



OXFORD CENTRE FOR COLLABORATIVE APPLIED MATHEMATICS

Report Number 09/10

**Landau-De Gennes theory of nematic liquid
crystals: the Oseen-Frank limit and beyond**

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Landau-De Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond

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December 16, 2008

Abstract

We study global minimizers of a continuum Landau-De Gennes energy functional for nematic liquid crystals, in three-dimensional domains, subject to uniaxial boundary conditions. We analyze the physically relevant limit of small elastic constant and show that global minimizers converge strongly, in $W^{1,2}$, to a global minimizer predicted by the Oseen-Frank theory for uniaxial nematic liquid crystals with constant order parameter. Moreover, the convergence is uniform in the interior of the domain, away from the singularities of the limiting Oseen-Frank global minimizer. We obtain results on the rate of convergence of the eigenvalues and the regularity of the eigenvectors of the Landau-De Gennes global minimizer.

We also study the interplay between biaxiality and uniaxiality in Landau-De Gennes global energy minimizers and obtain estimates for various related quantities such as the biaxiality parameter and the size of admissible strongly biaxial regions.

1 Introduction

Nematic liquid crystals are an intermediate phase of matter between the commonly observed solid and liquid states of matter [13]. The constituent nematic molecules translate freely as in a conventional liquid but whilst flowing, tend to align along certain locally preferred directions i.e. exhibit a certain degree of long-range orientational order. Nematic liquid crystals break the rotational symmetry of isotropic liquids; the resulting anisotropic properties make liquid crystals suitable for a wide range of physical applications and the subject of very interesting mathematical modelling [18].

There are three main continuum theories for nematic liquid crystals [18]. The simplest mathematical theory for nematic liquid crystals is the *Oseen-Frank* theory [11]. The Oseen-Frank theory is restricted to uniaxial nematic liquid crystal materials (liquid crystal materials with a single preferred direction of molecular alignment) with constant degree of orientational order. The state of a uniaxial nematic liquid crystal is described by a unit-vector field, $n(x) \in S^2$, which represents the preferred direction of molecular alignment. In the simplest setting, the liquid crystal energy reduces to:

$$\mathcal{F}_{OF}[n] = \int_{\Omega} n_{i,k}(x)n_{i,k}(x) dx, \quad (1)$$

the standard Dirichlet energy for vector-valued maps into the unit sphere. The equilibrium configurations (the physically observable configurations) correspond to minimizers of the \mathcal{F}_{OF} -energy, subject to the imposed boundary conditions. In particular, the minimizers of \mathcal{F}_{OF} are examples of S^2 -valued harmonic maps [18, 32]. The Oseen-Frank theory has been extensively studied in the literature, see the review [5], and there are rigorous results on the existence, regularity and singularities of Oseen-Frank minimizers.

The Oseen-Frank theory is limited in the sense that it can only account for point defects in liquid crystal systems but not the more complicated line and surface defects that are observed experimentally. A second,

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more comprehensive theory is the continuum *Ericksen theory* [8]. The Ericksen theory is also restricted to uniaxial liquid crystal materials but can account for spatially varying orientational order i.e. the state of the liquid crystal is described by a pair, $(s, n) \in \mathbb{R} \times S^2$, where $s \in \mathbb{R}$ is a real scalar order parameter that measures the degree of orientational ordering and n represents the direction of preferred molecular alignment. In the simplest setting, the corresponding energy functional is given by

$$\mathcal{F}_E[s, n] = \int_{\Omega} s(x)^2 |\nabla n(x)|^2 + k |\nabla s(x)|^2 + W_0(s) dx \quad (2)$$

where k is a material-dependent elastic constant and $W_0(s)$ is a bulk potential. The Ericksen theory is based on the premise that s vanishes wherever n has a singularity and this theory can account for all physically observable defects.

However Ericksen recognizes that his theory is but a simplified description of a possibly more complex situation (see [8]):

“There is the third possibility, that the three eigenvalues of Q are all distinct, giving what are called biaxial nematic configurations. Theories fitting MACMILLAN’S [11] format permit any of the three types of configurations to occur. Certainly it is not unreasonable to think that flows or other influences could convert a rather stable nematic configuration to one of the biaxial type, etc. I [19] am one of those who have argued that, near isotropic-nematic phase transitions, it should be quite easy to induce such changes. Accounting for such possibilities does add significant complications to the equations and the problems of analyzing them. Experimental information concerning the biaxial configurations is still quite slim and, for me, it is too early to think seriously about them. So, I will develop a theory representing a kind of compromise.”

The most general continuum theory for nematic liquid crystals is the *Landau-De Gennes* theory [13, 25] which can account for uniaxial and biaxial phases (biaxiality implies the existence of more than one preferred direction of molecular alignment). Indeed, this theory was one of the major reasons for awarding P.G. De Gennes a Nobel prize for physics in 1991. In the Landau-De Gennes framework, the state of a nematic liquid crystal is modelled by a symmetric, traceless 3×3 matrix $Q \in M^{3 \times 3}$, known as the *Q -tensor order parameter*. A nematic liquid crystal is said to be (a) *isotropic* when $Q = 0$, (b) *uniaxial* when the Q -tensor has two equal non-zero eigenvalues; a uniaxial Q -tensor can be written in the special form

$$Q = s \left(n \otimes n - \frac{1}{3} Id \right); \quad s \in \mathbb{R} \setminus \{0\}, \quad n \in S^2 \quad (3)$$

and (c) *biaxial* when Q has three distinct eigenvalues; a biaxial Q -tensor can always be represented as follows (see Proposition 1)

$$Q = s \left(n \otimes n - \frac{1}{3} Id \right) + r \left(m \otimes m - \frac{1}{3} Id \right) \quad s, r \in \mathbb{R}; \quad n, m \in S^2. \quad (4)$$

The Landau-De Gennes energy functional, $\mathcal{F}_{LG}[Q]$, is a nonlinear integral functional of Q and its spatial derivatives. We work with the simplest form of $\mathcal{F}_{LG}[Q]$, with Dirichlet boundary conditions, Q_b (refer to (11)), on three-dimensional domains $\Omega \subset \mathbb{R}^3$. We take $\mathcal{F}_{LG}[Q]$ to be [27]

$$\mathcal{F}_{LG}[Q] = \int_{\Omega} \frac{L}{2} |\nabla Q|^2(x) + f_B(Q(x)) dx \quad (5)$$

where $f_B(Q)$ is the bulk energy density that accounts for bulk effects, $|\nabla Q|^2 = \sum_{i,j,k=1}^3 Q_{ij,k} Q_{ij,k}$ is the elastic energy density that penalizes spatial inhomogeneities and $L > 0$ is a material-dependent elastic constant. We take $f_B(Q)$ to be a quartic polynomial in the Q -tensor components, since this is the simplest form of $f_B(Q)$ that allows for multiple local minima and a first-order nematic-isotropic phase transition [13, 32]. This form of $f_B(Q)$ has been widely-used in the literature and is defined as follows

$$f_B(Q) = \frac{\alpha(T - T^*)}{2} \text{tr}(Q^2) - \frac{b}{3} \text{tr}(Q^3) + \frac{c}{4} (\text{tr}Q^2)^2$$

where $\alpha, b, c \in \mathbb{R}$ are material-dependent positive constants, T is the absolute temperature and T^* is a characteristic liquid crystal temperature. We work in the low-temperature regime $T < T^*$ for which $\alpha(T - T^*) < 0$. Keeping this in mind, we recast the bulk energy density as follows:

$$f_B(Q) = -\frac{a^2}{2} \text{tr}(Q^2) - \frac{b^2}{3} \text{tr}(Q^3) + \frac{c^2}{4} (\text{tr}Q^2)^2, \quad (6)$$

where $a^2, b^2, c^2 \in \mathbb{R}^+$ are material-dependent and temperature-dependent positive constants. The equilibrium configurations (the physically observable configurations) then correspond to minimizers of $\mathcal{F}_{LG}[Q]$, subject to the imposed boundary conditions.

In the first part of the paper, we study the the limit of vanishing elastic constant $L \rightarrow 0$ for global minimizers, $Q^{(L)}$, of $\mathcal{F}_{LG}[Q]$. This study is in the spirit of the asymptotics for minimizers of Ginzburg-Landau functionals for superconductors [3]. The limit $L \rightarrow 0$ is a physically relevant limit since the elastic constant L is typically very small, of the order of 10^{-11} Joule/metre. [27].

We define a *limiting harmonic map* $Q^{(0)}$ as follows

$$Q^{(0)} = s_+ \left(n^{(0)} \otimes n^{(0)} - \frac{1}{3} Id \right)$$

where s_+ is defined in (10), $n^{(0)}$ is a minimizer of the Oseen-Frank energy, $\mathcal{F}_{OF}[n]$ in (1), subject to the fixed boundary condition $n = n_b \in C^\infty(\partial\Omega, \mathbb{S}^2)$ and Q_b and n_b are related as in (11). Our main results are:

- There exists a sequence of global minimizers $\{Q^{(L_k)}\}$ such that $Q^{(L_k)} \xrightarrow{L_k \rightarrow 0^+} Q^{(0)}$ strongly in the Sobolev space $W^{1,2}(\Omega, \mathbb{R}^9)$.
- The sequence $\{Q^{(L_k)}\}$ as above converges uniformly to $Q^{(0)}$ as $L_k \rightarrow 0$, in the interior of Ω , away from the (possible) singularities of $Q^{(0)}$.
- The bulk energy density, $f_B(Q^{(L_k)})$, converges uniformly to its minimum value away from the (possible) singularities of $Q^{(0)}$; the uniform convergence of the bulk energy density holds in the interior and up to the boundary, away from the (possible) singularities of $Q^{(0)}$.

These results show that the predictions of the Oseen-Frank theory (described by the limiting map $Q^{(0)}$) and the Landau-De Gennes theory agree away from the singularities of $Q^{(0)}$. The global minimizers, $Q^{(L)}$, are real analytic (see Proposition 13) and have no singularities as such. However, one of the most intriguing features of nematic liquid crystals are the optical ‘defects’ that appear in the Schlieren textures [13]. From a physical point of view, these defects are regions of rapid changes in the configurational properties of a nematic liquid crystal [13]. We conjecture that certain types of optical defects in $Q^{(L_k)}$ (for small L_k), when they exist, may be localized near the analytic singularities of the limiting map $Q^{(0)}$, since $Q^{(L_k)}$ can have strong variations only near the singularities of $Q^{(0)}$ (more precisely, the gradient, $\nabla Q^{(L_k)}$, cannot be bounded independently of L_k on any set containing a singularity of $Q^{(0)}$). There is existing literature on the location of singularities in harmonic maps [1] and this may allow one to predict the location of (optical) defects in a global Landau-De Gennes minimizer.

Our convergence results analyze the limit of vanishing elastic constant $L \rightarrow 0$. Physical situations are modelled by small *but non-zero* values of the elastic constant L . Thus our convergence results show that for L sufficiently small, the limiting harmonic map $Q^{(0)}$ provides but a ‘rough’ description of $Q^{(L)}$ i.e. $Q^{(L)}$ can be thought of as having a ‘leading’ uniaxial part plus a small biaxial perturbation, away from the singularities of $Q^{(0)}$. This small biaxial perturbation is of order $O(\sqrt{L})$ where $L \ll 1$ (see Section 5 for details). However, numerical simulations show that biaxiality may become prominent in the vicinity of defects [23, 28]. In the second part of our paper, we study biaxiality and their role in global minimizers $Q^{(L)}$, noting that biaxiality (if it exists) is one of the main differences between $Q^{(L)}$ and the limiting approximation $Q^{(0)}$. More precisely, in Propositions 11 and 12, we obtain estimates for the size of the regions where $Q^{(L_k)}$ can deviate significantly from $Q^{(0)}$ and on the size of admissible strongly biaxial regions in $Q^{(L)}$, in terms of the biaxiality parameter β (defined in (22)) and the material-dependent constants. While Proposition 11 may be relevant to the properties of $Q^{(L)}$ near the singular set of $Q^{(0)}$, Proposition 12 is relevant to the equilibrium properties away from the singular set of $Q^{(0)}$.

Using a simple nearest-neighbour projection argument (see Corollary 1), we show that the ‘leading eigendirection’, corresponding to the leading uniaxial part (see Section 5 for definitions) is smooth on any compact set K not containing any singularity of $Q^{(0)}$. Further, in Proposition 15, we also show that $Q^{(L)}$ is either (a) uniaxial everywhere (except for possibly a set of measure zero where Q can be isotropic) or (b) $Q^{(L)}$ is biaxial everywhere and can be uniaxial or isotropic only on sets of measure zero. It is known that as long as the number of distinct eigenvalues does not change, the eigenvectors of $Q^{(L)}$ enjoy the same degree of regularity as $Q^{(L)}$ itself [26]. In Corollary 2, we show that the eigenvectors are necessarily smooth everywhere except for possibly a zero-measure set where the number of distinct eigenvalues changes and therefore, if the eigenvectors of $Q^{(L)}$ suffer any discontinuities, these discontinuities must be localized on the uniaxial-biaxial, uniaxial-isotropic or biaxial-isotropic interfaces. This result may be relevant to the interpretation of optical data from experiments and we hope to explore this connection in future work.

Finally, we note that the Landau-De Gennes theory for uniaxial liquid crystal materials has strong analogies with the 3D version of the Ginzburg-Landau theory for superconductors [3]. The Ginzburg-Landau energy functional for a three-dimensional vector field, $u : \Omega \rightarrow \mathbb{R}^3$, is typically of the form

$$\mathcal{F}_{GL}[u] = \int_{\Omega} \frac{1}{2} |\nabla u|^2 + \frac{1}{4\epsilon^2} (1 - |u|^2)^2 dx \quad (7)$$

where $\epsilon > 0$ is a very small parameter. The functional \mathcal{F}_{GL} has been rigorously studied in the limit $\epsilon \rightarrow 0$ which is analogous to the limit $L \rightarrow 0$ in our problem. The new mathematical complexities in the Landau-De Gennes theory for nematic liquid crystals come from the high dimensionality of the target space and also from the possibility of biaxiality in global energy minimizers. Future challenges include a better understanding of the qualitative properties of global minimizers for small but non-vanishing values of L , a better description of $Q^{(L)}$ near the singularities of the limiting harmonic map $Q^{(0)}$, the regularity of the eigenvectors and eigenvalues, along with a deeper understanding of the appearance and role of biaxiality in global minimizers.

The paper is organized as follows - in Section 2, we introduce the conventions and notations that are used in the rest of the paper. In Section 3, we state two representation formulae for Q -tensors that are useful for subsequent computations in later sections. In Section 4, we study the properties of global energy minimizers in the limit $L \rightarrow 0$ and prove the convergence results. In Section 5, we discuss the consequences of our convergence results and their relevance to the bulk energy density, the biaxiality parameter, the eigenvalues and the eigenvectors of a global Landau-De Gennes minimizer. In Section 6, we derive estimates for the bulk energy density, obtain bounds for the size of admissible strongly biaxial regions and discuss the interplay between biaxiality and uniaxiality in a global energy minimizer.

2 Preliminaries

We take our domain, $\Omega \subset \mathbb{R}^3$, to be bounded and simply-connected with smooth boundary, $\partial\Omega$. Let $S_0 \subset \mathbb{M}^{3 \times 3}$ denote the space of Q -tensors, i.e.

$$S_0 \stackrel{def}{=} \{Q \in \mathbb{M}^{3 \times 3}; Q_{ij} = Q_{ji}, Q_{ii} = 0\}$$

where we have used the Einstein summation convention; the Einstein convention will be assumed in the rest of the paper. The corresponding matrix norm is defined to be

$$|Q| \stackrel{def}{=} \sqrt{\text{tr}Q^2} = \sqrt{Q_{ij}Q_{ij}}.$$

As stated in the introduction, we take the bulk energy density term to be

$$f_B(Q) = -\frac{a^2}{2} \text{tr}(Q^2) - \frac{b^2}{3} \text{tr}(Q^3) + \frac{c^2}{4} (\text{tr}(Q^2))^2$$

where $a^2, b^2, c^2 \in \mathbb{R}$ are material-dependent and temperature-dependent positive constants. One can readily verify that $f_B(Q)$ is bounded from below (see Proposition 8, [21]), and we define a non-negative bulk energy

density, $\tilde{f}_B(Q)$, that differs from $f_B(Q)$ by an additive constant as follows:

$$\tilde{f}_B(Q) = f_B(Q) - \min_{Q \in S_0} f_B(Q). \quad (8)$$

It is clear that $\tilde{f}_B(Q) \geq 0$ for all $Q \in S_0$ and the set of minimizers of $\tilde{f}_B(Q)$ coincides with the set of minimizers for $f_B(Q)$. In Proposition 8, we show that the function $\tilde{f}_B(Q)$ attains its minimum on the set of uniaxial Q -tensors with constant order parameter s_+ as shown below

$$\begin{aligned} \tilde{f}_B(Q) = 0 &\Leftrightarrow Q \in Q_{\min} \text{ where} \\ Q_{\min} &= \left\{ Q \in S_0, Q = s_+ \left(n \otimes n - \frac{1}{3} Id \right), n \in \mathbb{S}^2 \right\} \end{aligned} \quad (9)$$

with

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \quad (10)$$

We work with Dirichlet boundary conditions, referred to as *strong anchoring* in the liquid crystal literature [13]. The boundary condition $Q_b \in Q_{\min}$ is smooth and is given by

$$Q_b = s_+ \left(n_b \otimes n_b - \frac{1}{3} Id \right), \quad n_b \in C^\infty(\partial\Omega; \mathbb{S}^2). \quad (11)$$

We define our admissible space to be

$$\mathcal{A}_Q = \{ Q \in W^{1,2}(\Omega; S_0); Q = Q_b \text{ on } \partial\Omega, \text{ with } Q_b \text{ as in (11)} \}, \quad (12)$$

where $W^{1,2}(\Omega; S_0)$ is the Sobolev space of square-integrable Q -tensors with square-integrable first derivatives [9]. The corresponding $W^{1,2}$ -norm is given by $\|Q\|_{W^{1,2}(\Omega)} = \left(\int_\Omega |Q|^2 + |\nabla Q|^2 dx \right)^{1/2}$. In addition to the $W^{1,2}$ -norm, we also use the L^∞ -norm in this paper, defined to be $\|Q\|_{L^\infty(\Omega)} = \text{ess sup}_{x \in \Omega} |Q(x)|$.

We study global minimizers of a modified Landau-De Gennes energy functional, $\tilde{F}_{LG}[Q]$, in the admissible space \mathcal{A}_Q . The functional $\tilde{F}_{LG}[Q]$ differs from $\mathcal{F}_{LG}[Q]$ in (5) by an additive constant and is defined to be

$$\tilde{F}_{LG}[Q] = \int_\Omega \frac{L}{2} Q_{ij,k}(x) Q_{ij,k}(x) + \tilde{f}_B(Q(x)) dx. \quad (13)$$

For a fixed $L > 0$, let $Q^{(L)}$ denote a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible class, \mathcal{A}_Q . The existence of $Q^{(L)}$ is immediate from the direct methods in the calculus of variations [9]. The bulk energy density, $\tilde{f}_B(Q)$, is bounded from below, the energy density is convex in ∇Q and therefore, $\tilde{F}_{LG}[Q]$ is weakly sequentially lower semi-continuous. Moreover, it is clear that $\tilde{F}_{LG}[Q]$ and $\mathcal{F}_{LG}[Q]$ have the same set of global minimizers for a fixed set of material-dependent and temperature-dependent constants $\{a^2, b^2, c^2, L\}$.

The global minimizer $Q^{(L)}$ is a weak solution of the corresponding Euler-Lagrange equations [21]

$$L\Delta Q_{ij} = -a^2 Q_{ij} - b^2 \left(Q_{ik} Q_{kj} - \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right) + c^2 Q_{ij} \text{tr}(Q^2) \quad i, j = 1, 2, 3. \quad (14)$$

where the term $b^2 \frac{\delta_{ij}}{3} \text{tr}(Q^2)$ is a Lagrange multiplier that enforces the tracelessness constraint. It follows from standard arguments in elliptic regularity that $Q^{(L)}$ is actually a classical solution of (14) and $Q^{(L)}$ is smooth and real analytic (see also Section 6.2).

Finally, we introduce a “*limiting uniaxial harmonic map*” $Q^{(0)} : \Omega \rightarrow Q_{\min}$; $Q^{(0)}$ is defined to be a global minimizer (not necessarily unique) of $\tilde{F}_{LG}[Q]$ in the restricted class, $\mathcal{A}_Q \cap \{Q : \Omega \rightarrow S_0, Q(x) \in Q_{\min} \text{ a.e. } x \in \Omega\}$. Then $Q^{(0)}$ is necessarily of the form

$$Q^{(0)} = s_+ \left(n^{(0)} \otimes n^{(0)} - \frac{1}{3} Id \right), \quad (15)$$

where $n^{(0)}$ is a global minimizer of $\mathcal{F}_{OF}[n]$ (see [2], [4]),

$$\int_{\Omega} |\nabla n^0(x)|^2 dx = \min_{n \in \mathcal{A}_n} \int_{\Omega} |\nabla n(x)|^2 dx \quad (16)$$

in the admissible class $\mathcal{A}_n = \{n \in W^{1,2}(\Omega; S^2); n = n_b \text{ on } \partial\Omega\}$ and n_b and Q_b are related as in (11). This “limiting harmonic” map $Q^{(0)}$ is therefore obtained from an energy minimizer, n^0 , (not necessarily unique) within the Oseen-Frank theory for uniaxial nematic liquid crystals with constant order parameter (for more results about the relation between $n^{(0)}$ and $Q^{(0)}$ see [2]). It follows from standard results in harmonic maps [32] that $Q^{(0)}$ has at most a finite number of isolated point singularities (points where $n^{(0)}$ has singularities). In the following sections we will elaborate on the relation between $Q^{(L)}$ and $Q^{(0)}$.

