \nabla n = |\nabla n|^2(I - n \otimes n). \quad (5.22)$$

Applying both sides of the preceding equation to $\partial_1 n$ and $\partial_2 n$ yields the pair of vector equations

$$\alpha \partial_1 n + \beta \partial_2 n = \beta \partial_1 n + \gamma \partial_2 n = 0, \tag{5.23}$$

where $\alpha = |\partial_1 n|^2 - \frac{1}{2}|\nabla n|^2$, $\beta = \partial_1 n \cdot \partial_2 n$, and $\gamma = |\partial_2 n|^2 - \frac{1}{2}|\nabla n|^2$. The solvability conditions are $\alpha = \beta = \gamma = 0$, which are equivalent to the condition (5.1) for n to be conformal. \square

Proof of Theorem 5.1. (i) Without loss of generality we may assume that $Q \in H^1(\Omega, \mathcal{S}_*)$, since otherwise $\mathcal{E}_0(Q) = +\infty$. Since Ω is simply connected, it follows that $Q = s_+(n \otimes n - \frac{1}{3}I)$ for some $n \in H^1(\Omega, \mathbb{S}^2)$. Since we are seeking to establish a lower bound for the energy, we can assume without loss of generality that Q is global minimiser of \mathcal{E}_0 . From Remark 2.1, it follows that n is a minimising \mathbb{S}^2 -valued harmonic map, and without loss of generality we may assume that $n \cdot e_3 > 0$. The classical regularity result of Hélein [18] on two-dimensional harmonic maps implies that n is smooth up to the boundary. The following bound is standard (see, for instance, [6]):

$$\begin{aligned} \mathcal{E}_0[Q] &= s_+^2 \int_{\Omega} |\partial_1 n|^2 + |\partial_2 n|^2 \geq 2s_+^2 \int_{\Omega} |\partial_1 n| |\partial_2 n| \\ &\geq 2s_+^2 \left| \int_{\Omega} n \cdot (\partial_1 n \times \partial_2 n) \right| = 2s_+^2 |\mathcal{A}[n(\Omega)]|, \end{aligned} \tag{5.24}$$

where $\mathcal{A}(n(\Omega))$ denotes the oriented area $n(\Omega) \subset \mathbb{S}^2$. For completeness, we provide an argument. Let us introduce spherical polar coordinates for n ,

$$n = \sin \theta \cos \varphi e_1 + \sin \theta \sin \varphi e_2 + \cos \theta e_3, \tag{5.25}$$

and similarly for the C^1 -boundary conditions, $n_b = n|_{\partial\Omega} = \cos \varphi_b e_1 + \sin \varphi_b e_2$. We may express the oriented area in terms of spherical polar coordinates as

$$\mathcal{A}[n(\Omega)] = \int_{\Omega} n \cdot (\partial_1 n \times \partial_2 n) = \int_{\Omega} \sin \theta (\partial_1 \theta \partial_2 \varphi - \partial_2 \theta \partial_1 \varphi). \tag{5.26}$$

Let

$$F = (1 - \cos \theta)(\partial_2 \varphi e_1 - \partial_1 \varphi e_2). \tag{5.27}$$

Since n is smooth, F is smooth; this is in spite of the fact that $\nabla \varphi$ may have singularities where $\theta = 0$ or $\theta = \pi$, since F vanishes if $\theta = 0$ while $\theta = \pi$ is excluded by $n \cdot e_3 > 0$. Noting that $\sin \theta (\partial_1 \theta \partial_2 \varphi - \partial_2 \theta \partial_1 \varphi) = \nabla \cdot F$, we apply the divergence theorem in (5.26) to obtain

$$\mathcal{A}[n(\Omega)] = \int_{\partial\Omega} F \cdot \nu = \int_{\partial\Omega} \varphi'_b = 2\pi m, \tag{5.28}$$

where ν denotes the unit normal on $\partial\Omega$, φ'_b denotes the tangential derivative of φ_b , and m is the degree of $\exp(i\varphi)$, regarded as an \mathbb{S}^1 -valued map on $\partial\Omega$. This establishes the lower bound (5.7).

The first inequality in (5.24) is saturated if and only if $|\partial_1 n| = |\partial_2 n|$, and the second inequality is saturated if and only if $\partial_1 n$ and $\partial_2 n$ are orthogonal. As n is orthogonal to both $\partial_1 n$ and $\partial_2 n$, these two conditions are equivalent to the condition

$$\partial_2 n = \sigma n \times \partial_1 n, \quad \sigma = \pm 1. \tag{5.29}$$

The last inequality in (5.24) is saturated if and only if σ is constant, that is, with regard to Definition 5.1 if and only if n is conformal.

(ii) We are given that $n \in C^\infty(\Omega, \mathbb{S}^2)$ is a conformal minimising \mathbb{S}^2 -valued harmonic map with degree- m planar C^1 -boundary conditions $n_b = \cos \varphi_b e_1 + \cos \varphi_b e_2$. We will obtain an explicit formula for n in terms of its escape points, that is, points where n is parallel to e_3 , and thereby determine the special form that n_b must assume. For definiteness, we take m positive and (cf. Remark 2.1) $n \cdot e_3 > 0$, which together imply that $\sigma = 1$ in (5.29). The adjustments required for the alternative cases are explained at the end.