3 Representation formulae for Q -tensors

We have:

Proposition 1 *A matrix $Q \in S_0$ can be represented in the form*

$$Q = s(n \otimes n - \frac{1}{3}Id) + r(m \otimes m - \frac{1}{3}Id) \quad (17)$$

with n and m unit-length eigenvectors of Q , $n \cdot m = 0$ and

$$0 \leq r \leq \frac{s}{2} \quad \text{or} \quad \frac{s}{2} \leq r \leq 0 \quad (18)$$

The scalar order parameters r and s are piecewise linear combinations of the eigenvalues of Q .

Proof. From the spectral decomposition theorem we have

$$Q = \lambda_1 n_1 \otimes n_1 + \lambda_2 n_2 \otimes n_2 + \lambda_3 n_3 \otimes n_3 \quad (19)$$

where $\lambda_1, \lambda_2, \lambda_3$ are eigenvalues of Q and n_1, n_2, n_3 are the corresponding unit eigenvectors, pairwise perpendicular. We have $I = \sum_{i=1}^3 n_i \otimes n_i$ and the tracelessness condition implies that $\lambda_1 + \lambda_2 + \lambda_3 = 0$. Thus

$$Q = \lambda_1 n_1 \otimes n_1 + \lambda_2 n_2 \otimes n_2 - (\lambda_1 + \lambda_2)(I - n_1 \otimes n_1 - n_2 \otimes n_2)$$

We consider six regions $R_i^+, i = 1, \dots, 6$ in the (λ_1, λ_2) - plane which cover exactly half of the whole plane. This corresponds to the representation (17) with $0 \leq r \leq \frac{s}{2}$. The other half of the plane is covered by the regions $R_i^-, i = 1, \dots, 6$, (which are obtained by reflecting R_i^+ through the origin $(0, 0)$) and the regions R_i^- correspond to the representation (17), with $r, s \leq 0$.

We let $R_1^+ = \{(\lambda_1, \lambda_2) \in \mathbb{R}^2, -2\lambda_1 \leq \lambda_2, \lambda_1 \leq 0\}$. In this case $r \stackrel{def}{=} 2\lambda_1 + \lambda_2$ and $s \stackrel{def}{=} 2\lambda_2 + \lambda_1$ with $n \stackrel{def}{=} n_2, m \stackrel{def}{=} n_1$. One can directly verify that for r, s thus defined, we have

$$r = 2\lambda_1 + \lambda_2 \leq \frac{s}{2} = \lambda_2 + \frac{\lambda_1}{2}.$$

Interchanging λ_1 with λ_2 in the definition of r and s and m with n , we obtain the region $R_2^+ = \{(\lambda_1, \lambda_2); \lambda_2 \geq -\lambda_1/2; \lambda_2 \leq 0\}$.

Let $R_3^+ = \{(\lambda_1, \lambda_2) \in \mathbb{R}^2, \lambda_2 \leq 0, \lambda_2 \geq \lambda_1\}$. Taking $r \stackrel{def}{=} \lambda_2 - \lambda_1, s \stackrel{def}{=} -2\lambda_1 - \lambda_2, n \stackrel{def}{=} n_3, m \stackrel{def}{=} n_2$, one can check that

$$r = \lambda_2 - \lambda_1 \leq \frac{s}{2} = -\lambda_1 - \frac{\lambda_2}{2}.$$

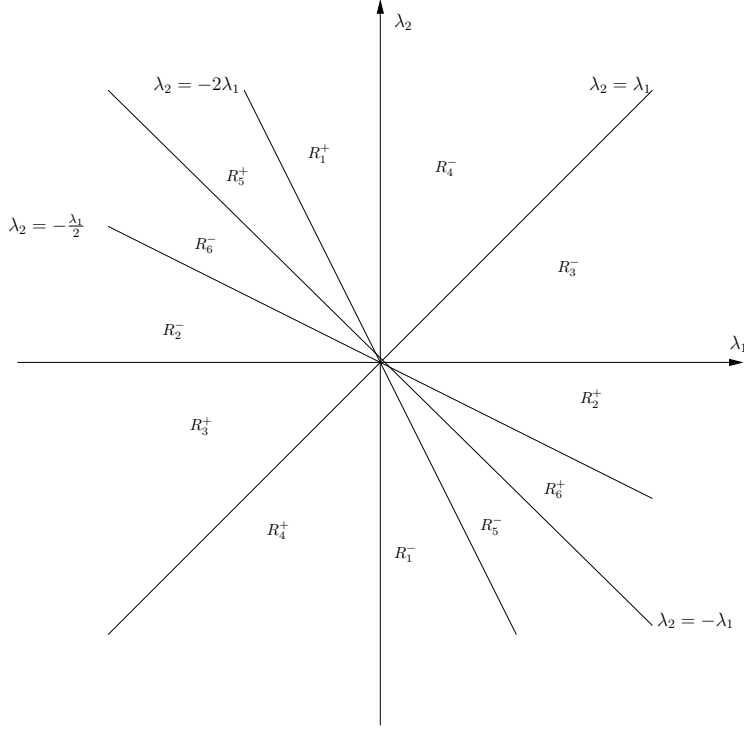


Figure 1: The λ_2, λ_1 plane and its regions

The region R_4^+ is obtained from interchanging λ_1 and λ_2 .

We have $R_5^+ = \{(\lambda_1, \lambda_2) \in \mathbb{R}^2, \lambda_1 \leq 0, -2\lambda_1 \geq \lambda_2 \geq -\lambda_1\}$ with $r \stackrel{def}{=} -2\lambda_1 - \lambda_2, s \stackrel{def}{=} \lambda_2 - \lambda_1, n = n_2$ and $m \stackrel{def}{=} n_3$. Again, it is straightforward to check that

$$r = -2\lambda_1 - \lambda_2 \leq \frac{\lambda_2}{2} - \frac{\lambda_1}{2}.$$

Interchanging λ_1 with λ_2 , we obtain the region R_6^+ .

Finally the remaining half of the (λ_1, λ_2) -plane is covered by the regions R_i^- (obtained from R_i^+ by changing the signs of the inequalities and keeping the definitions of r and s unchanged). For example, R_1^- is defined to be

$$R_1^- = \{(\lambda_1, \lambda_2) \in \mathbb{R}^2; \lambda_1 \geq 0, 2\lambda_1 \leq -\lambda_2\}$$

with $r = 2\lambda_1 + \lambda_2$ and $s = 2\lambda_2 + \lambda_1$. One can then directly check that

$$\frac{s}{2} \leq r \leq 0.$$

The remaining five regions R_i^- for $i = 2 \dots 6$ can be defined analogously. \square

Remark 1 *The representation formula (17) is known in the literature [25]. In Proposition 1, we state that it suffices to consider the two cases given by (18); we have not found references for this fact.*

In Proposition 2, we state a second representation formula for admissible $Q \in S_0$ and its relation to the representation formula (17). The representation formula (20) is known in the literature [22] and will be used in Section 5. For reader's convenience we provide a quick proof.

Proposition 2 (A second representation formula) A matrix $Q \in S_0$ can be represented as:

$$Q = S \left(n \otimes n - \frac{1}{3} Id \right) + R (m \otimes m - p \otimes p) \quad (20)$$

The vectors n, m and p are unit-length and pairwise perpendicular eigenvectors of Q with corresponding eigenvalues $\lambda_1, \lambda_2, \lambda_3$. The scalar order parameters S and R are given by

$$S = 3 \frac{\lambda_1}{2} \quad R = \frac{1}{2} (2\lambda_2 + \lambda_1). \quad (21)$$

Proof. We have the spectral decomposition of Q , namely

$$Q = \lambda_1 n \otimes n + \lambda_2 m \otimes m + \lambda_3 p \otimes p$$

with n, m, p pairwise perpendicular unit-length eigenvectors of Q and

$$Id = n \otimes n + m \otimes m + p \otimes p.$$

Combining the last two relations and taking $S = 3 \frac{\lambda_1}{2}, R = \frac{1}{2} (2\lambda_2 + \lambda_1)$ we obtain the claim. \square

4 The limiting harmonic map

4.1 The uniform convergence in the interior

Firstly, we recall that for a $Q \in S_0$ the biaxiality parameter $\beta(Q)$ (see for instance [23]) is defined to be

$$\beta(Q) = 1 - 6 \frac{(\text{tr} Q^3)^2}{(\text{tr} Q^2)^3} \quad (22)$$

The significance of $\beta(Q)$ as a measure of biaxiality is due to the following

Lemma 1 (i) The biaxiality parameter $\beta(Q) \in [0, 1]$ and $\beta(Q) = 0$ if and only if Q is purely uniaxial i.e. if Q is of the form, $Q = s (n \otimes n - \frac{1}{3} Id)$ for some $s \in \mathbb{R}, n \in \mathbb{S}^2$. (ii) The biaxiality parameter, $\beta(Q)$, can be bounded in terms of the ratio $\frac{r}{s}$, where (s, r) are the scalar order parameters in Proposition 1. These bounds are given by

$$\frac{1}{2} \left(1 - \sqrt{1 - \sqrt{\beta}} \right) \leq \frac{r}{s} \leq \frac{1}{2} \left(1 + \sqrt{1 - \sqrt{\beta}} \right). \quad (23)$$

Equivalently,

$$\frac{1 - \sqrt{1 - \sqrt{\beta}}}{3 + \sqrt{1 - \sqrt{\beta}}} \leq \frac{R}{S} \leq \frac{1 + \sqrt{1 - \sqrt{\beta}}}{3 - \sqrt{1 - \sqrt{\beta}}} \quad (24)$$

where (S, R) are the order parameters in Proposition 2. Further $\beta(Q) = 1$ if and only if $r = \frac{s}{2}$ or if and only if $\frac{R}{S} = \frac{1}{3}$. (iii) For an arbitrary $Q \in S_0$, we have that

$$-\frac{|Q|^3}{\sqrt{6}} \left(1 - \frac{\beta}{2} \right) \leq \text{tr} Q^3 \leq \frac{|Q|^3}{\sqrt{6}} \left(1 - \frac{\beta}{2} \right). \quad (25)$$

Proof: The proof of Lemma 1 is deferred to the Appendix. \square

The next proposition gives us apriori L^∞ bounds, independent of L .

Proposition 3 *Let $\Omega \subset \mathbb{R}^3$ be a bounded and simply-connected open set with smooth boundary. Let $Q^{(L)}$ be a global minimizer of the Landau-De Gennes energy functional (13), in the space (12).*

Then

$$\|Q^{(L)}\|_{L^\infty(\Omega)} \leq \sqrt{\frac{2}{3}}s_+ \quad (26)$$

where s_+ is defined in (10).

Proof. Proposition 3 has been proven in [21]; we reproduce the proof here for completeness.

The proof proceeds by contradiction. In the following we drop the superscript L for convenience. We assume that there exists a point $x^* \in \bar{\Omega}$ where $|Q|$ attains its maximum and $|Q(x^*)| > \sqrt{\frac{2}{3}}s_+$. On $\partial\Omega$, $|Q| = \sqrt{\frac{2}{3}}s_+$ by our choice of the boundary condition Q_b (note that if $Q \in Q_{min}$ then $|Q| = \sqrt{\frac{2}{3}}s_+$). If Q is a global minimizer of $\tilde{F}[Q]$ then Q is a classical solution (see Section 6.2 for regularity) of the Euler-Lagrange equations

$$L\Delta Q_{ij} = -a^2Q_{ij} - b^2\left(Q_{ip}Q_{pj} - \frac{1}{3}\text{tr}Q^2\delta_{ij}\right) + c^2(\text{tr}Q^2)Q_{ij}. \quad (27)$$

Since the function $|Q|^2 : \bar{\Omega} \rightarrow \mathbb{R}$ must attain its maximum at $x^* \in \Omega$, we necessarily have that

$$\Delta\left(\frac{1}{2}|Q|^2\right)(x^*) \leq 0 \quad (28)$$

We multiply both sides of (27) by Q_{ij} and obtain

$$L\Delta\left(\frac{1}{2}|Q|^2\right) = -a^2\text{tr}Q^2 - b^2\text{tr}Q^3 + c^2(\text{tr}Q^2)^2 + L|\nabla Q|^2. \quad (29)$$

We note that

$$-a^2\text{tr}(Q^2) - b^2\text{tr}(Q^3) + c^2(\text{tr}(Q^2))^2 \geq f(|Q|) \quad (30)$$

where

$$f(|Q|) = -a^2|Q|^2 - \frac{b^2}{\sqrt{6}}|Q|^3 + c^2|Q|^4, \quad (31)$$

since $\text{tr}(Q^3) \leq \frac{|Q|^3}{\sqrt{6}}$ from (25). One can readily verify that

$$f(|Q|) > 0 \quad \text{for } |Q| > \sqrt{\frac{2}{3}}s_+ \quad (32)$$

which together with (29) and (30) imply that

$$\Delta\left(\frac{1}{2}|Q|^2\right)(x) > 0 \quad (33)$$

for all interior points $x \in \Omega$, where $|Q(x)| > \sqrt{\frac{2}{3}}s_+$. This contradicts (28) and thus gives the conclusion. \square

In what follows, let $e_L(Q(x))$ denote the energy density $e_L(Q(x)) \stackrel{\text{def}}{=} \frac{1}{2}|\nabla Q|^2 + \frac{\tilde{f}_B(Q(x))}{L}$. We consider the normalized energy on balls $B(x, r) \subset \Omega = \{y \in \Omega; |x - y| \leq r\}$

$$\mathcal{F}(Q, x, r) \stackrel{\text{def}}{=} \frac{1}{r} \int_{B(x, r)} e_L(Q(x)) dx = \frac{1}{r} \int_{B(x, r)} \frac{\tilde{f}_B(Q)}{L} + \frac{1}{2}|\nabla Q|^2 dx. \quad (34)$$

We have:

Lemma 2 (*Monotonicity lemma*) Let $Q^{(L)}$ be a global minimizer of $\tilde{F}_{LG}[Q]$ in (13). Then

$$\mathcal{F}(Q^{(L)}, x, r) \leq \mathcal{F}(Q^{(L)}, x, R), \forall x \in \Omega, r \leq R, \text{ so that } B(x, R) \subset \Omega \quad (35)$$

Proof. The proof follows a standard pattern (see for instance [20]) and is a consequence of the Pohozaev identity. We assume, without loss of generality, that $x = 0$ and $0 < R < d(0, \partial\Omega)$, where d denotes the Euclidean distance. Since $Q^{(L)}$ is a global energy minimizer, it is a classical solution (see Section 6.2 for regularity) of the system (14):

$$\Delta Q_{ij} = \frac{1}{L} \left[\frac{\partial \tilde{f}_B(Q)}{\partial Q_{ij}} + b^2 \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right] \quad (36)$$

In (36) and in what follows, we drop the superscript L for convenience.

We multiply (36) by $x_k \cdot \partial_k Q_{ij}$, sum over repeated indices and integrate over $B(0, R)$ to obtain the following

$$\begin{aligned} 0 &= \int_{B(0,R)} Q_{ij, ll}(x) \cdot x_k \cdot \partial_k Q_{ij}(x) - \frac{1}{L} \frac{\partial \tilde{f}_B(Q(x))}{\partial Q_{ij}} \cdot x_k \cdot \partial_k Q_{ij}(x) - \frac{1}{L} b^2 \frac{\delta_{ij}}{3} \text{tr}(Q^2(x)) \cdot x_k \cdot \partial_k Q_{ij}(x) dx \\ &= \underbrace{\int_{B(0,R)} Q_{ij, ll}(x) \cdot x_k \cdot \partial_k Q_{ij}(x) dx}_I - \underbrace{\int_{B(0,R)} \frac{1}{L} \frac{\partial \tilde{f}_B(Q(x))}{\partial Q_{ij}} \cdot x_k \cdot \partial_k Q_{ij} dx}_{II} \quad (37) \end{aligned}$$

where we have used the tracelessness condition $Q_{ii} = 0$.

Integrating by parts, we have that:

$$\begin{aligned} I &= \int_{B(0,R)} Q_{ij, ll}(x) x_k \partial_k Q_{ij}(x) dx \\ &= - \int_{B(0,R)} Q_{ij, l} (\delta_{lk} Q_{ij, k}(x) + x_k Q_{ij, kl}(x)) dx + \int_{\partial B(0,R)} Q_{ij, l} x_k Q_{ij, k} \frac{x_l}{R} dx \\ &= - \int_{B(0,R)} Q_{ij, l}(x) Q_{ij, l}(x) dx + 3 \int_{B(0,R)} \frac{1}{2} Q_{ij, l}(x) Q_{ij, l}(x) dx \\ &\quad - \int_{\partial B(0,R)} \frac{Q_{ij, l}(x) Q_{ij, l}(x) x_k \cdot x_k}{2R} dx + \int_{\partial B(0,R)} \frac{(Q_{ij, k}(x) \cdot x_k)^2}{R} dx \quad (38) \end{aligned}$$

$$\begin{aligned} II &= \int_{B(0,R)} \frac{1}{L} \frac{\partial \tilde{f}_B(Q(x))}{\partial Q_{ij}} \cdot x_k \cdot \partial_k Q_{ij}(x) dx = \frac{1}{L} \int_{B(0,R)} \partial_k \tilde{f}_B(Q(x)) \cdot x_k dx \\ &= -\frac{3}{L} \int_{B(0,R)} \tilde{f}_B(Q(x)) dx + \frac{1}{L} \int_{\partial B(0,R)} \tilde{f}_B(Q(x)) \cdot \frac{x_k \cdot x_k}{R} dx \quad (39) \end{aligned}$$

Hence (37) becomes:

$$\begin{aligned} &- \int_{B(0,R)} \frac{Q_{ij, l}(x) Q_{ij, l}(x)}{2} + \frac{\tilde{f}_B(Q(x))}{L} dx + R \int_{\partial B(0,R)} \frac{Q_{ij, k}(x) Q_{ij, k}(x)}{2} + \frac{\tilde{f}_B(Q(x))}{L} dx \\ &= \frac{1}{R} \int_{\partial B(0,R)} (Q_{ij, k}(x) \cdot x_k)^2 dx + 2 \int_{B(0,R)} \frac{\tilde{f}_B(Q(x))}{L} dx \quad (40) \end{aligned}$$

We have

$$\begin{aligned} \frac{\partial}{\partial R} \left(\frac{1}{R} \int_{B(0,R)} \frac{Q_{ij,l}(x)Q_{ij,l}(x)}{2} + \frac{\tilde{f}_B(Q(x))}{L} dx \right) &= -\frac{1}{R^2} \int_{B(0,R)} \frac{Q_{ij,l}(x) \cdot Q_{ij,l}(x)}{2} + \frac{\tilde{f}_B(Q(x))}{L} dx \\ &\quad + \frac{1}{R} \int_{\partial B(0,R)} \frac{Q_{ij,l}(x) \cdot Q_{ij,l}(x)}{2} + \frac{\tilde{f}_B(Q(x))}{L} dx. \end{aligned} \quad (41)$$

The right-hand side of (41) is positive from (40) and hence the conclusion. \square

Lemma 3 (*$W^{1,2}$ convergence to harmonic maps*) *Let $\Omega \subset \mathbb{R}^3$ be a simply-connected bounded open set with smooth boundary. Let $Q^{(L)}$ be a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible class \mathcal{A}_Q defined in (12). Then there exists a sequence $L_k \rightarrow 0$ so that $Q^{(L_k)} \rightarrow Q^{(0)}$ strongly in $W^{1,2}(\Omega; S_0)$, where $Q^{(0)}$ is the limiting harmonic map defined in (15).*

Proof. Our proof follows closely, up to a point, the ideas of Proposition 1 in [3]. Firstly, we note that the limiting harmonic map $Q^{(0)}$ belongs to our admissible space \mathcal{A}_Q and since $Q^{(0)}(x) \in Q_{\min}$, a.e. $x \in \Omega$ (see Section 2) we have that $\tilde{f}_B(Q^{(0)}(x)) = 0$ a.e. $x \in \Omega$. Therefore

$$\int_{\Omega} \frac{1}{2} Q_{ij,k}^{(L)}(x) Q_{ij,k}^{(L)}(x) dx \leq \int_{\Omega} \frac{1}{2} Q_{ij,k}^{(L)}(x) Q_{ij,k}^{(L)}(x) + \frac{1}{L} \tilde{f}_B(Q^{(L)}(x)) dx \leq \int_{\Omega} \frac{1}{2} Q_{ij,k}^{(0)}(x) Q_{ij,k}^{(0)}(x) dx \quad (42)$$

The $Q^{(L)}$'s are subject to the same boundary condition, Q_b , for all L . Therefore (42) shows that the $W^{1,2}$ -norms of the $Q^{(L)}$'s are bounded uniformly in L . Hence there exists a weakly-convergent subsequence $Q^{(L_k)}$ such that $Q^{(L_k)} \rightharpoonup Q^{(1)}$ in $W^{1,2}$, for some $Q^{(1)} \in \mathcal{A}_Q$ as $L_k \rightarrow 0$. Using the lower semicontinuity of the $W^{1,2}$ norm with respect to the weak convergence, we have that

$$\int_{\Omega} |\nabla Q^{(1)}(x)|^2 dx \leq \int_{\Omega} |\nabla Q^{(0)}(x)|^2 dx \quad (43)$$

Relation (42) shows that $\int_{\Omega} \tilde{f}_B(Q^{(L_k)}(x)) dx \leq L_k \int_{\Omega} Q_{ij,k}^{(0)}(x) Q_{ij,k}^{(0)}(x) dx$ and hence $\int_{\Omega} \tilde{f}_B(Q^{(L_k)}(x)) dx \rightarrow 0$ as $L_k \rightarrow 0$. Taking into account that $\tilde{f}_B(Q) \geq 0, \forall Q \in S_0$ we have that, on a subsequence L_{k_j} , $\tilde{f}_B(Q^{(L_{k_j})}(x)) \rightarrow 0$ for almost all $x \in \Omega$. From Proposition 8, we know that $\tilde{f}_B(Q) = 0$ if and only if $Q \in Q_{\min}$ i.e. if $Q = s_+ (n \otimes n - \frac{1}{3} Id)$ for $n \in S^2$. On the other hand, the sequence $Q^{(L_k)}$ converges weakly in $W^{1,2}$ and, on a subsequence, strongly in L^2 to $Q^{(1)}$. Therefore, the weak limit $Q^{(1)}$ is of the form

$$Q^{(1)}(x) = s_+ \left(n^{(1)}(x) \otimes n^{(1)}(x) - \frac{1}{3} Id \right), \quad n^{(1)}(x) \in S^2, \text{ a.e. } x \in \Omega \quad (44)$$

It was proved in [2] (see also [4]) that if $Q^{(1)} \in W^{1,2}$ and the domain Ω is simply-connected, we can assume, without loss of generality, that $n^{(1)} \in W^{1,2}(\Omega, S^2)$ and its trace is n_b . Then (44) implies $|\nabla Q^{(1)}(x)|^2 = 2s_+^2 |\nabla n^{(1)}(x)|^2$ for a.e. $x \in \Omega$. Also, recalling the definition of $Q^{(0)}$ from Section 2 we have $|\nabla Q^{(0)}(x)|^2 = 2s_+^2 |\nabla n^{(0)}(x)|^2$ for a.e. $x \in \Omega$.

Combining (43) with (16) and the observations in the previous paragraph, we obtain $\int_{\Omega} |\nabla n^{(1)}(x)|^2 dx = \int_{\Omega} |\nabla n^{(0)}(x)|^2 dx$ and $\int_{\Omega} |\nabla Q^{(1)}(x)|^2 dx = \int_{\Omega} |\nabla Q^{(0)}(x)|^2 dx$. Then:

$$\int_{\Omega} |\nabla Q^{(0)}(x)|^2 dx \leq \liminf_{L_{k_j} \rightarrow 0} \int_{\Omega} |\nabla Q^{(L_{k_j})}(x)|^2 dx \leq \limsup_{L_{k_j} \rightarrow 0} \int_{\Omega} |\nabla Q^{(L_{k_j})}(x)|^2 dx \leq \int_{\Omega} |\nabla Q^{(0)}(x)|^2 dx,$$

which demonstrates that $\lim_{L_{k_j} \rightarrow 0} \|\nabla Q^{(L_{k_j})}\|_{L^2} = \|\nabla Q^{(0)}\|_{L^2}$. This together with the weak convergence $Q^{(L_{k_j})} \rightarrow Q^{(0)}$ suffices to show the strong convergence $Q^{(L_{k_j})} \rightarrow Q^{(0)}$ in $W^{1,2}$. \square

The following has an elementary proof, that will be omitted:

Lemma 4 *The function $\tilde{f}_B : S_0 \rightarrow \mathbb{R}_+$ is locally Lipschitz.*

We can now prove the uniform convergence of the bulk energy density in the interior, away from the singularities of the limiting harmonic map $Q^{(0)}$.

Proposition 4 *Let $\Omega \subset \mathbb{R}^3$ be a simply-connected bounded open set with smooth boundary. Let $Q^{(L)} \in W^{1,2}(\Omega, S_0)$ denote a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible class \mathcal{A}_Q . Assume that we have a sequence $\{Q^{(L_k)}\}_{k \in \mathbb{N}}$ so that $Q^{(L_k)} \rightarrow Q^{(0)}$ in $W^{1,2}(\Omega, S_0)$ as $L_k \rightarrow 0$.*

For any compact $K \subset \Omega$ such that $Q^{(0)}$ has no singularity in K we have

$$\lim_{L_k \rightarrow 0} \tilde{f}_B(Q^{(L_k)}(x)) = 0 \quad x \in K \quad (45)$$

and the limit is uniform on K .

Proof. *Lemma 3* shows that the strong limit $Q^{(0)}$ is a limiting harmonic map, as defined in Section 2, $Q^{(0)} = s_+(n^{(0)}(x) \otimes n^{(0)}(x) - \frac{1}{3}Id)$ where $n^{(0)}(x) \in W^{1,2}(\Omega, \mathbb{S}^2)$ a global energy minimizer of the harmonic map problem, subject to the boundary condition $n = n_b$ on $\partial\Omega$.

Let $\alpha_{L_k} = \tilde{f}_B(Q^{(L_k)}(x_0))$, for $x_0 \in K$ an arbitrary point. *Proposition 3* and *Lemma 4* imply that there exists a constant β (independent of x_0) so that

$$|\tilde{f}_B(Q^{(L)}(x)) - \tilde{f}_B(Q^{(L)}(y))| \leq \beta |Q^{(L)}(x) - Q^{(L)}(y)| \quad (46)$$

for any $x, y \in \Omega, L > 0$.

We then have

$$\begin{aligned} \alpha_{L_k} &\leq \tilde{f}_B(Q^{(L_k)}(x)) + \beta |Q^{(L_k)}(x) - Q^{(L_k)}(x_0)| \\ &\leq \tilde{f}_B(Q^{(L_k)}(x)) + \beta \|\nabla Q^{(L_k)}\|_{L^\infty(K')} |x - x_0| \leq \tilde{f}_B(Q^{(L_k)}(x)) + \frac{\tilde{C}\beta}{\sqrt{L_k}} |x - x_0|, \forall x \in K' \end{aligned} \quad (47)$$

where $K' \subset \Omega$ is a compact neighborhood of K to be precisely defined later. In the last relation above we use *Lemma A.1* from [3] and the apriori bound given by *Proposition 3*. For reader's convenience we recall that *Lemma A.1* in [3] states that if u is a scalar-valued function such that $-\Delta u = f$ on $\Omega \subset \mathbb{R}^n$ then $|\nabla u(x)|^2 \leq C \left(\|f\|_{L^\infty(\Omega)} \|u\|_{L^\infty(\Omega)} + \frac{1}{\text{dist}^2(x, \partial\Omega)} \|u\|_{L^\infty(\Omega)}^2 \right)$ where C is a constant that depends on n only. In our case the constant \tilde{C} depends on the dimension, $n = 3$, on a^2, b^2, c^2 and on the distance $\sup_{y \in K} d(y, \partial\Omega)$ only.

From (47) we have that

$$\alpha_{L_k} - \frac{\tilde{C}\beta\rho_k}{\sqrt{L_k}} \leq \tilde{f}_B(Q^{(L_k)}(x)), \forall x \in K', |x - x_0| < \rho_k \quad (48)$$

We argue similarly as in [3] and divide by L_k and integrate over $B_{\rho_k}(x_0)$ to obtain:

$$\frac{\rho_k^3}{L_k} \left(\alpha_{L_k} - \frac{\tilde{C}\beta\rho_k}{\sqrt{L_k}} \right) \leq \int_{B_{\rho_k}(x_0)} \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx \quad (49)$$

Take an arbitrary $\varepsilon > 0$. Recall that K is a compact set that does not contain singularities of $Q^{(0)}$. Then there exists a larger compact set K' , so that $K \subset K'$, that does not contain singularities either, and a constant $C_{K'}$ such that $|\nabla Q^{(0)}(x)|^2 < C_{K'}, \forall x \in K'$. For R_0 small enough, with $R_0 < \text{dist}(K, \partial\Omega)$ and such that $B(x_0, R_0) \subset K', \forall x_0 \in K$ we have

$$\frac{1}{R_0} \int_{B_{R_0}(x_0)} \frac{|\nabla Q^{(0)}(x)|^2}{2} dx \leq \frac{4\pi}{6} C_{K'} R_0^2 \leq \frac{\varepsilon}{3}, \forall x_0 \in K \quad (50)$$

We fix an R_0 as before. As $Q^{(L_k)} \rightarrow Q^{(0)}$ in $W^{1,2}$, we have that there exists an $\bar{L}_0 > 0$ so that:

$$\frac{1}{R_0} \int_{B_{R_0}(x_0)} \frac{|\nabla Q^{(L_k)}(x)|^2}{2} dx < \frac{1}{R_0} \int_{B_{R_0}(x_0)} \frac{|\nabla Q^{(0)}(x)|^2}{2} dx + \frac{\varepsilon}{3}, \text{ for } L_k < \bar{L}_0, \forall x_0 \in K \quad (51)$$

The arguments in [3] fail to work in our case as we have a three dimensional domain, unlike in the quoted paper, where the domain is two dimensional. In our case, using the monotonicity formula from *Lemma 2* and taking $\rho_k < R_0$ we obtain:

$$\int_{B_{\rho_k}(x_0)} \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx \leq \frac{\rho_k}{R_0} \int_{B_{R_0}(x_0)} \frac{|\nabla Q^{(L_k)}(x)|^2}{2} + \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx \leq \rho_k \left(\frac{2\varepsilon}{3} + \frac{\varepsilon}{3} \right) \quad (52)$$

for $L_k < \bar{L}_1$ with \bar{L}_1 small enough so that $\frac{1}{R_0} \int_{B_{R_0}(x_0)} \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx < \frac{\varepsilon}{3}$ (note that there exists such an \bar{L}_1 as the proof of *Lemma 3* shows that $\int_{\Omega} \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx = o(1)$ as $L_k \rightarrow 0$).

We take $\rho_k = \frac{\alpha_{L_k} \sqrt{L_k}}{2\tilde{C}\beta}$. Then, from (49) and (52) we obtain

$$\alpha_{L_k}^3 < 8(\tilde{C}\beta)^2 \varepsilon$$

for $L_k < \min\{\bar{L}_0, \bar{L}_1\}$. As $\varepsilon > 0$ is arbitrary and the estimate on $\alpha_{L_k} = \tilde{f}_B(Q^{(L_k)}(x_0))$, $x_0 \in K$ is obtained in a manner independent of x_0 , we have the claimed result. \square

We also need the following

Lemma 5 *There exists $\varepsilon_0 > 0$ so that:*

$$\frac{1}{\tilde{C}} \tilde{f}_B(Q) \leq \sum_{i,j=1}^3 \left(\frac{\partial \tilde{f}_B(Q)}{\partial Q_{ij}} + b^2 \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right)^2 \leq \tilde{C} \tilde{f}_B(Q) \quad (53)$$

$\forall Q \in S_0$ such that $|Q - s_+(n \otimes n - \frac{1}{3}Id)| \leq \varepsilon_0$, for some $n \in \mathbb{S}^2$

where $s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}$ and the constant \tilde{C} is independent of Q , but depends on a^2, b^2, c^2 .

Proof. Recall from Proposition 8, [21] that $\tilde{f}_B(Q) \geq 0$ and $\tilde{f}_B(Q) = 0 \leftrightarrow Q = s_+(n \otimes n - \frac{1}{3}Id)$ with $s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}$ and $n \in \mathbb{S}^2$.

Let the eigenvalues of Q be $x, y, -x - y$. We define $F(x, y) \stackrel{def}{=} -a^2(x^2 + y^2 + xy) + b^2xy(x + y) + c^2(x^2 + y^2 + xy)^2$ and $D \stackrel{def}{=} \min_{(x,y) \in \mathbb{R}^2} F(x, y)$. Then $\tilde{F}(x, y) \stackrel{def}{=} F(x, y) - D = \tilde{f}_B(Q)$.

Then $\tilde{F} = 0$ only at three pairs (x, y) namely $(-\frac{s_+}{3}, -\frac{s_+}{3}), (-\frac{s_+}{3}, 2\frac{s_+}{3})$ and $(2\frac{s_+}{3}, -\frac{s_+}{3})$.

On the other hand we have

$$\sum_{i,j=1}^3 \left(\frac{\partial \tilde{f}_B}{\partial Q_{ij}} + \frac{b^2 \delta_{ij}}{3} \text{tr}(Q^2) \right)^2 = a^4 \text{tr}(Q^2) + \left(\frac{b^4}{6} - 2a^2c^2 \right) (\text{tr}(Q^2))^2 + c^4 (\text{tr}(Q^2))^3 + 2a^2b^2 \text{tr}(Q^3) - 2b^2c^2 \text{tr}(Q^2) \text{tr}(Q^3) \quad (54)$$

(where we used the identity $\text{tr}(Q^4) = \frac{(\text{tr}(Q^2))^2}{2}$, valid for a traceless symmetric 3×3 matrix)

If we denote $h(Q) = \sum_{i,j=1}^3 \left(\frac{\partial \tilde{f}_B(Q)}{\partial Q_{ij}} + b^2 \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right)^2$ we have $h(Q) = H(x, y)$ where $H : \mathbb{R}^2 \rightarrow \mathbb{R}$ is given by

$$H(x, y) \stackrel{def}{=} 2a^4(x^2 + y^2 + xy) + 4\left(\frac{b^4}{6} - 2a^2c^2\right)(x^2 + y^2 + xy)^2 + 8c^4(x^2 + y^2 + xy)^3 \\ + 12b^2c^2xy(x+y)(x^2 + y^2 + xy) - 6a^2b^2xy(x+y)$$

We claim that there exist $\varepsilon_1, \varepsilon_2, \varepsilon_3 > 0$ so that

$$\frac{1}{\tilde{C}}\tilde{F}(x, y) \leq H(x, y) \leq \tilde{C}\tilde{F}(x, y), \forall (x, y) \in B_{\varepsilon_1}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right), B_{\varepsilon_2}\left(-\frac{s_+}{3}, 2\frac{s_+}{3}\right), B_{\varepsilon_3}\left(2\frac{s_+}{3}, -\frac{s_+}{3}\right) \quad (55)$$

which gives the conclusion.

We prove the inequality (55) only for $(x, y) \in B_{\varepsilon_1}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right)$; the other two cases can be dealt with similarly.

Careful computations show:

$$H\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{\partial H}{\partial x}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{\partial H}{\partial y}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = 0$$

$$\frac{\partial^2 H}{\partial y^2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{\partial^2 H}{\partial x^2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = 4(b^4 + 6a^2c^2)\frac{b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 2a^2c^2}}{24c^4}$$

$$\frac{\partial^2 H}{\partial x\partial y}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = -2(b^4 - 12a^2c^2)\frac{b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 24a^2c^2}}{24c^4}$$

$$\tilde{F}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{\partial \tilde{F}}{\partial x}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{\partial \tilde{F}}{\partial y}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = 0$$

$$\frac{\partial^2 \tilde{F}}{\partial y^2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{\partial^2 \tilde{F}}{\partial x^2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{1}{4c^2}(b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 24a^2c^2})$$

$$\frac{\partial^2 \tilde{F}}{\partial x\partial y}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = 3a^2$$

Let $(x_0, y_0) = \left(-\frac{s_+}{3}, -\frac{s_+}{3}\right)$. We have

$$\frac{H(x, y)}{\tilde{F}(x, y)} = \frac{H_1(x, y) + R_H(x, y)}{\tilde{F}_1(x, y) + R_{\tilde{F}}(x, y)}$$

where $H_1(x, y) = (x - x_0)^2 \frac{\partial^2 H}{\partial x^2}(x_0, y_0) + 2(x - x_0)(y - y_0) \frac{\partial^2 H}{\partial x\partial y}(x_0, y_0) + (y - y_0)^2 \frac{\partial^2 H}{\partial y^2}(x_0, y_0)$ and $\tilde{F}_1(x, y) = (x - x_0)^2 \frac{\partial^2 \tilde{F}}{\partial x^2}(x_0, y_0) + 2(x - x_0)(y - y_0) \frac{\partial^2 \tilde{F}}{\partial x\partial y}(x_0, y_0) + (y - y_0)^2 \frac{\partial^2 \tilde{F}}{\partial y^2}(x_0, y_0)$ with $R_H, R_{\tilde{F}}$ the remainders in the Taylor expansions around (x_0, y_0) .

From the definition of Taylor expansions, we have that there exists $\varepsilon_0 > 0$ so that on $B_{\varepsilon_1}(x_0, y_0)$ we have

$$|R_H(x, y)| \leq \frac{1}{2}H_1(x, y) \text{ and } |R_{\tilde{F}}(x, y)| \leq \frac{1}{2}\tilde{F}_1(x, y), \forall (x, y) \in B_{\varepsilon_1}(x_0, y_0) \quad (56)$$

On the other hand we have

$$\tilde{F}_1(x, y) \frac{1}{8(b^4 + 6a^2c^2)} \leq H_1(x, y) \leq \tilde{F}_1(x, y)8(b^4 + 6a^2c^2) \forall (x, y) \in \mathbb{R}^2 \quad (57)$$

hence, combining (56) and (57), we get:

$$\tilde{F}(x, y) \frac{1}{24(b^4 + 6a^2c^2)} \leq H(x, y) \leq \tilde{F}(x, y) 24(b^4 + 6a^2c^2), \forall (x, y) \in B_{\varepsilon_1}(-\frac{s_+}{3}, -\frac{s_+}{3}) \quad (58)$$

which yields claim (55) for $(x, y) \in B_{\varepsilon_1}(-\frac{s_+}{3}, -\frac{s_+}{3})$. The other two cases can be analyzed analogously. \square

We continue by proving a Bochner-type inequality that is crucial for the derivation of uniform (in L) Lipschitz bounds, away from the singularities of the limiting harmonic map. This type of inequalities were first used (to the best of our knowledge) in the context of harmonic maps (see [29] and the references there) and later adapted to other, more complicated contexts (see for instance [6]). The main difficulty in the proof of Proposition 5 (to follow) is the derivation of the next lemma.

Lemma 6 *There exists $\varepsilon_0 > 0$ and a constant $C > 0$, independent of L , so that for $Q^{(L)}$ a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible space \mathcal{A}_Q , we have*

$$-\Delta e_L(Q^{(L)})(x) \leq C e_L^2(Q^{(L)})(x) \quad (59)$$

provided there exists a ball $B_{\rho(x)}(x)$ for some $\rho(x) > 0$ such that $|Q^{(L)}(y) - s_+(m(y) \otimes m(y) - \frac{1}{3}Id)| < \varepsilon_0$ with $m(y) \in \mathbb{S}^2$, for all $y \in B_{\rho(x)}(x)$.

Proof. In the following we drop the superscript L for convenience. We have:

$$\begin{aligned} & -\Delta \left(\frac{Q_{ij,k} Q_{ij,k}}{2} \right) = -\Delta(Q_{ij,k}) Q_{ij,k} - Q_{ij,kl} Q_{ij,kl} \leq \\ & \leq -\partial_k \left[\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) + \frac{b^2 \delta_{ij}}{3L} \text{tr}(Q^2) \right] Q_{ij,k} = -\partial_k \left[\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) \right] Q_{ij,k} \end{aligned} \quad (60)$$

On the other hand:

$$\begin{aligned} -\Delta \left[\frac{1}{L} \tilde{f}_B(Q(x)) \right] &= -\partial_k \left(\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) \partial_k Q_{ij} \right) = -\partial_k \left[\left[\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) + \frac{b^2 \delta_{ij}}{3L} \text{tr}(Q^2) \right] \partial_k Q_{ij} \right] \\ &= - \underbrace{\left(\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) + \frac{b^2 \delta_{ij}}{3L} \text{tr}(Q^2) \right)}_{\stackrel{\text{def}}{=} Z} \times \underbrace{\Delta Q_{ij}}_{=Z} - \partial_k \left(\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) \right) Q_{ij,k} \\ &\leq -\partial_k \left(\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) \right) Q_{ij,k} \end{aligned} \quad (61)$$

We take $\varepsilon_1 > 0$ a small number, to be made precise later. For any such ε_1 we can pick $\varepsilon_0 > 0$ small enough so that if the eigenvalues of $Q(x)$ are $(\lambda, \mu, -\lambda - \mu)$ then one of the three numbers $(\lambda + \frac{s_+}{3})^2 + (\mu + \frac{s_+}{3})^2 + (\lambda + \mu + 2\frac{s_+}{3})^2$, $(\lambda + \frac{s_+}{3})^2 + (\mu - 2\frac{s_+}{3})^2 + (\lambda + \mu - \frac{s_+}{3})^2$, $(\lambda - 2\frac{s_+}{3})^2 + (\mu + \frac{s_+}{3})^2 + (\lambda + \mu - \frac{s_+}{3})^2$ is less than or equal to ε_1 (this can be done because the eigenvalues are continuous functions of matrices, [17], and the matrix $s_+(n \otimes n - \frac{1}{3}Id)$ has eigenvalues $-\frac{s_+}{3}$, $-\frac{s_+}{3}$ and $2\frac{s_+}{3}$). Note moreover that we need to choose ε_0 to be smaller than the choice (of ε_0) in Lemma 5 as we will need to use that lemma in the remainder of this proof.