For $a \in \Omega$, we denote by g_a the solution of the Laplace equation (5.5), and we let h_a denote a harmonic conjugate of g_a . Then $g_a + ih_a$ is holomorphic on Ω . Let w denote the stereographic projection of n , as in (5.2). It is straightforward to verify that the conformal condition (5.29) is equivalent to the Cauchy-Riemann equations

$$\operatorname{Re} \partial_1 w = \operatorname{Im} \partial_2 w, \quad \operatorname{Re} \partial_2 w = -\operatorname{Im} \partial_1 w. \tag{5.30}$$

Also, $n \cdot e_3 > 0$ implies that w is bounded. Therefore, w is complex holomorphic on Ω . We have that $\operatorname{Im} \int_{\partial\Omega} d \log w = \int_{\partial\Omega} \varphi'_b = 2\pi m$. It follows that w has precisely m zeros in Ω , counted with multiplicity. Let $\mathbf{a} = (a_{(1)}, \dots, a_{(m)}) \in \Omega^m$ denote these zeros, and let

$$f = w \prod_{j=1}^m \frac{\exp(g_{a_{(j)}} + ih_{a_{(j)}})}{x - a_{(j)}}. \tag{5.31}$$

Then f is holomorphic and nonvanishing on Ω . It follows that $\log f$ is holomorphic on Ω , so that $\operatorname{Re} \log f$ is harmonic, that is, $\Delta(\operatorname{Re} \log f) = 0$. Also, since $|w| = 1$ on $\partial\Omega$, it follows that $\operatorname{Re} \log f$ vanishes on $\partial\Omega$. But then $\operatorname{Re} \log f$ must vanish identically, which implies that $\operatorname{Im} \log f$ is constant, that is, $f = \exp(i\alpha)$ for some $\alpha \in \mathbb{R}$. Therefore,

$$w = e^{i\alpha} \prod_{j=1}^m \frac{x - a_{(j)}}{\exp(g_{a_{(j)}} + ih_{a_{(j)}})}, \tag{5.32}$$

which is equivalent to (5.6) for $m > 0$ and $n \cdot e_3 > 0$. The boundary condition (5.8) is obtained by setting $x \in \partial\Omega$ and stereographic projection.

The transformation $m \mapsto -m$ while leaving $n \cdot e_3$ unchanged is achieved by $w \mapsto \bar{w}$; we note that \bar{w} is antiholomorphic. The transformation $(n_1, n_2, n_3) \mapsto (n_1, n_2, -n_3)$ while leaving m unchanged is achieved by $w \mapsto 1/\bar{w}$; we note that $1/\bar{w}$ is antimeromorphic with poles but no zeros. Finally, simultaneously changing the signs of m and $n \cdot e_3$ is achieved by $w \mapsto 1/w$. \square

Remark 5.2. The lower bound (5.7) can be established for general H^1 maps (thus bypassing the regularity result of Helein [18]) by performing the arguments in the proof for smooth maps and using the density of smooth maps into H^1 maps for $2d$ domains (see Schoen and Uhlenbeck [32]).

5.3. The case $b^2 = 0$

For $b^2 = 0$, we have from Eq. (4.7) that the Landau-de Gennes minimiser is given to leading order by $\sqrt{2/3} s_+ \sum_{j=1}^3 (c_0 \cdot e_j) F_j$, where $c_0 \in H^1(\Omega, \mathbb{S}^2)$ is (weakly) harmonic. In analogy with the $b^2 \neq 0$ case, we can obtain explicit results for a special family of planar boundary conditions for which c_0 is conformal. In this case, the escape points, which parameterise the family, are points where Q_0 is oblate uniaxial (rather than prolate uniaxial) with director e_3 .

Theorem 5.2. *Let $\Omega \subset \mathbb{R}^2$ be a bounded, simply-connected domain with C^1 boundary, and let $Q_b \in C^1(\partial\Omega, \mathcal{B}_Q)$ be a degree- k uniaxial planar Q -tensor field on the boundary $\partial\Omega$.*

(i) *For $Q \in H^1(\Omega, \mathcal{S}_0)$ with $Q|_{\partial\Omega} = Q_b$, we have that*

$$\mathcal{E}_0[Q] \geq \frac{4}{9} s_+^2 \pi |k|, \tag{5.33}$$

with equality if and only if

$$Q = \sqrt{2/3} s_+ \sum_{j=1}^3 (c_0 \cdot e_j) F_j \tag{5.34}$$

and c_0 is conformal with $c_0 \cdot e_3 < 0$.

(ii) *The field c_0 is conformal with $c_0 \cdot e_3 < 0$ if and only its stereographic projection (5.2) is given by*

$$w_{0;a}(x) = \sqrt{3} \prod_{j=1}^{|k|} \frac{\exp(g_{a_{(j)}} + i h_{a_{(j)}})}{x - a_{(j)}}, \quad \mathbf{a} = (a_{(1)}, \dots, a_{(|k|)}) \in \Omega^{|k|}, \tag{5.35}$$

for $k > 0$, and by $\bar{w}_{0;a}$ for $k < 0$. The corresponding boundary conditions are given by $Q_{b;a} = s_+(n_{b;a} \otimes n_{b;a} - \frac{1}{3}I)$, where

$$n_{b;a} = \cos \phi_a e_1 + \sin \phi_a e_2, \quad \phi_a = \frac{1}{2} \operatorname{sgn} k \sum_{j=1}^{|k|} \arg(x - a_{(j)}) - h_{a_{(j)}}. \tag{5.36}$$

The proof is essentially the same as for Theorem 5.1, and hence is omitted. We note the two different ways in which an \mathbb{S}^2 -valued harmonic map is associated with a Q -tensor field, namely quadratically via (2.10) for uniaxial Q -tensors when $b^2 \neq 0$, and linearly via (4.7) when $b = 0$. The latter allows for the representation of non-orientable boundary conditions.

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