For the matrix $Q(x)$, let us denote its eigenvectors by $n_1(x), n_2(x), n_3(x)$ and let $\lambda_1(x), \lambda_2(x), \lambda_3(x) = -\lambda_1(x) - \lambda_2(x)$ denote the corresponding eigenvalues. From the preceding discussion, we can, without loss of generality, assume that

$$(\lambda_1 + \frac{s_+}{3})^2 + (\lambda_2 + \frac{s_+}{3})^2 + (\lambda_1 + \lambda_2 + 2\frac{s_+}{3})^2 < \varepsilon_1 \quad (62)$$

We define the matrix

$$Q^x \stackrel{def}{=} -\frac{s_+}{3}n_1(x) \otimes n_1(x) - \frac{s_+}{3}n_2(x) \otimes n_2(x) + \frac{2s_+}{3}n_3(x) \otimes n_3(x)$$

(Note that there exists a $m(x) \in \mathbb{S}^2$ so that $Q^x = s_+(m(x) \otimes m(x) - \frac{1}{3}Id)$).

Taking into account (62) and the fact that $Q(x)$ and Q^x have the same eigenvectors, we have :

$$\text{tr}(Q(x) - Q^x)^2 = (\lambda_1 + \frac{s_+}{3})^2 + (\lambda_2 + \frac{s_+}{3})^2 + (\lambda_1 + \lambda_2 + 2\frac{s_+}{3})^2 < \varepsilon_1 \quad (63)$$

Using the of Taylor expansion of $\frac{1}{2}\frac{\partial^2 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}}(Q(x))$ around Q^x we obtain:

$$\frac{1}{2}\frac{\partial^2 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}}(Q(x)) = \frac{1}{2}\frac{\partial^2 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}}(Q^x) + \frac{1}{2}\frac{\partial^3 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}\partial Q_{pq}}(Q^x)(Q_{pq}(x) - Q_{pq}^x) + \mathcal{R}^{ijmn}(Q^x, Q(x)) \quad (64)$$

where $\mathcal{R}^{ijmn}(Q^x, Q(x))$ is the remainder.

From (64) we have:

$$\begin{aligned} & -\partial_k \left(\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) \right) Q_{ij,k} = -\frac{1}{L} \frac{\partial^2 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}} Q_{mn,k} Q_{ij,k} = \\ & = \underbrace{-\frac{1}{L} \frac{\partial^2 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}}(Q^x) Q_{mn,k} Q_{ij,k}}_{\leq 0} - \frac{1}{L} \frac{\partial^3 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}\partial Q_{pq}}(Q^x)(Q_{pq}(x) - Q_{pq}^x) Q_{ij,k} Q_{mn,k} - \\ & \qquad \qquad \qquad - \frac{1}{L} \mathcal{R}^{ijmn}(Q(x), Q^x) Q_{ij,k} Q_{mn,k} \leq \\ & \leq \frac{C_0 \delta}{L^2} \sum_{i,j,m,n=1}^3 \left(\frac{\partial^3 \tilde{f}_B}{\partial Q_{ij}\partial Q_{mn}\partial Q_{pq}}(Q^x) \right)^2 (Q_{pq}(x) - Q_{pq}^x)^2 \\ & \qquad \qquad \qquad + \frac{C_0 \delta}{L^2} \sum_{i,j,m,n=1}^3 (\mathcal{R}^{ijmn})^2(Q(x), Q^x) + \frac{1}{\delta} |\nabla Q|^4 \leq \\ & \leq \frac{\delta}{L^2} \sum_{i,j,m,n=1}^3 \left[\bar{C}_0 \left(\frac{\partial^3 f}{\partial Q_{ij}\partial Q_{mn}\partial Q_{pq}}(Q^x) \right)^2 + 1 \right] (Q_{pq}(x) - Q_{pq}^x)^2 \frac{1}{\delta} |\nabla Q|^4 \\ & \qquad \qquad \qquad \leq \frac{C_1 \delta}{L^2} \text{tr}(Q(x) - Q^x)^2 + \frac{1}{\delta} |\nabla Q|^4 \quad (65) \end{aligned}$$

where $0 < \delta < 1$ and C_0, \bar{C}_0, C_1 are independent of L and x . For the first term in the second line above we use the fact that the Hessian matrix of a function $\tilde{f}_B(Q)$ is non-negative definite at a global minimum (which holds true in our case as well, as one can easily check, even though we have $\tilde{f}_B(Q)$ restricted to the linear space S_0).

Let us recall (from the proof of the previous lemma) the definitions of F and \tilde{F} . Then, for a matrix $Q \in S_0$ with eigenvalues $(\lambda_1, \lambda_2, -\lambda_1 - \lambda_2)$ we have

$$\tilde{f}_B(Q) = \tilde{F}(\lambda_1, \lambda_2) \quad (66)$$

We claim that for $\varepsilon_1 > 0$ small enough there exists C_2 independent of L, λ_1, λ_2 so that

$$\begin{aligned} & C_2 \left((\lambda_1 + \frac{s_+}{3})^2 + (\lambda_2 + \frac{s_+}{3})^2 + (\lambda_1 + \lambda_2 + 2\frac{s_+}{3})^2 \right) \leq \tilde{F}(\lambda_1, \lambda_2) \\ & \text{for all } (\lambda_1, \lambda_2) \text{ so that } (\lambda_1 + \frac{s_+}{3})^2 + (\lambda_2 + \frac{s_+}{3})^2 + (\lambda_1 + \lambda_2 + 2\frac{s_+}{3})^2 < \varepsilon_1. \quad (67) \end{aligned}$$

Careful computations show:

$$\begin{aligned}\tilde{F}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) &= \frac{\partial \tilde{F}}{\partial \lambda_1}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{\partial \tilde{F}}{\partial \lambda_2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = 0 \\ \frac{\partial^2 \tilde{F}}{\partial \lambda_2^2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) &= \frac{\partial^2 \tilde{F}}{\partial \lambda_1^2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) = \frac{1}{4c^2}(b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 24a^2c^2}) \\ \frac{\partial^2 \tilde{F}}{\partial \lambda_1 \partial \lambda_2}\left(-\frac{s_+}{3}, -\frac{s_+}{3}\right) &= 3a^2\end{aligned}$$

Using a Taylor expansion around $(\lambda_1, \lambda_2) = (-\frac{s_+}{3}, -\frac{s_+}{3})$ we have

$$\begin{aligned}\tilde{F}(\lambda_1, \lambda_2) &= \frac{1}{8c^2} \left(b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 24a^2c^2} \right) \left[\left(\lambda_1 + \frac{s_+}{3} \right)^2 + \left(\lambda_2 + \frac{s_+}{3} \right)^2 \right] + \\ &\quad + 3a^2 \left(\lambda_1 + \frac{s_+}{3} \right) \left(\lambda_2 + \frac{s_+}{3} \right) + R(\lambda_1, \lambda_2) \geq \\ &\geq \frac{1}{2} \left\{ \frac{1}{8c^2} \left(b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 24a^2c^2} \right) \left[\left(\lambda_1 + \frac{s_+}{3} \right)^2 + \left(\lambda_2 + \frac{s_+}{3} \right)^2 \right] + 3a^2 \left(\lambda_1 + \frac{s_+}{3} \right) \left(\lambda_2 + \frac{s_+}{3} \right) \right\} \quad (68)\end{aligned}$$

where $R(\lambda_1, \lambda_2)$ is the remainder in the Taylor expansion, and the inequality holds *provided* that the remainder R is small enough. We choose $\varepsilon_1 > 0$ to be small enough so that if $(\lambda_1 + \frac{s_+}{3})^2 + (\lambda_2 + \frac{s_+}{3})^2 + (\lambda_1 + \lambda_2 + 2\frac{s_+}{3})^2 < \varepsilon_1$ then R is small enough and the inequality above holds.

As the quadratic form $\frac{1}{16c^2} (b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 24a^2c^2}) [(\lambda_1 + \frac{s_+}{3})^2 + (\lambda_2 + \frac{s_+}{3})^2] + \frac{3}{2}a^2(\lambda_1 + \frac{s_+}{3})(\lambda_2 + \frac{s_+}{3})$ is positive definite, there exists a $C_2 > 0$, depending only on a^2, b^2 and c^2 such that

$$\begin{aligned}\frac{1}{2} \left\{ \frac{1}{8c^2} \left(b^4 + 12a^2c^2 + b^2\sqrt{b^4 + 24a^2c^2} \right) \left[\left(\lambda_1 + \frac{s_+}{3} \right)^2 + \left(\lambda_2 + \frac{s_+}{3} \right)^2 \right] + 3a^2 \left(\lambda_1 + \frac{s_+}{3} \right) \left(\lambda_2 + \frac{s_+}{3} \right) \right\} &\geq \\ &\geq C_2 \left(\left(\lambda_1 + \frac{s_+}{3} \right)^2 + \left(\lambda_2 + \frac{s_+}{3} \right)^2 + \left(\lambda_1 + \lambda_2 + \frac{2s_+}{3} \right)^2 \right) \quad \forall (\lambda_1, \lambda_2) \in \mathbb{R}^2\end{aligned}$$

Combining this last inequality with (68) we obtain the claim (67).

The relation (67) together with (66) and (63) show that $\text{tr}(Q(x) - Q^x)^2 \leq C_3 \tilde{f}_B(Q(x))$ for some C_3 independent of L and x , which combined with (65) shows

$$-\partial_k \left(\frac{1}{L} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(Q(x)) \right) Q_{ij,k} \leq \frac{\delta C_4}{L^2} \tilde{f}_B(Q(x)) + \frac{1}{\delta} |\nabla Q(x)|^4$$

with C_4 a constant independent of L and x and any $\delta > 0$. This last inequality together with (60) and (61) show:

$$-\Delta e_L + \frac{1}{L^2} \sum_{i,j=1}^3 \left(\frac{\partial \tilde{f}_B}{\partial Q_{ij}} + \frac{b^2 \delta_{ij}}{3} \text{tr}(Q^2) \right)^2 \leq \frac{\delta C_4}{L^2} \tilde{f}_B(Q) + \frac{1}{\delta} |\nabla Q|^4$$

Taking into account *Lemma 5* and choosing δ small enough (depending only on C_4 and the constant \tilde{C} from *Lemma 5*) we can absorb the term $\frac{\delta C_4}{L^2} \tilde{f}_B(Q)$ on the right hand side into the left hand side and obtain

$$-\Delta e_L \leq \frac{1}{\delta} |\nabla Q|^4,$$

giving the desired conclusion. \square

Lemma 7 Let $\Omega \subset \mathbb{R}^3$ be a simply-connected bounded open set with smooth boundary. Let $Q^{(L_k)} \in W^{1,2}(\Omega, S_0)$ be a sequence of global minimizers for the energy $\tilde{F}_{LG}[Q]$ in the admissible space \mathcal{A}_Q . Assume that as $L_k \rightarrow 0$ we have $Q^{(L_k)} \rightarrow Q^{(0)}$ in $W^{1,2}(\Omega, S_0)$.

Let $K \subset \Omega$ be a compact set which contains no singularity of $Q^{(0)}$. There exists $C_1 > 0, C_2 > 0, \bar{L}_0 > 0$ (all constants independent of L_k) so that if for $a \in K, 0 < r < d(a, \partial K)$ we have

$$\frac{1}{r} \int_{B_r(a)} e_{L_k}(Q^{(L_k)}(x)) dx \leq C_1$$

then

$$r^2 \sup_{B_{\frac{r}{2}}(a)} e_{L_k}(Q^{(L_k)}) \leq C_2.$$

for all $L_k < \bar{L}_0$.

Proof. Taking into account our assumptions on the sequence $(Q^{(L_k)})_{k \in \mathbb{N}}$, Proposition 4 shows that for any given $\tilde{\varepsilon}_0$ smaller than ε_0 in Lemma 5 and also smaller than the ε_0 in Lemma 6, we have that there exists a \bar{L}_0 so that for $L_k < \bar{L}_0$ we have

$$\|Q^{(L_k)}(x) - s_+ \left(n(x) \otimes n(x) - \frac{1}{3} Id \right)\| \leq \tilde{\varepsilon}_0, \forall x \in K, \text{ for some } n(x) \in \mathbb{S}^2 \quad (69)$$

We continue reasoning similarly as in [29]. We fix an arbitrary $L_k < \bar{L}_0$ and an $a \in \Omega$ and take a $r > 0$ so that $0 < r < \min\{d(a, \partial\Omega), d(a, K)\}$. We let $r_1 > 0$ and $x_1 \in B_{r_1}(a)$ be such that

$$\max_{0 \leq s \leq \frac{2}{3}r} \left(\frac{2}{3}r - s \right)^2 \max_{B_s(a)} e_{L_k}(Q^{(L_k)}) = \left(\frac{2}{3}r - r_1 \right)^2 \max_{B_{r_1}(a)} e_{L_k}(Q^{(L_k)}) = \left(\frac{2}{3}r - r_1 \right)^2 e_{L_k}(Q^{(L_k)}(x_1))$$

Define $e_1^{(L_k)} \stackrel{def}{=} \max_{B_{r_1}(a)} e_{L_k}(Q^{(L_k)})$. Then:

$$\begin{aligned} \max_{B_{\frac{2}{3}r - r_1}(x_1)} e_{L_k}(Q^{(L_k)}) &\leq \max_{B_{\frac{2}{3}r + r_1}(a)} e_{L_k}(Q^{(L_k)}) \\ &\leq \frac{(2/3 \cdot r - r_1)^2 \max_{B_{r_1}(a)} e_{L_k}(Q^{(L_k)})}{(2/3 \cdot r - (2/3 \cdot r + r_1)/2)^2} = 4 \max_{B_{r_1}(a)} e_{L_k}(Q^{(L_k)}) = 4e_1^{(L_k)} \end{aligned} \quad (70)$$

where for the first inequality we use the fact that $B_{\frac{2}{3}r - r_1}(x_1) \subset B_{\frac{2}{3}r + r_1}(a)$ and for the second inequality, we use the definition of r_1 .

Let $r_2 = \frac{(2/3 \cdot r - r_1) \sqrt{e_1^{(L_k)}}}{2}$ and define $R^{(L_k)}(x) = Q^{(L_k)} \left(x_1 + \frac{x}{\sqrt{e_1^{(L_k)}}} \right)$. We let $\bar{L}_k = e_1^{(L_k)} L_k$ and then

$$e_{\bar{L}_k}(R^{(L_k)}) = \frac{1}{2} |\nabla R^{(L_k)}|^2 + \frac{\tilde{f}_B(R^{(L_k)})}{\bar{L}_k} = \frac{1}{2} \frac{|\nabla Q^{(L_k)}|^2}{e_1^{(L_k)}} + \frac{\tilde{f}_B(Q^{(L_k)})}{e_1^{(L_k)} L_k} = \frac{1}{e_1^{(L_k)}} e_{L_k}(Q^{(L_k)})$$

Equation (70) then implies

$$\max_{x \in B_{r_2}(0)} e_{\bar{L}_k}(R^{(L_k)}) = \max_{x \in B_{\frac{2}{3}r - r_1}(x_1)} \frac{e_{L_k}(Q^{(L_k)}(x))}{e_1^{L_k}} \leq 4$$

where the equality above follows from the definition of r_2 and $R^{(L_k)}$ and the inequality above follows from equation (70). Thus, we have

$$\max_{B_{r_2}(0)} e_{\bar{L}_k}(R^{(L_k)}) \leq 4, e_{\bar{L}_k}(R^{(L_k)})(0) = 1 \quad (71)$$

where $R^{(L_k)}$ satisfies the following system of elliptic PDEs

$$\bar{L}_k R_{ij,kk}^{(L_k)} = -a^2 R_{ij}^{(L_k)} - b^2 \left(R_{ik}^{(L_k)} R_{kj}^{(L_k)} - \frac{\delta_{ij}}{3} \text{tr}((R^{(L_k)})^2) \right) + c^2 R_{ij}^{(L_k)} \text{tr}((R^{(L_k)})^2) \quad (72)$$

We now claim that

$$r_2 \leq 1 \quad (73)$$

It is clear that $r_2 \leq 1$ implies the conclusion. Let us assume for contradiction that $r_2 > 1$. Then we claim that there exists a constant $C > 0$, independent of L_k , so that

$$1 \leq C \int_{B_1} e_{\bar{L}_k}(R^{(L_k)})(x) dx \quad (74)$$

The matrix $R^{(L_k)}$ satisfies the system (72) (which is the rescaled version of (14)); using relation (69) and the definition of $R^{(L_k)}$ as well as the fact that $r_2 > 1$, we can apply *Lemma 6* to $e_{\bar{L}_k}(R^{(L_k)})$ and obtain

$$-\Delta e_{\bar{L}_k}(R^{(L_k)})(x) \leq C e_{\bar{L}_k}^2(R^{(L_k)})(x) \stackrel{(71)}{\leq} 4C e_{\bar{L}_k}(R^{(L_k)})(x), \forall x \in B_1(0)$$

Combining (71) and the Harnack inequality (see for instance [31], Ch.14, Thm. 9.3) along with the above relation we obtain (74).

We have

$$\begin{aligned} \int_{B_1} e_{\bar{L}_k}(R^{(L_k)})(x) dx &\leq \frac{1}{r_2} \int_{B_{r_2}(0)} \frac{|\nabla R^{(L_k)}(x)|^2}{2} + \frac{\tilde{f}_B(R^{(L_k)}(x))}{L_k e_1^{(L_k)}} dx = \\ &= \frac{2}{2/3 \cdot r - r_1} \int_{B_{(2/3 \cdot r - r_1)/2}(x_1)} e_{L_k}(Q^{(L_k)})(x) dx \leq \frac{3}{r} \int_{B_{r/3}(x_1)} e_{L_k}(Q^{(L_k)})(x) dx \\ &\leq \frac{3}{r} \int_{B_r(a)} e_{L_k}(Q^{(L_k)})(x) dx \leq 3C_1 \end{aligned} \quad (75)$$

where for the first inequality we use the monotonicity inequality (Lemma 2) and the assumption that $r_2 \geq 1$ (note that the equation satisfied by $R^{(L_k)}$, equation (72) is the same as the equation satisfied by $Q^{(L_k)}$, up to a different elastic constant, hence the use of Lemma 2 here is justified). For the equality in relation (75) we use the change of variables $y = x_1 + \frac{x}{\sqrt{e_1^{L_k}}}$ and use the relation: $e_{\bar{L}_k}(R^{(L_k)}) = \frac{1}{e_1^{(L_k)}} e_{L_k}(Q^{(L_k)})$. For the

second inequality in (75) we use the monotonicity inequality and the fact that $\frac{2/3r - r_1}{2} \leq \frac{r}{3}$. For the third inequality in (75) we use the fact that $B_{r/3}(x_1) \subset B_r(a)$ since $|x_1 - a| < r_1 < \frac{2}{3}r$. The last step in (75) follows from the hypothesis of the Lemma.

Choosing C_1 small enough we reach a contradiction with (74) which in turn implies that $r_2 \leq 1$ and hence the conclusion. \square

We can now prove the uniform convergence of $Q^{(L_k)}$ away from singularities of the limiting harmonic map $Q^{(0)}$:

Proposition 5 *Let $\Omega \subset \mathbb{R}^3$ be a simply-connected bounded open set with smooth boundary. Let $Q^{(L_k)} \in W^{1,2}(\Omega, S_0)$ be a sequence of global minimizers for the energy $\tilde{F}_{LG}[Q]$ in the admissible space \mathcal{A}_Q . Assume that as $L_k \rightarrow 0$ we have $Q^{(L_k)} \rightarrow Q^{(0)}$ in $W^{1,2}(\Omega, S_0)$.*

Let $K \subset \Omega$ be a compact set which contains no singularity of $Q^{(0)}$. Then

$$\lim_{k \rightarrow \infty} Q^{(L_k)}(x) = Q^{(0)}(x), \text{ uniformly for } x \in K \quad (76)$$

Proof. From the hypothesis and *Proposition 4* we have that $\tilde{f}_B(Q^{(L_k)}(x)) \rightarrow 0$ uniformly in K . Thus for any $\varepsilon_0 > 0$ there exists a $\bar{L}_0 > 0$ such that for $L_k < \bar{L}_0$ we have that $|Q^{(L_k)}(x) - s_+(n(x) \otimes n(x) - \frac{1}{3}Id)| < \varepsilon_0$ for all $x \in K$ (and for each $x \in K$, we have $n(x) \in \mathbb{S}^2$). Thus we can apply *Lemmas 5, 6 and 7*.

In order to show the uniform convergence it suffices to show that we have uniform (independent of L_k) Lipschitz bounds on $Q^{(L_k)}(x)$ for $x \in K$. We reason similarly to the proof in *Proposition 4* (see also [6]). We first claim that there exists an $\varepsilon_1 > 0$ so that

$$\forall \varepsilon \in (0, \varepsilon_1), \text{ there exists } r_0(\varepsilon) \text{ depending only on } \varepsilon, \Omega, K, \text{ and boundary data } Q_b \text{ so that}$$

$$\frac{1}{r_0} \int_{K \cap B_{r_0}(x)} \frac{1}{2} |\nabla Q^{(L_k)}(x)|^2 + \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx \leq \varepsilon, \forall x \in K, \text{ provided that } L_k < L_*(\varepsilon, r_0(\varepsilon)) \quad (77)$$

In order to prove the claim let us first recall that $Q^{(0)}$ has no singularities on the compact set K . Thus there exists a larger compact set K' with $K \subset K'$ and a constant $C > 0$ so that $|\nabla Q^{(0)}(x)| \leq C, \forall x \in K'$. We choose $\varepsilon_1 > 0$ so that $B(x, \varepsilon_1) \cap K \subset K'$ hence for an arbitrary $\varepsilon \in (0, \varepsilon_1)$ there exists $r_0(\varepsilon) > 0$ so that

$$\frac{1}{r_0} \int_{K \cap B_{r_0}(x)} \frac{1}{2} |\nabla Q^{(0)}(x)|^2 dx < \frac{\varepsilon}{3}$$

provided that $x \in K$ and $r_0(\varepsilon)$ is chosen small enough. We also have, from the $W^{1,2}(\Omega, S_0)$ convergence of $Q^{(L_k)}$ to $Q^{(0)}$, that there exists $\bar{L}(\varepsilon)$ so that

$$\frac{1}{r_0} \int_{K \cap B_{r_0}(x)} \frac{1}{2} |\nabla Q^{(L_k)}(x)|^2 dx \leq \frac{1}{r_0} \int_{K \cap B_{r_0}(x)} \frac{1}{2} |\nabla Q^{(0)}(x)|^2 dx + \frac{\varepsilon}{3}, \forall L_k < \bar{L}(\varepsilon)$$

Recall from the proof of *Lemma 3* that $\lim_{L_k \rightarrow 0} \int_{\Omega} \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx = 0$. Hence there exists $\tilde{L}(\varepsilon)$ so that $\frac{1}{r_0} \int_{\Omega} \frac{\tilde{f}_B(Q^{(L_k)}(x))}{L_k} dx < \frac{\varepsilon}{3}, \forall L_k < \tilde{L}(\varepsilon)$. Letting $L_*(\varepsilon, r_0(\varepsilon)) = \min\{\bar{L}, \tilde{L}\}$ and combining the two relations above we obtain the claim (77).

Choosing $\varepsilon > 0$ smaller than the constant C_1 from *Lemma 7*, we apply *Lemma 7* to conclude that $|\nabla Q^{(L_k)}(x)|$ can be bounded, independently of L_k , on the set K . The uniform convergence result now follows. \square

4.2 The analysis near the boundary

In this section we consider the behaviour of a global minimizer $Q^{(L)}$ near the boundary, $\partial\Omega$, in the limit $L \rightarrow 0$. For $x^0 \in \partial\Omega$ we define the region Ω_r to be:

$$\Omega_r \stackrel{\text{def}}{=} \Omega \cap B_r(x^0), r > 0. \quad (78)$$

Lemma 8 *Let Ω be a simply-connected, bounded open set with Lipschitz boundary. There exists a constant $D > 0$, depending only on Ω , and a constant $r_0 > 0$ such that for all $r < r_0$ and for any $x^0 \in \partial\Omega$, we have:*

$$\mathcal{H}^2(\partial\Omega \cap B_r(x^0)) \leq Dr^2. \quad (79)$$

Proof. Since Ω has Lipschitz boundary, we have that for any $x^0 \in \partial\Omega$, there exists a $\lambda(x^0) > 0$ and an orthonormal coordinate system $X = (x_1, x_2, x_3)$ such that $x^0 = (0, 0, 0)$ and there exists a Lipschitz function, $f_{x^0} : \mathbb{R}^2 \rightarrow \mathbb{R}$, with the property

$$\mathcal{U}_{x^0} \stackrel{\text{def}}{=} \{x \in \Omega, |x_i| < \lambda(x^0), i = 1, 2, 3\} = \{x \in \mathbb{R}^3, x_3 < f_{x^0}(x_1, x_2), |x_i| < \lambda(x^0), i = 1, 2, 3\}.$$

As Ω is bounded, it is necessarily uniformly Lipschitz (see for instance [10]). Hence, for each $x^0 \in \partial\Omega$, we can choose the system of coordinates as before such that there exists a constant $\bar{c} > 0$, independent of x^0 , so that $\|\nabla f_{x^0}\| \leq \bar{c}, \forall x^0 \in \partial\Omega$.

Letting $r_0 \stackrel{\text{def}}{=} \lambda$ we have:

$$\mathcal{H}^2(\partial\Omega \cap B_r(x^0)) \leq \int_{[-r,r]^2} \sqrt{1 + |\nabla f_{x^0}(x_1, x_2)|^2} dx_1 dx_2 \leq \int_{[-r,r]^2} \sqrt{1 + \bar{c}^2} dx_1 dx_2 = 4\sqrt{1 + \bar{c}^2} r^2$$

$\forall r < r_0$. \square

We have a boundary analogue of the interior monotonicity lemma, *Lemma 2*, namely :

Lemma 9 (*boundary monotonicity*) *Let Ω be a simply-connected bounded open set with smooth boundary. Let $Q^{(L)}$ be a global minimizer of $F_{LG}[Q]$ in the admissible class \mathcal{A}_Q . Let*

$$\mathcal{E}_r = \frac{1}{r} \int_{\Omega_r} \frac{|\nabla Q^{(L)}|^2}{2} + \frac{\tilde{f}_B(Q^{(L)})}{L} dV \quad (80)$$

Then there exists $r_0 > 0$ so that

$$\frac{d}{dr} \mathcal{E}_r \geq -C(a^2, b^2, c^2, Q_b, r_0, \Omega), \forall 0 < r < r_0 \quad (81)$$

where the positive constant C is independent of L .

Proof. *Step 1* We assume that the domain Ω is star-shaped. Then the proof of (81) closely follows the arguments in [20] combined with an idea from [3].

Recall that $Q^{(L)}$ satisfies the equation:

$$\Delta Q_{ij}^{(L)} = \frac{1}{L} \left[\frac{\partial \tilde{f}_B(Q^{(L)})}{\partial Q_{ij}^{(L)}} + b^2 \frac{\delta_{ij}}{3} \text{tr}(Q^{(L)})^2 \right] \quad (82)$$

In what follows, we drop the superscript L for convenience.

We multiply both sides of (82) by $(x_p - x_p^0)Q_{ij,p}$ and integrate over Ω_r . Then

$$\int_{\Omega_r} Q_{ij,kk}(x_p - x_p^0)Q_{ij,p} dx = \int_{\partial\Omega_r} Q_{ij,k}Q_{ij,p}(x_p - x_p^0)n_k d\sigma - \int_{\Omega_r} |\nabla Q|^2 + Q_{ij,k}Q_{ij,kp}(x_p - x_p^0) dx \quad (83)$$

where n is the unit outward normal to $\partial\Omega_r$ and $d\sigma$ is the area element on $\partial\Omega_r$.

The integral $\int_{\partial\Omega_r} Q_{ij,k}Q_{ij,p}(x_p - x_p^0)n_k d\sigma$ is evaluated by considering the contributions from $\partial\Omega \cap B_r(x^0)$ and $\Omega \cap \partial B_r(x^0)$ separately. On $\Omega \cap \partial B_r$, $n(x) = \frac{x - x^0}{|x - x^0|}$ so that

$$\int_{\Omega \cap \partial B_r} Q_{ij,k}Q_{ij,p}(x_p - x_p^0)n_k d\sigma = \int_{\Omega \cap \partial B_r} r \left| \frac{\partial Q}{\partial n} \right|^2 d\sigma.$$

Similarly

$$\int_{\partial\Omega\cap B_r} Q_{ij,k}Q_{ij,p}(x_p - x_p^0)n_k d\sigma = \int_{\partial\Omega\cap B_r} (x - x^0) \cdot n \left| \frac{\partial Q}{\partial n} \right|^2 + (x - x^0) \cdot \tau \frac{\partial Q_b}{\partial \tau} \cdot \frac{\partial Q}{\partial n} d\sigma$$

where $\tau(x) \in \mathbb{S}^2$ is the tangential direction to the boundary at $x \in \partial\Omega$.

In order to estimate $\int_{\Omega_r} Q_{ij,k}Q_{ij,kp}(x_p - x_p^0) dx$ we note that

$$Q_{ij,k}Q_{ij,kp}(x_p - x_p^0) = \frac{\partial}{\partial x_p} \left[(x_p - x_p^0) \frac{1}{2} |\nabla Q|^2 \right] - \frac{3}{2} |\nabla Q|^2$$

and therefore

$$\int_{\Omega_r} |\nabla Q|^2 + Q_{ij,k}Q_{ij,kp}(x_p - x_p^0) dx = \int_{\partial\Omega_r} (x_p - x_p^0) \frac{1}{2} |\nabla Q|^2 n_p d\sigma - \int_{\Omega_r} \frac{1}{2} |\nabla Q|^2 dx.$$

The surface integral over $\partial\Omega_r$ can again be expressed in terms of separate contributions from $\partial\Omega \cap B_r(x^0)$ and $\Omega \cap \partial B_r(x^0)$.

Combining the above, we have

$$\begin{aligned} \int_{\Omega_r} Q_{ij,kk}(x_p - x_p^0)Q_{ij,p} dx &= \int_{\Omega_r} \frac{|\nabla Q|^2}{2} dx + r \left(\int_{\Omega\cap\partial B_r} \left| \frac{\partial Q}{\partial n} \right|^2 - \frac{|\nabla Q|^2}{2} d\sigma \right) + \\ &+ \int_{\partial\Omega\cap B_r} (x - x^0) \cdot n \left[\frac{1}{2} \left| \frac{\partial Q}{\partial n} \right|^2 - \frac{1}{2} \left| \frac{\partial Q_b}{\partial \tau} \right|^2 \right] d\sigma + \int_{\partial\Omega\cap B_r} (x - x^0) \cdot \tau \frac{\partial Q_b}{\partial \tau} \cdot \frac{\partial Q}{\partial n} d\sigma. \end{aligned} \quad (84)$$

In (84), we use the fact that $|\nabla Q|^2 = \left| \frac{\partial Q}{\partial n} \right|^2 + \left| \frac{\partial Q_b}{\partial \tau} \right|^2$ on $\partial\Omega$.

Using the same sort of arguments as above, we compute

$$\frac{1}{L} \int_{\Omega_r} \frac{\partial \tilde{f}_B}{\partial Q_{ij}}(x_p - x_p^0)Q_{ij,p} dx = \frac{1}{L} \int_{\Omega_r} \frac{\partial}{\partial x_p} \left[\tilde{f}_B(Q)(x_p - x_p^0) \right] - 3\tilde{f}_B(Q) dx \quad (85)$$

where $\tilde{f}_B(Q) = \tilde{f}_B(Q_b) = 0$ on $\partial\Omega$ (from our choice of the boundary condition Q_b in (11)).

Equating (84) and (85) we obtain

$$\begin{aligned} &\int_{\Omega_r} \frac{|\nabla Q|^2}{2} dx + r \left(\int_{\Omega\cap\partial B_r} \left| \frac{\partial Q}{\partial n} \right|^2 - \frac{|\nabla Q|^2}{2} d\sigma \right) + \\ &+ \int_{\partial\Omega\cap B_r} (x - x^0) \cdot n \left[\frac{1}{2} \left| \frac{\partial Q}{\partial n} \right|^2 - \frac{1}{2} \left| \frac{\partial Q_b}{\partial \tau} \right|^2 \right] d\sigma + \int_{\partial\Omega\cap B_r} (x - x^0) \cdot \tau \frac{\partial Q_b}{\partial \tau} \cdot \frac{\partial Q}{\partial n} d\sigma = \\ &= \int_{\Omega\cap\partial B_r} r \frac{\tilde{f}_B(Q)}{L} d\sigma - 3 \int_{\Omega_r} \frac{\tilde{f}_B(Q)}{L} dx. \end{aligned} \quad (86)$$

We multiply both sides of (86) by $\frac{1}{r^2}$ and after some re-arrangement, obtain

$$\begin{aligned} &-\frac{1}{r^2} \int_{\Omega_r} \frac{|\nabla Q|^2}{2} + \frac{\tilde{f}_B(Q)}{L} dx + \frac{1}{r} \int_{\Omega\cap\partial B_r} \frac{|\nabla Q|^2}{2} + \frac{\tilde{f}_B(Q)}{L} d\sigma = \\ &= \frac{1}{r} \int_{\Omega\cap\partial B_r} \left| \frac{\partial Q}{\partial n} \right|^2 d\sigma + \frac{2}{r^2} \int_{\Omega_r} \frac{\tilde{f}_B(Q)}{L} dx + \\ &+ \frac{1}{2r^2} \int_{\partial\Omega\cap B_r} (x - x^0) \cdot n \left[\left| \frac{\partial Q}{\partial n} \right|^2 - \left| \frac{\partial Q_b}{\partial \tau} \right|^2 \right] d\sigma + \frac{1}{r^2} \int_{\partial\Omega\cap B_r} (x - x^0) \cdot \tau \frac{\partial Q_b}{\partial \tau} \cdot \frac{\partial Q}{\partial n} d\sigma. \end{aligned} \quad (87)$$

For a star-shaped domain $(x - x^0) \cdot n \geq 0$ on $\partial\Omega$. Therefore, the negative contributions to the right hand side of (87) are $-\frac{1}{2r^2} \int_{\partial\Omega \cap B_r} (x - x^0) \cdot n \left| \frac{\partial Q_b}{\partial \tau} \right|^2 d\sigma$ and potentially $\frac{1}{r^2} \int_{\partial\Omega \cap B_r} (x - x^0) \cdot \tau \frac{\partial Q_b}{\partial \tau} \cdot \frac{\partial Q}{\partial n} d\sigma$. The first integral can be easily estimated since Q_b is known. Using the fact that $\left| \frac{\partial Q_b}{\partial \tau} \right|^2 \leq Cs_+^2$ for some $C > 0$ (as $Q_b \in C^\infty(\partial\Omega)$ by hypothesis) where s_+ is defined in (10), we have that

$$\frac{1}{2r^2} \int_{\partial\Omega \cap B_r} |(x - x^0) \cdot n| \left| \frac{\partial Q_b}{\partial \tau} \right|^2 d\sigma \leq Cr s_+^2. \quad (88)$$

Here we have used $|(x - x^0) \cdot n| \leq r$ and *Lemma 8*.

Using Cauchy-Schwarz, we have

$$\frac{1}{r^2} \int_{\partial\Omega \cap B_r} (x - x^0) \cdot \tau \frac{\partial Q_b}{\partial \tau} \cdot \frac{\partial Q}{\partial n} d\sigma \leq \frac{1}{r} \left(\int_{\partial\Omega \cap B_r} \left| \frac{\partial Q_b}{\partial \tau} \right|^2 d\sigma \right)^{1/2} \left(\int_{\partial\Omega \cap B_r} \left| \frac{\partial Q}{\partial n} \right|^2 d\sigma \right)^{1/2}. \quad (89)$$

The first integral on the right hand side is easily dealt with i.e. $\int_{\partial\Omega \cap B_r} \left| \frac{\partial Q_b}{\partial \tau} \right|^2 d\sigma \leq Cs_+^2 r^2$, from *Lemma 8*.

The second integral involving $\left| \frac{\partial Q}{\partial n} \right|^2$ is estimated using *Lemma 10*:

$$\int_{\partial\Omega \cap B_r} \left| \frac{\partial Q}{\partial n} \right|^2 d\sigma \leq G(Q_b, \Omega)$$

where $G > 0$ is a constant independent of L .

Combining the above we have that

$$-\frac{1}{r^2} \int_{\Omega_r} \frac{|\nabla Q|^2}{2} + \frac{\tilde{f}_B(Q)}{L} dx + \frac{1}{r} \int_{\Omega \cap \partial B_r} \frac{|\nabla Q|^2}{2} + \frac{\tilde{f}_B(Q)}{L} d\sigma \geq -Cr s_+^2 - G'(a^2, b^2, c^2, \Omega) \quad (90)$$

where C and G' are positive constants independent of L . We note that

$$\frac{d}{dr} \mathcal{E}_r = -\frac{1}{r^2} \int_{\Omega_r} \frac{|\nabla Q|^2}{2} + \frac{\tilde{f}_B(Q)}{L} dx + \frac{1}{r} \int_{\Omega \cap \partial B_r} \frac{|\nabla Q|^2}{2} + \frac{\tilde{f}_B(Q)}{L} d\sigma \quad (91)$$

and the above holds for any $0 < r < r_0$ where r_0 is the constant from *Lemma 8*. Therefore

$$\frac{d}{dr} \mathcal{E}_r \geq -G''(a^2, b^2, c^2, Q_b, r_0, \Omega)$$

where $G'' > 0$ is independent of L .

Step 2: General domain Ω .

We do not assume that the domain Ω is star-shaped and take into account the perturbation terms induced by omitting this assumption. As in [20], the boundary regularity of the domain implies that

$$(x - x^0) \cdot n \geq |(x - x^0) \cdot n| - cr^2 \quad (92)$$

where $c > 0$ is independent of r or $x^0 \in \partial\Omega$. Then

$$\frac{1}{2r^2} \int_{\partial\Omega \cap B_r} (x - x^0) \cdot n \left| \frac{\partial Q}{\partial n} \right|^2 d\sigma \geq \frac{1}{2r^2} \int_{\partial\Omega \cap B_r} |(x - x^0) \cdot n| \left| \frac{\partial Q}{\partial n} \right|^2 d\sigma - \frac{c}{2} \int_{\partial\Omega \cap B_r} \left| \frac{\partial Q}{\partial n} \right|^2 d\sigma. \quad (93)$$

The inequality (81) now follows from *Lemma 10*. \square

Lemma 10 *Let $Q^{(L)}$ be a minimizer of $\tilde{F}_{LG}[Q]$ in \mathcal{A}_Q (see (12)) for a fixed $L > 0$. Then*

$$\int_{\partial\Omega} \left| \frac{\partial Q^{(L)}}{\partial n} \right|^2 d\sigma \leq G(Q_b, \Omega) \quad (94)$$

where $G > 0$ only depends on the boundary condition Q_b and Ω .

Proof. The proof follows closely the arguments of Proposition 3 in [3]. Let $V : \Omega \rightarrow \mathbb{R}^3$ be a smooth vector field on Ω such that $V = n$ on $\partial\Omega$. We drop the superscript L for convenience. We multiply (14) by $V_p Q_{ij,p}$ and note that

$$\int_{\Omega} Q_{ij,kk} Q_{ij,p} V_p \, dx = \int_{\partial\Omega} \left| \frac{\partial Q}{\partial n} \right|^2 \, d\sigma - \int_{\Omega} Q_{ij,k} \frac{\partial}{\partial x_k} (Q_{ij,p} V_p) \, dx. \quad (95)$$

Proceeding similarly as in [3], we have that

$$\begin{aligned} \int_{\Omega} Q_{ij,k} \frac{\partial}{\partial x_k} (Q_{ij,p} V_p) \, dx &= \int_{\Omega} Q_{ij,k} Q_{ij,kp} V_p + \int_{\Omega} Q_{ij,k} Q_{ij,k} \frac{\partial V_p}{\partial x_p} \, dx \\ &= \int_{\partial\Omega} \frac{|\nabla Q|^2}{2} \, d\sigma + O(s_+^2), \quad \text{as } L \rightarrow 0 \end{aligned} \quad (96)$$

Thus,

$$\int_{\Omega} Q_{ij,kk} Q_{ij,p} V_p \, dx = \int_{\partial\Omega} \left| \frac{\partial Q}{\partial n} \right|^2 \, d\sigma - \int_{\partial\Omega} \frac{|\nabla Q|^2}{2} \, d\sigma + O(s_+^2), \quad \text{as } L \rightarrow 0 \quad (97)$$

On the other hand,

$$\frac{1}{L} \int_{\Omega} Q_{ij,p} V_p \frac{\partial \tilde{f}_B(Q)}{\partial Q_{ij}} \, dx = -\frac{1}{L} \int_{\Omega} \tilde{f}_B(Q) \nabla \cdot V \, dx \leq O(s_+^2), \quad \text{as } L \rightarrow 0 \quad (98)$$

since $\frac{1}{L} \int_{\Omega} \tilde{f}_B(Q) \, dV \leq C(\Omega) s_+^2$ from energy minimality and $\tilde{f}_B(Q_b) = 0$ by our choice of Q_b .

Equating (97) and (98), we obtain

$$\int_{\partial\Omega} \left| \frac{\partial Q}{\partial n} \right|^2 \, d\sigma - \int_{\partial\Omega} \frac{|\nabla Q|^2}{2} \, d\sigma = \frac{1}{2} \int_{\partial\Omega} \left| \frac{\partial Q}{\partial n} \right|^2 - \left| \frac{\partial Q_b}{\partial \tau} \right|^2 \, d\sigma \leq C(\Omega) s_+^2 \quad (99)$$

and (94) now follows. \square

We now prove the uniform convergence of the bulk energy density, $\tilde{f}_B(Q^{(L)})$, to its minimal value, on compact subsets, $K \subset \bar{\Omega}$, that do not contain defects of the limiting harmonic map $Q^{(0)}$. This extends the result in Proposition 4 where the uniform convergence is proven only for $K \subset \Omega$.

Proposition 6 *Let $Q^{(L)}$ denote a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible space \mathcal{A}_Q defined in (12). Consider a sequence $\{Q^{(L_k)}\}_{k \in \mathbb{N}}$ which converges to a limiting harmonic map $Q^{(0)}$ strongly in $W^{1,2}(\Omega, S_0)$ as $L_k \rightarrow 0$.*

Let $x^0 \in \partial\Omega$ be a boundary point. We assume that the region Ω_r in (78) contains no singularity of the limiting harmonic map $Q^{(0)}$. Then

$$\lim_{L_k \rightarrow 0} \tilde{f}_B(Q^{(L_k)}(x)) = 0 \quad \forall x \in \Omega_r \quad (100)$$

and the limit is uniform on Ω_r .

Proof. We set $\alpha = \tilde{f}_B(Q^{(L_k)}(x^0)) \geq 0$. Consider the region $\Omega_\rho \subset \Omega_r$ where $\rho < r \leq r_0$ (here r_0 is the constant from Lemmas 8 and 9). Then the boundary monotonicity inequality (81) implies that

$$\mathcal{E}_\rho \leq \mathcal{E}_r + C(a^2, b^2, c^2, Q_b, \Omega)(r - \rho) \quad (101)$$

for $\rho < r < r_0$.

Take an arbitrary $\varepsilon > 0$. Recall that $Q^{(L_k)} \rightarrow Q^{(0)}$ in $W^{1,2}$ as $L_k \rightarrow 0$ and Ω_r contains no singularities of $Q^{(0)}$. Using the same arguments as in Proposition 4, we have that there exists an $r_1 < \min\{r_0, \varepsilon\}$ and $\bar{L} > 0$ (both depending on ε) so that for $L_k < \bar{L}$

$$\frac{1}{r_1} \int_{\Omega_{r_1}} \frac{1}{2} |\nabla Q^{(L_k)}|^2 \, dx \leq \varepsilon$$

Similarly, we have that there exists an $\tilde{L} > 0$ (depending on ε) so that

$$\frac{1}{r_1} \int_{\Omega_{r_1}} \frac{\tilde{f}_B(Q^{(L_k)})}{L_k} dV \leq \varepsilon$$

for $L_k < \tilde{L}$ (see the proof of Lemma 3). Combining the above, we obtain

$$\frac{1}{\rho} \int_{\Omega_\rho} \frac{\tilde{f}_B(Q^{(L_k)})}{L_k} dx \leq \mathcal{E}_\rho \leq C' \varepsilon \quad (102)$$

for any $\rho < r_1$ and for $L_k < \min\{\bar{L}, \tilde{L}\}$ where the constant $C' > 0$ is independent of L_k .

Using arguments very close to those in [3] (Lemma A.2 and the way it is used in Step B.1 of the proof of Theorem 1) together with Proposition 3, one can easily obtain:

$$\|\nabla Q^{(L_k)}\|_{L^\infty(\Omega)} \leq \frac{H(a^2, b^2, c^2, \Omega)}{\sqrt{L_k}}. \quad (103)$$

On the other hand, $\tilde{f}_B(Q)$ is a Lipschitz function of the Q -tensor and one can infer the following from (103) and Proposition 3:

$$\|\nabla \tilde{f}_B(Q^{(L_k)})\|_{L^\infty} \leq \frac{D(a^2, b^2, c^2, \Omega)}{\sqrt{L_k}} \quad (104)$$

so that

$$\tilde{f}_B(Q^{(L_k)}(x)) \geq \alpha - \frac{D(a^2, b^2, c^2, \Omega)}{\sqrt{L_k}} \rho \quad \forall x \in \Omega_\rho. \quad (105)$$

We take

$$\rho = \frac{\alpha \sqrt{L_k}}{2D(a^2, b^2, c^2, \Omega)}.$$

There exists a constant $\gamma(\Omega)$ so that

$$|\Omega_\rho| \geq \gamma(\Omega) \rho^3$$

(see also [3] for the 2D version of the above) Combining the above with (105), we obtain the following inequality

$$\frac{1}{\rho} \int_{\Omega_\rho} \frac{\tilde{f}_B(Q^{(L_k)})}{L_k} dx \geq \frac{\gamma \rho^2}{L_k} \left(\alpha - \frac{D(a^2, b^2, c^2, \Omega)}{\sqrt{L_k}} \rho \right) = \gamma \frac{\alpha^3}{D'(a^2, b^2, c^2, \Omega)} \quad (106)$$

where the constant $D' > 0$ is independent of L_k . Combining (102) and (106), we have that

$$\alpha^3 \leq D''(a^2, b^2, c^2, Q_b, \Omega) \varepsilon \quad (107)$$

where $D'' > 0$ is independent of L_k . The upper bound (107) is independent of x^0 and $\varepsilon > 0$ was chosen arbitrarily. Therefore, Proposition 6 now follows. \square

5 Consequences of the convergence results

In this section, we discuss some consequences of the convergence results in Propositions 4, 5, and 6. We consider a sequence of global minimizers $\{Q^{(L_k)}\}_{k \in \mathbb{N}}$ converging to a limiting harmonic map $Q^{(0)}$. From Proposition 5, we have that for a ball $B(x, r_0) \subset \Omega$, where $B(x, r_0)$ does not contain any singularities of $Q^{(0)}$

$$\left| Q^{(L_k)}(y) - Q^{(0)}(y) \right| \leq \varepsilon(L_k) \quad y \in B(x, r_0) \quad (108)$$

where $\epsilon(L_k) \rightarrow 0^+$ as $L_k \rightarrow 0$. Further, the small energy regularity in Lemma 7 implies that for L_k sufficiently small,

$$e_{L_k} \left(Q^{(L_k)}(y) \right) = \frac{\tilde{f}_B(Q^{(L_k)}(y))}{L_k} + \frac{1}{2} \left| \nabla Q^{(L_k)}(y) \right|^2 \leq C(a^2, b^2, c^2, \Omega) \quad y \in B(x, r_0) \quad (109)$$

where $C > 0$ is a positive constant independent of L_k . Therefore, for sufficiently small L_k , one has

$$\begin{aligned} |\nabla Q^{(L_k)}(y)|^2 &\leq C(a^2, b^2, c^2, \Omega) \\ \tilde{f}_B(Q^{(L_k)}(y)) &\leq C(a^2, b^2, c^2, \Omega) L_k \quad y \in B(x, r_0). \end{aligned} \quad (110)$$

One immediate consequence of the uniform convergence in (108) and the bounds in (110) is the following

Lemma 11 *Let $Q^{(L)}$ denote a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible class \mathcal{A}_Q . Consider a sequence $\{Q^{(L_k)}\}_{k \in \mathbb{N}}$ which converges to a limiting harmonic map $Q^{(0)}$ strongly in $W^{1,2}(\Omega, S_0)$ as $L_k \rightarrow 0$. Let $x \in \bar{\Omega}$ be such that $B(x, r_0) \cap \bar{\Omega}$ (for r_0 smaller than the r_0 used in Lemma 8), does not contain any singularities of the limiting map $Q^{(0)}$. Then*

$$\begin{aligned} Q^{(L_k)}(y) &= S^{(L_k)} \left(n^{(L_k)} \otimes n^{(L_k)} - \frac{1}{3} Id \right) + R^{(L_k)} \left(m^{(L_k)} \otimes m^{(L_k)} - p^{(L_k)} \otimes p^{(L_k)} \right) \\ \text{where } |S^{(L_k)} - s_+| &\leq \epsilon_1(L_k), \quad |R^{(L_k)}| \leq \epsilon_2(L_k) \end{aligned} \quad (111)$$

with $n^{(L_k)}, m^{(L_k)}$ and $p^{(L_k)}$ unit eigenvectors of $Q^{(L_k)}$, and $\epsilon_1(L_k), \epsilon_2(L_k) \rightarrow 0^+$ as $L_k \rightarrow 0$. Secondly, if $x \in \Omega$ is an interior point such that $B(x, r_0) \subset \Omega$ does not contain any singularities of $Q^{(0)}$, then we also have that

$$(n^{(L_k)} \cdot n^{(0)})^2 \geq 1 - \epsilon_3(L_k) \quad (112)$$

where $\epsilon_3(L_k) \rightarrow 0^+$ as $L_k \rightarrow 0$ and $n^{(0)}$ has been defined in (16).

Proof The representation (111) is a direct consequence of Propositions 2, 4 and 6. In the following we drop the superscripts L_k for convenience, but keep the superscript 0 in $Q^{(0)}$ and $n^{(0)}$. From Proposition 4 and Proposition 6, we have that

$$\tilde{f}_B(Q(y)) \rightarrow 0 \quad \text{as } L_k \rightarrow 0$$

for $y \in B(x, r_0) \cap \bar{\Omega}$ where $B(x, r_0) \cap \bar{\Omega}$ does not contain any singularities of $Q^{(0)}$. The bulk energy density $\tilde{f}_B(Q)$ is a smooth function of the order parameters (S, R) in Proposition 2. Therefore, as $\tilde{f}_B(Q(y)) \rightarrow 0$, the corresponding order parameters (S, R) approach the bulk energy minimum defined by $(S, R) = (s_+, 0)$ and the inequalities (111) follow. Further, if $B(x, r_0) \subset \Omega$, then the uniform convergence (108) holds. A direct computation shows that for

$$Q = S \left(n \otimes n - \frac{1}{3} Id \right) + R (m \otimes m - p \otimes p),$$

we have

$$\left| Q(y) - Q^{(0)}(y) \right|^2 = \frac{2}{3} (S^2 + s_+^2) - 2Ss_+ \left[(n \cdot n^{(0)})^2 - \frac{1}{3} \right] + 2R^2 - 2s_+R \left((m \cdot n^{(0)})^2 - (p \cdot n^{(0)})^2 \right).$$

The lower bound on $(n \cdot n^{(0)})^2$ now follows from (108) and the fact that $|S - s_+| \leq \epsilon_1(L_k), |R| \leq \epsilon_2(L_k)$ for sufficiently small values of L_k . \square

Proposition 7 *Let $Q^{(L)}$ denote a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible space \mathcal{A}_Q . Consider a sequence $\{Q^{(L_k)}\}_{k \in \mathbb{N}}$ which converges to a limiting harmonic map $Q^{(0)}$ strongly in $W^{1,2}(\Omega, S_0)$ as $L_k \rightarrow 0$. Then $Q^{(L_k)}$ converges uniformly to the limiting harmonic map $Q^{(0)}$, away from the singular set of $Q^{(0)}$, in the interior of Ω . Let $K \subset \Omega$ be an interior subset that does not contain any singularities of $Q^{(0)}$. Then (i)*

$$\begin{aligned} \beta(Q^{(L_k)}(y)) &\leq CL_k \\ \left| Q^{(L_k)}(y) - \sqrt{\frac{2}{3}} s_+ \right| &\leq D\sqrt{L_k} \quad y \in K \end{aligned} \quad (113)$$

where C and D are positive constants independent of L_k . (ii)(rate of convergence of eigenvalues) Let $\{\lambda_i^{(L_k)}\}$ denote the set of eigenvalues of $Q^{(L_k)}$ and $\{\lambda_i\}$ denote the set of eigenvalues of $Q^{(0)}$. Then

$$\left| \lambda_i^{(L_k)}(y) - \lambda_i(y) \right|^2 \leq \alpha(a^2, b^2, c^2) L_k \quad y \in K; \quad i = 1 \dots 3 \quad (114)$$

where α is a positive constant independent of L_k .

Proof (i) This follows directly from (110) and Proposition 9. In Proposition 9, we obtain a lower bound for $\tilde{f}_B(Q)$ in terms of $|Q|$ and β and in (110) we have an upper bound for $\tilde{f}_B(Q)$ in terms of L_k as shown below

$$\left[\frac{\frac{2}{3}c^2s_+^2 + a^2}{2} \right] \left(|Q| - \sqrt{\frac{2}{3}}s_+ \right)^2 + \frac{b^2}{6\sqrt{6}}\beta(Q)|Q|^3 \leq \tilde{f}_B(Q(y)) \leq C(a^2, b^2, c^2, \Omega) L_k \quad y \in K$$

(ii) In the following we drop the superscripts “ (L_k) ” for convenience. From (110), we have the following upper bound for the bulk energy density on the set $K \subset \Omega$

$$\tilde{f}_B(Q(y)) \leq C L_k \quad y \in K$$

where C is a positive constant independent of L_k . Using the representation formula (111), we have that

$$Q = S \left(n \otimes n - \frac{1}{3} Id \right) + R (m \otimes m - p \otimes p) \quad (115)$$

where

$$|S - s_+| \leq \epsilon_4(L_k) = o(1) \quad (116)$$

and

$$|R| \leq \epsilon_5(L_k) = o(1). \quad (117)$$

A direct computation shows that

$$Q_{ij}Q_{ij} = \frac{2}{3}S^2 + 2R^2 \quad Q_{ip}Q_{pj}Q_{ij} = \frac{2S^3}{9} - 2SR^2. \quad (118)$$

From (116) and (117), we represent Q on the subset $K \subset \Omega$ as follows:

$$Q = (s_+ + \epsilon) \left(n \otimes n - \frac{1}{3} Id \right) + \gamma (m \otimes m - p \otimes p) \quad (119)$$

where $|\epsilon|, |\gamma| = o(1)$. Using (118), we find that

$$|Q|^2 = \frac{2}{3} (s_+^2 + \epsilon^2 + 2s_+\epsilon) + 2\gamma^2$$

and from the maximum principle (Proposition 3),

$$|Q(x)|^2 \leq \frac{2}{3}s_+^2 \quad x \in K.$$

This necessarily implies that $\epsilon \leq 0$.

The bulk energy density \tilde{f}_B is given by

$$\tilde{f}_B(Q) = \frac{a^2}{3} (s_+^2 - S^2) + \frac{2b^2}{27} (s_+^3 - S^3) - \frac{c^2}{9} (s_+^4 - S^4) - a^2R^2 + \frac{2b^2}{3}SR^2 + \frac{2c^2}{3}S^2R^2 + c^2R^4 \quad (120)$$

where we have merely expressed $\text{tr}Q^2$ and $\text{tr}Q^3$ in terms of the order parameters S and R . We write the bulk energy density as the sum of two contributions -

$$\tilde{f}_B(Q) = F(S) + G(S, R) \quad (121)$$

where

$$F(S) = \frac{a^2}{3} (s_+^2 - S^2) + \frac{2b^2}{27} (s_+^3 - S^3) - \frac{c^2}{9} (s_+^4 - S^4)$$

and

$$G(S, R) = -a^2 R^2 + \frac{2b^2}{3} S R^2 + \frac{2c^2}{3} S^2 R^2 + c^2 R^4.$$

The function $F(S)$ is analyzed in (149); the function $F(S)$ is bounded from below by

$$F(S) \geq D(a^2, b^2, c^2) (S - s_+)^2, \quad D(a^2, b^2, c^2) \geq 0 \quad (122)$$

Similarly, since $2c^2 s_+^2 = b^2 s_+ + 3a^2$ and $0 < s_+ - S = o(1)$ (for L_k sufficiently small), we have the following inequality

$$-a^2 R^2 + \frac{2b^2}{3} S R^2 + \frac{2c^2}{3} S^2 R^2 \geq \frac{b^2 s_+}{2} \gamma^2. \quad (123)$$

Combining (122), (123) and (110), we obtain the following

$$D(a^2, b^2, c^2) \epsilon^2 + \frac{b^2}{2} s_+ \gamma^2 + c^2 \gamma^4 \leq \tilde{f}_B(Q(x)) \leq C L_k \quad (124)$$

from which we deduce

$$\epsilon^2 \leq C_1 L_k \quad \text{and} \quad \gamma^2 \leq C_2 L_k,$$

where C_1, C_2 are positive constants independent of L_k . The inequalities (114) now follow. \square

Next, we have a lemma about the leading eigenvector n in the representation (111).

Lemma 12 *Let $Q = S(n \otimes n - \frac{1}{3} Id) + R(m \otimes m - p \otimes p)$ with $S > 8|R|$ and $n, m, p \in \mathbb{S}^2$, pairwise perpendicular. Then the minimum of*

$$\left| Q - s_+ \left(a \otimes a - \frac{1}{3} Id \right) \right|^2$$

with $a \in \mathbb{S}^2$ is attained by $a = \pm n$.

Proof. A direct computation shows that

$$\begin{aligned} \left| Q - s_+ \left(a \otimes a - \frac{1}{3} Id \right) \right|^2 &= \frac{2}{3} (S^2 + s_+^2 + S s_+) + 2R^2 - 2S s_+ (n \cdot a)^2 - 2s_+ R \left((m \cdot a)^2 - (p \cdot a)^2 \right) \\ &= \frac{2}{3} (S^2 + s_+^2 + S s_+) + 2R^2 + 2s_+ R - 2s_+ (S + R) (n \cdot a)^2 - 4s_+ R (m \cdot a)^2 \end{aligned} \quad (125)$$

where in the last line of (125), we use the equality $(n \cdot a)^2 + (m \cdot a)^2 + (p \cdot a)^2 = 1$. Since $S > 8|R|$, one can immediately verify that (125) is minimized for $(n \cdot a)^2 = 1$ or equivalently $a = \pm n$. \square

We can now provide a result about the regularity the leading ‘‘eigendirection’’ $n \otimes n \in M^{3 \times 3}$ where $n \in \mathbb{S}^2$ is the leading eigenvector. For a thorough discussion about the relationships between the regularity of the eigenvector $n \in \mathbb{S}^2$ and that of the eigendirection $n \otimes n \in M^{3 \times 3}$ see [2].

Corollary 1 *Let $Q^{(L)}$ denote a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible class \mathcal{A}_Q . Consider a sequence $\{Q^{(L_k)}\}_{k \in \mathbb{N}}$ which converges to a limiting harmonic map $Q^{(0)}$ strongly in $W^{1,2}(\Omega, S_0)$ as $L_k \rightarrow 0$. Let $K \subset \Omega$ be a compact subset of Ω that does not contain singularities of the limiting map $Q^{(0)}$. Then, for L_k small enough (depending on K), $Q^{(L_k)}$ can be represented as in (111) on the set $K \subset \Omega$ and the leading eigendirection $n^{(L_k)} \otimes n^{(L_k)} \in C^\infty(K; M^{3 \times 3})$.*

Proof From (111), we can represent $Q^{(L_k)}$ as

$$Q^{(L_k)}(x) = S^{(L_k)} \left(n^{(L_k)} \otimes n^{(L_k)} - \frac{1}{3} Id \right) + R^{(L_k)} \left(m^{(L_k)} \otimes m^{(L_k)} - p^{(L_k)} \otimes p^{(L_k)} \right)$$

where $|S^{(L_k)} - s_+| = o(1)$, $|R^{(L_k)}| = o(1)$, and $n^{(L_k)}, m^{(L_k)}, p^{(L_k)} \in \mathbb{S}^2$ are the eigenvectors of $Q^{(L_k)}$.

Let $\pi(Q)$ be the nearest neighbor projection onto the manifold of global minimizers of the bulk energy density, denoted by $Q_{\min} = \{s_+ (a \otimes a - \frac{1}{3} Id), a \in \mathbb{S}^2\}$ as in (9). Namely, $\pi(Q)$ associates with each Q' , (in a neighborhood of the manifold Q_{\min}) an element $Q^* \in Q_{\min}$ such that

$$|Q' - Q^*| = \min_{Q \in Q_{\min}} |Q' - Q|.$$

The projection π is defined only in a neighborhood of the manifold Q_{\min} and moreover $\pi(Q') \in C^\infty(S_0, Q_{\min})$ (see, for instance, [6]). The Lemma 11 and Lemma 12 show that in our case

$$\pi(Q^{(L_k)}) = s_+ \left(n^{(L_k)} \otimes n^{(L_k)} - \frac{1}{3} Id \right).$$

Therefore, the tensor

$$(n^{(L_k)} \otimes n^{(L_k)} - \frac{1}{3} Id) \in C^\infty(K, S_0),$$

(since s_+ is a constant) and the conclusion of the lemma now follows. \square

6 Biaxiality and uniaxiality

6.1 The bulk energy density

Our first proposition concerns the stationary points of the bulk energy density.

Proposition 8 [21] *Consider the bulk energy density $\tilde{f}_B(Q)$ given by*

$$\tilde{f}_B(Q) = -\frac{a^2}{2} \text{tr} Q^2 - \frac{b^2}{3} \text{tr} Q^3 + \frac{c^2}{4} (\text{tr} Q^2)^2 + \frac{a^2}{3} s_+^2 + \frac{2b^2}{27} s_+^3 - \frac{c^2}{9} s_+^4. \quad (126)$$

Then $\tilde{f}_B(Q)$ attains its minimum for uniaxial Q -tensors of the form

$$Q = s_+ \left(n \otimes n - \frac{1}{3} \right), \quad (127)$$

where

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2} \quad (128)$$

and $n : \Omega \rightarrow S^2$ is a unit eigenvector of Q .

Proof. Proposition 8 has been proven in [21] and we reproduce the proof in the *Appendix* for completeness. \square

In the following proposition, we estimate $\tilde{f}_B(Q)$ in terms of $|Q|$ and the biaxiality parameter $\beta(Q)$.

Proposition 9 *Let $Q \in S_0$. Then the bulk energy density $\tilde{f}_B(Q)$ is bounded from below by*

$$\tilde{f}_B(Q) \geq \left[\frac{\frac{2}{3}c^2s_+^2 + a^2}{2} \right] \left(|Q| - \sqrt{\frac{2}{3}s_+} \right)^2 + \frac{b^2}{6\sqrt{6}} \beta(Q) |Q|^3 \quad (129)$$

where s_+ has been defined in (128).

Proof. From Lemma 1, we have the inequality,

$$\text{tr}Q^3 = |Q|^3 \sqrt{\left(\frac{1-\beta}{6}\right)} \leq \frac{|Q|^3}{\sqrt{6}} \left(1 - \frac{\beta}{2}\right) \text{ for } Q \in S_0.$$

From the definition of $\tilde{f}_B(Q)$ and s_+ in (126) and (128), we can obtain a lower bound for $\tilde{f}_B(Q)$ in terms of $|Q|$ and $\beta(Q)$ as follows i.e.

$$\tilde{f}_B(Q) = -\frac{a^2}{2}|Q|^2 - \frac{b^2}{3\sqrt{6}}|Q|^3\sqrt{1-\beta} + \frac{c^2}{4}|Q|^4 + \frac{a^2}{2}\left(\sqrt{\frac{2}{3}}s_+\right)^2 + \frac{b^2}{3}\frac{2s_+^3}{9} - \frac{c^2}{4}\left(\sqrt{\frac{2}{3}}s_+\right)^4 \quad (130)$$

$$\geq \left[-\frac{a^2}{2}|Q|^2 - \frac{b^2}{3\sqrt{6}}|Q|^3 + \frac{c^2}{4}|Q|^4 + \frac{a^2}{3}s_+^2 + \frac{2b^2}{27}s_+^3 - \frac{c^2}{9}s_+^4\right] + \frac{b^2}{6\sqrt{6}}\beta(Q)|Q|^3. \quad (131)$$

The bracketed term in (131) can be further simplified by carrying out a series of calculations. Consider the function

$$f(u) = -\frac{a^2}{2}u^2 - \frac{b^2}{3\sqrt{6}}u^3 + \frac{c^2}{4}u^4. \quad (132)$$

The stationary points of $f(u)$ are solutions of the algebraic equation

$$f'(u) = u\left(c^2u^2 - \frac{b^2}{\sqrt{6}}u - a^2\right) = 0 \quad (133)$$

and one can readily verify that $f(u)$ attains its minimum for

$$u_{\min} = \sqrt{\frac{2}{3}}s_+ \quad (134)$$

The bracketed term in (131) is non-negative by virtue of (132)–(134). Further, let $\delta = |Q| - \sqrt{\frac{2}{3}}s_+$ where $c^2\frac{2}{3}s_+^2 = \frac{b^2}{\sqrt{6}}\sqrt{\frac{2}{3}}s_+ + a^2$ by the definition of s_+ . Then

$$\left[-\frac{a^2}{2}|Q|^2 - \frac{b^2}{3\sqrt{6}}|Q|^3 + \frac{c^2}{4}|Q|^4 + \frac{a^2}{3}s_+^2 + \frac{2b^2}{27}s_+^3 - \frac{c^2}{9}s_+^4\right] = \quad (135)$$

$$= \delta \left[-a^2\sqrt{\frac{2}{3}}s_+ - \frac{\sqrt{2}b^2}{3\sqrt{3}}s_+^2 + \frac{2\sqrt{2}}{3\sqrt{3}}c^2s_+^3\right] + \delta^2 \left[-\frac{a^2}{2} - \frac{b^2}{3}s_+ + s_+^2c^2\right] + \delta^3 \left[c^2\sqrt{\frac{2}{3}}s_+ - \frac{b^2}{3\sqrt{6}}\right] + \frac{c^2}{4}\delta^4. \quad (136)$$

The coefficient of δ vanishes from the definition of s_+ in (128). The coefficients of δ^2 and δ^3 are positive since

$$-\frac{a^2}{2} - \frac{b^2}{3}s_+ + s_+^2c^2 \geq \left[\frac{\frac{2}{3}c^2s_+^2 + a^2}{2}\right] \\ \sqrt{\frac{2}{3}}c^2s_+ - \frac{b^2}{3\sqrt{6}} \geq \frac{2b^2}{3\sqrt{6}}. \quad (137)$$

We substitute (137) into (135) to obtain

$$\left[-\frac{a^2}{2}|Q|^2 - \frac{b^2}{3\sqrt{6}}|Q|^3 + \frac{c^2}{4}|Q|^4 + \frac{a^2}{3}s_+^2 + \frac{2b^2}{27}s_+^3 - \frac{c^2}{9}s_+^4\right] \geq \\ \geq \delta^2 \left[\frac{\frac{2}{3}c^2s_+^2 + a^2}{2}\right] \quad (138)$$

and on combining (138) with (131), the lower bound (129) follows. \square

The bulk energy density, $\tilde{f}_B(Q)$, can be equivalently expressed in terms of the order parameters s and r in Proposition 1, as shown below

Proposition 10 *Let $Q \in S_0$ be represented as in Proposition 1*

$$Q = s \left(n \otimes n - \frac{1}{3} Id \right) + r \left(m \otimes m - \frac{1}{3} Id \right)$$

with either $0 \leq r \leq \frac{s}{2}$ or $\frac{s}{2} \leq r \leq 0$. Case (i) Non-negative order parameters, $0 \leq r \leq \frac{s}{2}$ with $0 \leq s \leq s_+$, where s_+ is defined in (128). Then the bulk energy density, $\tilde{f}_B(Q)$, is bounded from below by

$$\tilde{f}_B(Q) \geq (s_+ - s)^2 \gamma(a^2, b^2, c^2) + \frac{r(s-r)}{9} (3a^2 + b^2s - 2c^2s^2) + \frac{5b^2}{27} r^2s \quad 0 \leq s \leq s_+ \quad (139)$$

where $\gamma(a^2, b^2, c^2)$ is an explicitly computable positive constant.

Case (ii) Non-negative order parameters, $0 \leq r \leq \frac{s}{2}$ and $s \geq s_+$. Then

$$\tilde{f}_B(Q) \geq \left[\frac{\frac{2}{3}c^2s_+^2 + a^2}{2} \right] \min \left\{ \frac{2}{3} (s - s_+)^2, \frac{1}{6} (\sqrt{3}s - 2s_+)^2 \right\} + \tau b^2 s_+^3 \left(\frac{r^2(s-r)^2}{s^4} \right) \quad (140)$$

where τ is an explicitly computable positive constant, independent of a^2, b^2, c^2 .

Case (iii) If $\frac{s}{2} \leq r \leq 0$, then

$$\tilde{f}_B(Q) = \tilde{f}_B(-Q) + \frac{2b^2}{27} (2|s|^3 + 2|r|^3 - 3s^2|r| - 3|s|r^2), \quad (141)$$

where $-Q \in S_0$ has positive order parameters $0 \leq -r \leq -\frac{s}{2}$ and $\tilde{f}_B(-Q)$ can be estimated using (139) and (140). In particular,

$$\tilde{f}_B(Q) \geq -\frac{a^4}{4c^2} - \frac{s_+^3}{3} \left(\frac{b^2}{9} - \frac{c^2}{3} s_+ \right) > 0 \quad (142)$$

for Q -tensors with $\frac{s}{2} \leq r \leq 0$.

Proof. From Proposition 1, it suffices to consider the two cases $0 \leq r \leq \frac{s}{2}$ and $\frac{s}{2} \leq r \leq 0$.

Case (i): We can explicitly express the bulk energy density, $\tilde{f}_B(Q)$, in terms of s and r as follows -

$$\begin{aligned} \tilde{f}_B(Q) = & -\frac{a^2}{3} (s^2 + r^2 - sr) - \frac{b^2}{27} (2s^3 + 2r^3 - 3s^2r - 3sr^2) + \\ & + \frac{c^2}{9} (s^4 + r^4 + 3s^2r^2 - 2sr^3 - 2s^3r) + \frac{a^2}{3} s_+^2 + \frac{2b^2}{27} s_+^3 - \frac{c^2}{9} s_+^4, \end{aligned} \quad (143)$$

where we have expressed $\text{tr}Q^2$ and $\text{tr}Q^3$ in terms of s and r

$$\text{tr}Q^2 = \frac{2}{3} (s^2 + r^2 - sr)$$

and

$$\text{tr}Q^3 = \frac{1}{9} (2s^3 + 2r^3 - 3s^2r - 3sr^2).$$

The function $\tilde{f}_B(Q)$ consists of two components -

$$\begin{aligned} \tilde{f}_B(Q) = & F(s) + G(s, r) \quad \text{where} \\ F(s) = & -\frac{a^2}{3} (s^2 - s_+^2) - \frac{2b^2}{27} (s^3 - s_+^3) + \frac{c^2}{9} (s^4 - s_+^4) \\ G(s, r) = & \frac{a^2}{3} (sr - r^2) + \frac{b^2}{27} (3s^2r + 3sr^2 - 2r^3) + \frac{c^2}{9} (-2s^3r + 3s^2r^2 - 2sr^3 + r^4). \end{aligned} \quad (144)$$

Recalling that $2c^2s_+^2 = b^2s_+ + 3a^2$ (from the definition of s_+ in (128)), the function $F(s)$ can be expressed in terms of $\delta = s_+ - s \geq 0$ as follows -

$$F(s) = \frac{\delta}{27} (18a^2s_+ + 6b^2s_+^2 - 12c^2s_+^3) + \delta^2 \left(\frac{3b^2}{27}s_+ + \frac{18a^2}{27} + \delta \left(\frac{2b^2}{27} - \frac{4c^2}{9}s_+ + \frac{c^2}{9}\delta \right) \right). \quad (145)$$

The coefficient of δ vanishes by virtue of the definition of s_+ in (128). We note that the function

$$G(\delta) = \delta \left(\frac{2b^2}{27} - \frac{4c^2}{9}s_+ + \frac{c^2}{9}\delta \right) \quad (146)$$

attains a minimum for

$$\delta_{\min} = 2s_+ - \frac{b^2}{3c^2} > s_+ \quad (147)$$

and, therefore,

$$G(\delta) \geq G(s_+) = \frac{1}{27} (2b^2s_+ - 9c^2s_+^2). \quad (148)$$

We substitute (148) into (145) to obtain the following lower bound for $F(s)$ -

$$F(s) \geq \frac{c^2s_+^2 + 3a^2}{27} (s_+ - s)^2. \quad (149)$$

We can analyze the function $G(s, r)$, in (144), in an analogous manner. Let $\gamma = \frac{r}{s} \in [0, \frac{1}{2}]$. Then

$$G(s, r) = \gamma s^2 \left[\frac{a^2}{3} + \frac{3b^2}{27}s - \frac{2c^2}{9}s^2 \right] + \gamma^2 s^2 \left[-\frac{a^2}{3} + \frac{3b^2}{27}s + \frac{3c^2}{9}s^2 \right] + \gamma^3 s^3 \left[-\frac{2b^2}{27} - \frac{2c^2s}{9} + \gamma \frac{c^2s}{9} \right] \quad (150)$$

The coefficient of γ is non-negative for all $s \leq s_+$. Using the inequality $\gamma \leq \frac{1}{2}$, one readily obtains the following lower bound for $G(s, r)$ -

$$\begin{aligned} G(s, r) &\geq \gamma s^2 \left[\frac{a^2}{3} + \frac{3b^2}{27}s - \frac{2c^2}{9}s^2 \right] + \gamma^2 s^2 \left[-\frac{a^2}{3} + \frac{2b^2}{27}s + \frac{2c^2}{9}s^2 \right] \geq \\ &\geq \frac{r(s-r)}{9} (3a^2 + b^2s - 2c^2s^2) + \frac{5b^2}{27} r^2 s. \end{aligned} \quad (151)$$

Combining (149) and (151), the lower bound for $0 \leq s \leq s_+$ in (139) follows.

Case(ii) The case $s \geq s_+$ can be dealt with similarly. For any $Q \in S_0$ with $0 \leq r \leq \frac{s}{2}$, we have that

$$\frac{s}{\sqrt{2}} \leq |Q| = \sqrt{\frac{2}{3}} \sqrt{(s^2 + r^2 - sr)} \leq \sqrt{\frac{2}{3}} s. \quad (152)$$

For $s \geq s_+$, $|Q|^3 \geq \frac{s_+^3}{2\sqrt{2}}$ and

$$\beta(Q) \geq \eta \left(\frac{r^2(s-r)^2}{s^4} \right) \quad (153)$$

where $\beta(Q)$ is the biaxiality parameter defined in (22) and η is a positive constant independent of a^2, b^2 or c^2 or L . Combining (152), (153) and (129), we readily obtain the lower bound

$$\begin{aligned} \tilde{f}_B(Q) &\geq \left[\frac{\frac{2}{3}c^2s_+^2 + a^2}{2} \right] \left(|Q| - \sqrt{\frac{2}{3}}s_+ \right)^2 + \frac{b^2}{6\sqrt{6}} \beta(Q) |Q|^3 \geq \\ &\geq \left[\frac{\frac{2}{3}c^2s_+^2 + a^2}{2} \right] \min \left\{ \frac{2}{3} (s - s_+)^2, \frac{1}{6} (\sqrt{3}s - 2s_+)^2 \right\} + \tau b^2 s_+^3 \left(\frac{r^2(s-r)^2}{s^4} \right) \end{aligned} \quad (154)$$

where τ is an explicitly computable positive constant.

Case (iii) Finally, we consider $Q \in S_0$ with negative order parameters $\frac{s}{2} \leq r \leq 0$. In this case, one can directly check that

$$\operatorname{tr}Q^3 = \frac{1}{9}(2s^3 + 2r^3 - 3s^2r - 3sr^2) \leq 0$$

and therefore,

$$\begin{aligned} \tilde{f}_B(Q) &= -\frac{a^2}{2}|Q|^2 - \frac{b^2}{3}\operatorname{tr}Q^3 + \frac{c^2}{4}|Q|^4 + \frac{a^2}{3}s_+^2 + \frac{2b^2}{27}s_+^3 - \frac{c^2}{9}s_+^4 \\ &= -\frac{a^2}{2}|Q|^2 - \frac{b^2}{3}\operatorname{tr}(-Q)^3 + \frac{c^2}{4}|Q|^4 + \frac{a^2}{3}s_+^2 + \frac{2b^2}{27}s_+^3 - \frac{c^2}{9}s_+^4 + \frac{2b^2}{3}|\operatorname{tr}Q^3|, \end{aligned} \quad (155)$$

since $\frac{b^2}{3}\operatorname{tr}(-Q)^3 = -\frac{b^2}{3}\operatorname{tr}Q^3$ and $-\frac{b^2}{3}\operatorname{tr}Q^3 = \frac{b^2}{3}|\operatorname{tr}Q^3|$. The inequality (141) follows from (155) upon expressing $\operatorname{tr}Q^3$ in terms of s and r .

For (142), it suffices to note that for $s, r \leq 0$, $\operatorname{tr}Q^3 \leq 0$ and therefore,

$$\begin{aligned} \tilde{f}_B(Q) &\geq -\frac{a^2}{2}|Q|^2 + \frac{c^2}{4}|Q|^4 + \frac{a^2}{3}s_+^2 + \frac{2b^2}{27}s_+^3 - \frac{c^2}{9}s_+^4 = \\ &= -\frac{a^2}{3}(s^2 + r^2 - sr) + \frac{c^2}{9}(s^2 + r^2 - sr)^2 - \frac{s_+^3}{3}\left(\frac{b^2}{9} - \frac{c^2}{3}s_+\right). \end{aligned}$$

A straightforward computation shows that the function

$$-\frac{a^2}{3}(s^2 + r^2 - sr) + \frac{c^2}{9}(s^2 + r^2 - sr)^2 \geq -\frac{a^4}{4c^2}$$

and

$$\frac{s_+^3}{3}\left(\frac{b^2}{9} - \frac{c^2}{3}s_+\right) < -\frac{a^4}{4c^2}.$$

The inequality (142) now follows. \square

Remark 2 One can readily obtain lower bounds for $\tilde{f}_B(Q)$ in terms of the order parameters (S, R) in Proposition 2, following the methods outlined in Proposition 10. The details are omitted here for brevity.

Remark 3 Relation (142) shows that if $f_B(Q^{(L_k)}(x)) \rightarrow 0$ as $L_k \rightarrow 0$ then $Q^{(L_k)}$ cannot have an (s, r) representation with $\frac{s}{2} < r < 0$, if L_k is sufficiently small.

In view of Propositions 3 and 9, we can make qualitative predictions about the size of regions where a global Landau-De Gennes minimizer Q^* can have $|Q^*| \ll \sqrt{\frac{2}{3}}s_+$ and the size of regions where Q^* can be strongly biaxial.

Proposition 11 Let Q^* be a global minimizer of $\tilde{F}_{LG}[Q]$ in (13), in the admissible class \mathcal{A}_Q defined in (12). Let $\Omega^* = \left\{x \in \Omega; |Q^*(x)| \leq \frac{1}{2}\sqrt{\frac{2}{3}}s_+\right\}$. Then

$$|\Omega^*| \leq \alpha \frac{L}{(c^2s_+^2 + a^2)} \int_{\Omega} |\nabla n^{(0)}(x)|^2 dx, \quad (156)$$

where $n^{(0)}$ is defined in (16) and α is an explicitly computable positive constant independent of a^2, b^2, c^2 or L .

Proof. From Proposition 9, we have that

$$\tilde{f}_B(Q^*(x)) \geq \frac{1}{\alpha}(c^2s_+^2 + a^2)s_+^2, \quad x \in \Omega^* \quad (157)$$

for some explicitly computable positive constant α , since $|Q^*| \leq \frac{1}{2}\sqrt{\frac{2}{3}}s_+ = \frac{1}{\sqrt{6}}s_+$ on Ω^* . On the other hand, recalling the definition of $Q^{(0)}$ in (15) and since Q^* is a global minimizer of $\tilde{F}_{LG}[Q]$, we have that

$$\int_{\Omega^*} \tilde{f}_B(Q^*(x)) dx \leq \mathcal{F}_{LG}[Q^{(0)}] = \int_{\Omega} \tilde{f}_B(Q^{(0)}) + \frac{L}{2}|\nabla Q^{(0)}|^2 dx = Ls_+^2 \int_{\Omega} |\nabla n^{(0)}|^2 dx, \quad (158)$$

since $\tilde{f}_B(Q^{(0)}) = 0$ everywhere in Ω . Substituting (157) into (158), we obtain

$$\frac{1}{\alpha} (c^2 s_+^2 + a^2) s_+^2 |\Omega^*| \leq Ls_+^2 \int_{\Omega} |\nabla n^{(0)}|^2 dx, \quad (159)$$

from which the inequality (156) follows. \square

Proposition 12 *Let Q^* be a global minimizer of $\tilde{F}_{LG}[Q]$ in (13), in the admissible class \mathcal{A}_Q defined in (12). Let $\Omega^\lambda = \{x \in \Omega; |Q^*(x)| \geq \frac{1}{2}\sqrt{\frac{2}{3}}s_+, \beta(Q(x)) > \lambda\}$ for some positive constant λ . Then,*

$$|\Omega^\lambda| \leq \alpha \frac{L}{\lambda s_+ b^2} \int_{\Omega} |\nabla n^{(0)}|^2 dx \quad (160)$$

where $n^{(0)}$ is defined in (16) and α is an explicitly computable positive constant independent of a^2, b^2, c^2 or L .

Proof. From Proposition 9, we have that

$$\tilde{f}_B(Q^*(x)) \geq \frac{b^2}{6\sqrt{6}}\beta(Q^*(x))|Q^*(x)|^3 \geq \frac{1}{\alpha}b^2\lambda s_+^3 \quad x \in \Omega^\lambda \quad (161)$$

for some explicitly computable positive constant α , since $|Q^*| \geq \frac{1}{2}\sqrt{\frac{2}{3}}s_+ = \frac{1}{\sqrt{6}}s_+$ on Ω^λ . On the other hand, recalling the definition of $Q^{(0)}$, (15), and since Q^* is a global minimizer of $\tilde{F}_{LG}[Q]$, we have that

$$\int_{\Omega^\lambda} \tilde{f}_B(Q^*(x)) dx \leq \int_{\Omega} \tilde{f}_B(Q^{(0)}) + \frac{L}{2}|\nabla Q^{(0)}|^2 dx = Ls_+^2 \int_{\Omega} |\nabla n^{(0)}|^2 dx \quad (162)$$

since $\tilde{f}_B(Q^{(0)}) = 0$ everywhere in Ω . Substituting (161) into (162), we obtain

$$\frac{1}{\alpha}b^2\lambda s_+^3 |\Omega^\lambda| \leq Ls_+^2 \int_{\Omega} |\nabla n^{(0)}|^2 dx, \quad (163)$$

from which the inequality (160) follows. \square

Proposition 11 is relevant to the size of defect cores in global energy minimizers whereas Proposition 12 is relevant to the equilibrium behaviour far away from the defect cores.

6.2 Analyticity and uniaxiality

We define a new biaxiality parameter $\tilde{\beta}(Q)$ as follows:

$$\tilde{\beta}(Q) \stackrel{def}{=} (\text{tr}(Q^2))^3 - 6(\text{tr}(Q^3))^2.$$

Then $\tilde{\beta}(Q) \geq 0$ with $\tilde{\beta}(Q) = 0$ if and only if Q is uniaxial i.e. $Q = s(n \otimes n - \frac{1}{3}Id)$ for some $s \in \mathbb{R} \setminus \{0\}, n \in \mathbb{S}^2$ or $Q = 0$. The function $\tilde{\beta}(Q)$ is a real analytic function of Q and this is particularly important given that global energy minimizers of the functional \mathcal{F} (subject to smooth boundary conditions) are real analytic:

Proposition 13 *Let Ω be a simply-connected bounded open set. Let $Q^{(L)}$ be a global energy minimizer of $\tilde{F}_{LG}[Q]$ in (13) in the admissible space \mathcal{A}_Q . Then $Q^{(L)}$ is real analytic in Ω .*

Proof.

We drop the superscript L from $Q^{(L)}$ for convenience. As $-\frac{a^2}{2}\text{tr}(Q^2) - \frac{b^2}{3}\text{tr}(Q^3) + \frac{c^2}{4}(\text{tr}Q^2)^2$ is bounded from below (see also the *Appendix*) we have that there exists an H^1 global energy minimizer satisfying the Euler-Lagrange system:

$$L\Delta Q_{ij} = -a^2 Q_{ij} - b^2 \left(Q_{ik} Q_{kj} - \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right) + c^2 Q_{ij} \text{tr}(Q^2)$$

For Q an H^1 solution of the equation one uses $H^1 \hookrightarrow L^6$ (in \mathbb{R}^3) and Hölder's inequality to obtain that the right hand side of each equation is in L^2 . Elliptic regularity gives that $Q \in H^2 \hookrightarrow W^{1,6} \hookrightarrow L^\infty$ hence the right hand side of the equation is in H^1 . Elliptic regularity gives $Q \in H^3$ and one can continue bootstrapping to obtain the full regularity allowed by the regularity of boundary data and that of the domain.

In order to prove the analyticity we use a general abstract result due to A.Friedman,[12]. We define growth classes as follows: let M_n be a sequence of positive numbers. Then a function $F : C^\infty(D) \rightarrow \mathbb{C}$, with $D \subset \mathbb{R}^d$ an open set, belongs to the class $C\{M_n; D\}$ if for any closed subset $D_0 \subset D$ there exist constants H_0, H with

$$|\partial^j F(x)| \leq H_0 H^j M_j, x \in D_0$$

where we have used multiindex-notation ($\partial^j F = \partial_1^{j_1} \dots \partial_d^{j_d} F; j = \sum_{i=1}^d j_i$). Let us observe that $C\{n!; D\}$ is the class of functions analytic in D .

In [12] the following theorem is proved for general elliptic systems:

Proposition 14 ([12],p.45) *Let $u(x)$ be a real solution of the elliptic system*

$$\Phi_l(x; u, \nabla u, \nabla^2 u, \dots, \nabla^{2m} u) = 0, x \in \Omega \subset \mathbb{R}^d; u \in \mathbb{R}^N, l = 1, \dots, N$$

in $\Omega \subset \mathbb{R}^d$. Let E be some open set containing $E_1 \stackrel{\text{def}}{=} \{u(x), \nabla u(x), \dots, \nabla^{2m} u(x); x \in \Omega\}$. Assume that:

- (i) $\Phi_l \in C\{M_n; \Omega \times E\}$ and that the M_n satisfy the monotonicity conditions
- (ii) $\binom{n}{i} M_i M_{n-i} \leq A M_n; 0 \leq i \leq n, n \in \mathbb{N}$ for some $A > 0$.

If $u \in C^{2m+\alpha}(\Omega), 0 < \alpha < 1$ then $u \in C\{M_{n-2m+1}; \Omega\}$ (where $M_{-i} = 1$ for $i \in \mathbb{N}$)

In our case, for the system (14) we have $m = 1$ and Φ_l is analytic hence of class $C\{n!; \Omega\}$. The constants $M_n = n!$ satisfy the monotonicity conditions (ii) in the theorem, with $A = 1$. We have that $Q \in C^\infty(\Omega)$ and hence by the theorem Q is in the class $C\{(n-1)!; \Omega\}$ therefore real analytic. \square

Proposition 15 *Let Q be a real analytic function $Q : \Omega \subset \mathbb{R}^3 \rightarrow S_0$. Then the set where Q is uniaxial or isotropic is either the whole of Ω or has zero Lebesgue measure.*

Proof. If there is no $x \in \Omega$ such that $\tilde{\beta}(Q(x)) \neq 0$ then Q is uniaxial or isotropic everywhere. If there exists a $P \in \Omega$ such that $\tilde{\beta}(Q(P)) \neq 0$ then let us consider the lines passing through P . The restriction of Q to any such line is real analytic and then so is $\tilde{\beta}(Q)$. Thus $\tilde{\beta}(Q)$ has at most countably many zeroes on such a line. We claim that this implies that the set of zeroes of $\tilde{\beta}(Q)$ in Ω is of measure zero.

We assume, without loss of generality, that $P = 0$. We denote $N^* = N \setminus \{0\}$ and decompose $\mathbb{R}^n \cap \Omega = \bigcup_{n \in \mathbb{N}^*} \left(\overline{B_{\frac{1}{n}}} \setminus \overline{B_{\frac{1}{n+1}}} \cap \Omega \right) \cup \left(\bigcup_{n \in \mathbb{N}^*} \left(\overline{B_{n+1}} \setminus \overline{B_n} \cap \Omega \right) \right)$. We claim that for any $n, \frac{1}{n} \in \mathbb{N}^*$ the set $\left(\tilde{\beta}(Q) \right)^{-1}(0) \cap \left(\Omega \cap \overline{B_{\frac{1}{n}}} \setminus \overline{B_{\frac{1}{n+1}}} \right)$ is a set of measure zero. This implies that $\tilde{\beta}(Q)^{-1}(0) \cap \Omega$, which is a countable union of sets as before, is also a set of measure zero.

We consider the bi-Lipschitz functions

$$f_n : \left[\frac{1}{n+1}, \frac{1}{n} \right] \times \underbrace{[0, \pi] \times \dots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi] \rightarrow \overline{B_{\frac{1}{n}}} \setminus \overline{B_{\frac{1}{n+1}}}, \forall n, \frac{1}{n} \in \mathbb{N}$$

that realize the change of coordinates from polar to usual cartesian coordinates.

We have that $f_n^{-1} \left(\tilde{\beta}(Q)^{-1}(0) \cap \Omega \cap \overline{B_{\frac{1}{n}} \setminus B_{\frac{1}{n+1}}} \right) \subset \left[\frac{1}{n+1}, \frac{1}{n} \right] \times \underbrace{[0, \pi] \times \cdots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi)$. We recall that the Lebesgue measure μ on the n -dimensional product space $\left[\frac{1}{n+1}, \frac{1}{n} \right] \times \underbrace{[0, \pi] \times \cdots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi)$ is the completion of the product measure $\mu_1 \times \mu_2$ where μ_1 is the 1 dimensional Lebesgue measure on $\left[\frac{1}{n+1}, \frac{1}{n} \right]$ and μ_2 is the $n-1$ dimensional Lebesgue measure on $\underbrace{[0, \pi] \times \cdots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi)$. Then for any set $E \subset \left[\frac{1}{n+1}, \frac{1}{n} \right] \times \underbrace{[0, \pi] \times \cdots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi)$ we have

$$(\mu_1 \times \mu_2)(E) = \int_{\underbrace{[0, \pi] \times \cdots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi)} \mu_1(E^y) \mu_2(dy)$$

where $E^y = \{x \in \left[\frac{1}{n+1}, \frac{1}{n} \right], (x, y_1, \dots, y_{n-1}) \in E\} \subset \left[\frac{1}{n+1}, \frac{1}{n} \right]$. In our case, letting

$$E \stackrel{\text{def}}{=} f_n^{-1} \left(\tilde{\beta}(Q)^{-1}(0) \cap \Omega \cap \overline{B_{\frac{1}{n}} \setminus B_{\frac{1}{n+1}}} \right)$$

we have that E^y is made of finitely many points for almost all $y \in \underbrace{[0, \pi] \times \cdots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi)$ (as a consequence of the first paragraph in this proof; because E^y is just the set of the distances to P of the uniaxial or isotropic points that are in $\Omega \cap \overline{B_{\frac{1}{n}} \setminus B_{\frac{1}{n+1}}}$, on a segment through P , segment that has in polar coordinates the direction $y \in \underbrace{[0, \pi] \times \cdots \times [0, \pi]}_{n-2 \text{ times}} \times [0, 2\pi)$). Thus $\mu_1(E^y) = 0, \mu_2 - a.e. y$ hence $\mu_1 \times \mu_2(E) = 0$ thus $\mu(E) = 0$.

As bi-Lipschitz functions carry sets of measure zero into sets of measure zero we have that $\tilde{\beta}(Q)^{-1}(0) \cap \Omega \cap \overline{B_{\frac{1}{n}} \setminus B_{\frac{1}{n+1}}}$ is a set of measure zero. On the other hand $\tilde{\beta}(Q)^{-1}(0) \cap \Omega$ is a countable union of sets as before, hence it has measure zero. \square

Corollary 2 *Let $Q^{(L)}$ be a global minimizer of $\tilde{F}_{LG}[Q]$ in the admissible class \mathcal{A}_Q . Then there exists a set of measure zero, possibly empty, Ω_0 in Ω such that the eigenvectors of $Q^{(L)}$ are smooth at all points $x \in \Omega \setminus \Omega_0$. The uniaxial-biaxial interfaces, isotropic-uniaxial or isotropic-biaxial interfaces are contained in Ω_0 .*

Proof. The global minimizer $Q^{(L)} \in C^\infty(\Omega; \mathcal{A})$. The eigenvectors of $Q^{(L)}$ have the same degree of regularity as $Q^{(L)}$ on sets $K \subset \Omega$, where $Q^{(L)}$ has the same number of distinct eigenvalues i.e. where $Q^{(L)}$ is either biaxial or uniaxial or isotropic, [26], but not necessarily otherwise [17]. If $Q^{(L)}$ is uniaxial everywhere then $\Omega_0 = \emptyset$. If $Q^{(L)}$ is either uniaxial or isotropic on the whole of Ω (i.e. $\tilde{\beta}(Q^{(L)}) = 0$ in Ω), with $Q^{(L)} \neq 0$ at some point in Ω , then let $\tilde{\Omega} = \{x \in \Omega, Q^{(L)}(x) = 0\}$ denote the zero-set of $Q^{(L)}$. Let us observe that $\tilde{\Omega} = (|Q|^2)^{-1}(0)$ and $|Q|^2$ is an analytic function. By an argument similar to the proof of Proposition 15 and since $Q(x) \neq 0$ for at least one point $x \in \Omega$, we have that $\tilde{\Omega}$ has measure zero and we take $\Omega_0 \stackrel{\text{def}}{=} \tilde{\Omega}$.

If $Q^{(L)}$ is biaxial somewhere then Proposition 15 shows that the set of points where $\tilde{\beta}(Q) = 0$ has measure zero. We denote this set by Ω_0 and observe that $\Omega \setminus \Omega_0$ is an open set and the eigenvectors have the same regularity as $Q^{(L)}$ on $\Omega \setminus \Omega_0$, see [26]. \square

7 Acknowledgements

A. Majumdar was supported by a Royal Commission for the Exhibition of 1851 Research Fellowship till October 2008. She is now supported by Award No. KUK-C1-013-04, made by King Abdullah University of

Science and Technology (KAUST). A. Zarnescu is supported by the EPSRC Grant EP/E010288/1 - Equilibrium Liquid Crystal Configurations: Energetics, Singularities and Applications. We thank John Ball and Christof Melcher for stimulating discussions.

Appendix

Proposition 16 [21] Consider the bulk energy density $f_B(Q)$ given by

$$f_B(Q) = -\frac{a^2}{2} \text{tr}Q^2 - \frac{b^2}{3} \text{tr}Q^3 + \frac{c^2}{4} (\text{tr}Q^2)^2. \quad (164)$$

Then $f_B(Q)$ attains its minimum for uniaxial Q -tensors of the form

$$Q = s_+ \left(n \otimes n - \frac{1}{3} \right), \quad (165)$$

where $n : \Omega \rightarrow S^2$ is a unit eigenvector of Q and

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \quad (166)$$

Proof. Proposition 16 has been proven in [21]. We reproduce the proof here for completeness.

We recall that for a symmetric, traceless matrix Q of the form

$$Q = \sum_{i=1}^3 \lambda_i e_i \otimes e_i,$$

$\text{tr}Q^n = \sum_{i=1}^3 \lambda_i^n$ subject to the tracelessness condition so that the bulk energy density f_B in (164) only depends on the eigenvalues λ_1, λ_2 and λ_3 . Then the stationary points of the bulk energy density f_B are given by the stationary points of the function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ defined by

$$f(\lambda_1, \lambda_2, \lambda_3) = -\frac{a^2}{2} \sum_{i=1}^3 \lambda_i^2 - \frac{b^2}{3} \sum_{i=1}^3 \lambda_i^3 + \frac{c^2}{4} \left(\sum_{i=1}^3 \lambda_i^2 \right)^2 - 2\delta \sum_{i=1}^3 \lambda_i. \quad (167)$$

where we have recast f_B in terms of the eigenvalues and introduced a Lagrange multiplier δ for the tracelessness condition.

The equilibrium equations are given by a system of three algebraic equations

$$\frac{\partial f}{\partial \lambda_i} = 0 \Leftrightarrow -a^2 \lambda_i - b^2 \lambda_i^2 + c^2 \left(\sum_{k=1}^3 \lambda_k^2 \right) \lambda_i = 2\delta \quad \text{for } i = 1 \dots 3, \quad (168)$$

or equivalently

$$(\lambda_i - \lambda_j) \left[-a^2 - b^2 (\lambda_i + \lambda_j) + c^2 \sum_{k=1}^3 \lambda_k^2 \right] = 0 \quad 1 \leq i < j \leq 3. \quad (169)$$

Let $\{\lambda_i\}$ be a solution of the system (168) with three distinct eigenvalues $\lambda_i \neq \lambda_2 \neq \lambda_3$. We consider equation (169) for the pairs (λ_1, λ_2) and (λ_1, λ_3) . This yields two equations

$$\begin{aligned} -a^2 - b^2 (\lambda_1 + \lambda_2) + c^2 \sum_{k=1}^3 \lambda_k^2 &= 0 \\ -a^2 - b^2 (\lambda_1 + \lambda_3) + c^2 \sum_{k=1}^3 \lambda_k^2 &= 0 \end{aligned} \quad (170)$$

from which we obtain

$$-b^2(\lambda_2 - \lambda_3) = 0, \quad (171)$$

contradicting our initial hypothesis $\lambda_2 \neq \lambda_3$. We, thus, conclude that a stationary point of the bulk energy density must have at least two equal eigenvalues and therefore correspond to either a uniaxial or isotropic liquid crystal state.

We consider an arbitrary uniaxial state given by $(\lambda_1, \lambda_2, \lambda_3) = (\frac{2s}{3}, -\frac{s}{3}, -\frac{s}{3})$ and the corresponding Q-tensor is $Q = s(e_1 \otimes e_1 - \frac{1}{3}Id)$. The function f_B is then a quartic polynomial in the order parameter s ie.

$$f_B(s) = \frac{s^2}{27}(-9a^2 - 2b^2s + 3c^2s^2) \quad (172)$$

and the stationary points are solutions of the algebraic equation $\frac{df_B}{ds} = 0$,

$$\frac{df_B}{ds} = \frac{1}{27}(-18a^2s - 6b^2s^2 + 12c^2s^3) = 0. \quad (173)$$

The cubic equation (173) admits three solutions;

$$s = 0 \quad \text{and} \quad s_{\pm} = \frac{b^2 \pm \sqrt{b^4 + 24a^2c^2}}{4c^2} \quad (174)$$

where

$$f_B(0) = 0 \quad \text{and} \quad f_B(s_+) < f_B(s_-) < 0. \quad (175)$$

Symmetry considerations show that we obtain the same set of stationary points for the remaining two uniaxial choices. The global minimizer is, therefore, a uniaxial Q-tensor of the form

$$Q = s_+ \left(n \otimes n - \frac{1}{3}Id \right), \quad n \in \mathbb{S}^2 \quad (176)$$

where s_+ has been defined in (166).□

Lemma 13 *Let $Q \in S_0$. We define the biaxiality parameter $\beta(Q)$ to be*

$$\beta(Q) = 1 - 6 \frac{(\text{tr}Q^3)^2}{(\text{tr}Q^2)^3}. \quad (177)$$

(i) *The biaxiality parameter $\beta(Q) \in [0, 1]$ and $\beta(Q) = 0$ if and only if Q is purely uniaxial i.e. if Q is of the form, $Q = s(n \otimes n - \frac{1}{3}Id)$ for some $s \in \mathbb{R}, n \in \mathbb{S}^2$. (ii) *The biaxiality parameter, $\beta(Q)$, can be bounded in terms of the ratio $\frac{r}{s}$, where (s, r) are the scalar order parameters in Proposition 1. These bounds are given by**

$$\frac{1}{2} \left(1 - \sqrt{1 - \sqrt{\beta}} \right) \leq \frac{r}{s} \leq \frac{1}{2} \left(1 + \sqrt{1 - \sqrt{\beta}} \right). \quad (178)$$

Equivalently,

$$\frac{1 - \sqrt{1 - \sqrt{\beta}}}{3 + \sqrt{1 - \sqrt{\beta}}} \leq \frac{R}{S} \leq \frac{1 + \sqrt{1 - \sqrt{\beta}}}{3 - \sqrt{1 - \sqrt{\beta}}} \quad (179)$$

*where (S, R) are the order parameters in Proposition 2. Further $\beta(Q) = 1$ if and only if $r = \frac{s}{2}$ or if and only if $\frac{R}{S} = \frac{1}{3}$. (iii) *For an arbitrary $Q \in S_0$, we have that**

$$-\frac{|Q|^3}{\sqrt{6}} \left(1 - \frac{\beta}{2} \right) \leq \text{tr}Q^3 \leq \frac{|Q|^3}{\sqrt{6}} \left(1 - \frac{\beta}{2} \right). \quad (180)$$

Proof: (i) The quantity $\beta(Q)$ is known as the biaxiality parameter in the liquid crystal literature [23] and it is well-known that $\beta(Q) \in [0, 1]$. We present a simple proof here for completeness.

Following Proposition 1, we represent an arbitrary $Q \in S_0$ as

$$Q = s \left(n \otimes n - \frac{1}{3} Id \right) + r \left(m \otimes m - \frac{1}{3} Id \right) \quad 0 \leq r \leq \frac{s}{2} \text{ or } \frac{s}{2} \leq r \leq 0. \quad (181)$$

Since $6 \frac{(\text{tr}Q^3)^2}{(\text{tr}Q^2)^3} \geq 0$, the inequality $\beta(Q) \leq 1$ is trivial. To show $\beta(Q) \geq 0$, we use the representation (181) to express $\text{tr}Q^3$ and $\text{tr}Q^2$ in terms of the order parameters s and r .

$$\begin{aligned} \text{tr}Q^3 &= \frac{1}{9} (2s^3 + 2r^3 - 3s^2r - 3sr^2) \\ \text{tr}Q^2 &= \frac{2}{3} (s^2 + r^2 - sr) \end{aligned} \quad (182)$$

A straightforward calculation shows that

$$(\text{tr}Q^3)^2 = \frac{1}{81} (4s^6 + 4r^6 - 12s^5r - 12sr^5 + 26s^3r^3 - 3s^4r^2 - 3s^2r^4)$$

and

$$(\text{tr}Q^2)^3 = \frac{8}{27} (s^6 + r^6 - 3s^5r - 3sr^5 - 7s^3r^3 + 6s^2r^4 + 6s^4r^2).$$

One can then directly verify that

$$(\text{tr}Q^2)^3 - 6 (\text{tr}Q^3)^2 = 2s^2r^2 (s - r)^2 \geq 0 \quad (183)$$

as required. It follows immediately from (183) that $\beta(Q) = 0$ if and only if either $s = 0, r = 0$ or $s = r$. From (181), the three cases, $s = 0, r = 0$ and $s = r$, correspond to uniaxial nematic states (in fact all uniaxial states can be described by one of these three conditions) and therefore, $\beta(Q) = 0$ if and only if Q is uniaxial.

(ii) From Proposition 1, it suffices to consider Q -tensors with either $0 \leq r \leq \frac{s}{2}$ or $\frac{s}{2} \leq r \leq 0$. Let $\gamma = \frac{r}{s}$, then $\gamma \in [0, \frac{1}{2}]$ for the two cases under consideration. The biaxiality parameter, $\beta(Q)$, can be expressed in terms of the ratio γ as follows

$$\frac{(2 - 3\gamma - 3\gamma^2 + 2\gamma^3)^2}{(1 - \gamma + \gamma^2)^3} = 4(1 - \beta). \quad (184)$$

From (183), we have that

$$(2 - 3\gamma - 3\gamma^2 + 2\gamma^3)^2 = 4(1 - \gamma + \gamma^2)^3 - 27\gamma^2(1 - \gamma)^2, \quad (185)$$

which in turn, yields the following equality

$$\frac{27\gamma^2(1 - \gamma)^2}{(1 - \gamma + \gamma^2)^3} = 4\beta. \quad (186)$$

Noting that for $\gamma \in [0, \frac{1}{2}]$, the polynomial $1 - \gamma + \gamma^2 \geq \frac{3}{4}$, we obtain the following upper bound

$$\beta \leq 16\gamma^2(1 - \gamma)^2 \quad (187)$$

and the bounds (178) readily follow from (187).

One can readily see from (186) that $\beta(Q) = 1$ if and only if $\frac{r}{s} = \frac{1}{2}$. The bounds (179) follow directly from (178) on noting that

$$r = 2R \text{ and } s = S + R.$$

One can see directly from (179) that if $\beta = 1$, then $\frac{R}{S} = \frac{1}{3}$. On the other hand, if $\frac{R}{S} = \frac{1}{3}$, then $\frac{r}{s} = \frac{1}{2}$ and (186) implies that $\beta(Q) = 1$. The claims in (ii) now follow.

(iii) From the definition of the biaxiality parameter in (177), we necessarily have that

$$\operatorname{tr}Q^3 = \pm \frac{|Q|^3}{\sqrt{6}} \sqrt{1 - \beta(Q)}. \quad (188)$$

It is easily checked that

$$\sqrt{1 - \beta} \leq 1 - \frac{\beta}{2} \quad (189)$$

The bounds (180) follow from combining (188) and (189) .□

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