Uniaxiality in the Landau-de Gennes theory of nematic liquid crystals

Apala Majumdar*

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Abstract

We study uniaxial energy minimizers within the Landau-de Gennes theory for nematic liquid crystals, subject to Dirichlet boundary conditions. Topological defects in such minimizers correspond to the zeros of the corresponding equilibrium field. We consider two-dimensional and three-dimensional domains separately and study the correspondence between Landau-de Gennes theory and Ginzburg-Landau theory for superconductors. We obtain results for the location and dimensionality of the defect set, the minimizer profile near the defect set and study the qualitative properties of uniaxial energy minimizers away from the defect set, in the physically relevant case of vanishing elastic constant. In the three-dimensional case, we establish the $C^{1,\alpha}$-convergence of uniaxial minimizers to a limiting harmonic map, away from the defect set, for some $0 < \alpha < 1$. Some generalizations for biaxial minimizers are also discussed. This work is motivated by the study of defects in liquid crystalline systems and their applications.

1 Introduction

Nematic liquid crystals are examples of mesophases whose physical properties are intermediate between those of a typical liquid and a crystalline solid [10]. The constituent rod-like molecules have no translational order but exhibit a certain degree of long-range orientational ordering. Consequently, liquid crystals are anisotropic media and this makes them suitable for a wide range of physical applications and the subject of very interesting mathematical modelling [13].

The Landau-de Gennes theory is a general continuum theory for nematic liquid crystals [10, 28]. It describes the state of a nematic liquid crystal by a symmetric, traceless $3 \times 3$ matrix - the $Q$-tensor order parameter, that is defined in terms of anisotropic macroscopic quantities, such as the magnetic susceptibility and the dielectric anisotropy. Nematic liquid crystals are said to be in the (a) biaxial phase when $Q$ has three distinct eigenvalues, (b) uniaxial phase when $Q$ has a pair of equal non-zero eigenvalues and (c) isotropic phase when $Q$ has three equal eigenvalues or equivalently when $Q = 0$. For a general biaxial phase, $Q$ can be written in the form [15, 20]

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

(1)

*Mathematical Institute, University of Oxford, 24-29 St. Giles', OX1 3LB, U.K.
where $s, r$ are scalar order parameters, $\mathbf{n}, \mathbf{m}$ are eigenvectors of $\mathbf{Q}$ and $\mathbf{I}$ is the $3 \times 3$ identity matrix. In the uniaxial phase, $\mathbf{Q}$ takes the simpler form of

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

(2)

where $s$ is a scalar order parameter that measures the degree of orientational ordering about the distinguished eigenvector $\mathbf{n}$.

The Landau-de Gennes energy functional, $\mathcal{I}_{\text{LG}}$, is a nonlinear integral functional of $\mathbf{Q}$ and its spatial derivatives. In the absence of any surface energies or external fields, $\mathcal{I}_{\text{LG}}$ is given by \cite{10, 20}

$$
\mathcal{I}_{\text{LG}}[\mathbf{Q}] = \int_\Omega \frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{f_B(\mathbf{Q})}{L} \, dV
$$

(3)

where $\Omega$ is the domain, $f_B(\mathbf{Q})$ is the bulk energy density that dictates the preferred phase - isotropic, uniaxial or biaxial, $L$ is a positive material-dependent elastic constant and $|\nabla \mathbf{Q}|^2$ is an elastic energy density that penalizes spatial inhomogeneities. The equilibrium, physically observable configurations correspond to either global or local Landau-de Gennes energy minimizers, subject to the imposed boundary conditions.

In this paper, we study uniaxial global minimizers (of the form (2)) of the Landau-de Gennes energy functional. There is the very important underlying question - do uniaxial global minimizers actually exist \cite{15}? This is an open question but there is substantial numerical and experimental evidence to show that global energy minimizers are largely uniaxial almost everywhere, in the sense that they have a small degree of biaxiality. Therefore, a rigorous study of uniaxial global minimizers is the first step in the mathematical analysis of arbitrary global minimizers and the interplay between biaxiality and uniaxiality. Secondly, stable uniaxial configurations do exist, at least for certain temperature regimes and certain physically realistic choices of the material-dependent constants \cite{19, 23, 25}. Some of our results extend to stable uniaxial configurations with appropriately bounded energy and can then be used to understand these configuration structures and the nature of their singularities. We also point out that there are two widely-used continuum theories for purely uniaxial liquid crystal phases - the Oseen-Frank theory and the Ericksen theory, both of which have received considerable attention amongst the mathematical analysts and the numerical modellers \cite{5, 12, 14, 8}. In fact, uniaxiality is one of the most frequently used assumptions in the theoretical study of liquid crystalline systems, even in the context of applications.

We assume that uniaxial global minimizers exist for each $L > 0$ and then establish various properties of such uniaxial global minimizers throughout the paper. The paper is organized as follows. In Section 2 we introduce some basic notation and terminology. In Section 3 we study Landau-de Gennes minimizers on two-dimensional (2D) domains and establish a 1−1 correspondence between Landau-de Gennes theory and Ginzburg-Landau theory. In Section 4 we recall useful results from \cite{15} that are crucial for the development of this paper. We study uniaxial Landau-de Gennes minimizers on three-dimensional (3D) domains in the low-temperature regime. There are important differences between the 2D and 3D cases and the standard Ginzburg-Landau techniques do not extend to the 3D case. We derive the governing equations for uniaxial global minimizers and obtain qualitative information about topological defects. The scalar order parameter ‘$s$’ necessarily vanishes at the defect locations. The defect locations are prescribed in terms of the singular set of a limiting harmonic map and using asymptotic methods, we show that the leading eigenvector $\mathbf{n}$ (see (2)) necessarily has a radial-hedgehog type of profile in the immediate neighbourhood of each isolated point defect. Our result is analogous to a powerful result on singularity profiles in \cite{5}.  


where the authors work within the Oseen-Frank theory for uniaxial liquid crystals with constant order parameter $s$. In Section 5, we study the qualitative properties of uniaxial global minimizers away from the defect set, in the limit $L \to 0^+$. The elastic constant $L$ to typically several orders of magnitude smaller than the other material-dependent constants and hence the $L \to 0$ limit is physically realistic [22]. We adapt the small energy regularity theorem of [7] to the Landau-de Gennes framework and prove the $C^{1, \alpha}$-convergence of uniaxial global minimizers to a limiting harmonic map, away from the defect set, as $L \to 0$. This convergence result encodes quantitative information about the corresponding scalar order parameter. In Section 6, we discuss various generalizations of our results to uniaxial solutions with bounded energy and to the completely general biaxial case. The uniaxial case in 3D can be viewed as a generalized Ginzburg-Landau theory from $\mathbb{R}^3$ to $\mathbb{R}^3$ although there are important technical differences. However, the biaxial case presents a whole host of new mathematical difficulties; there are five degrees of freedom in the biaxial case and the additional degrees of freedom give us more possibilities, particularly in the context of defects. The methods in this paper contribute to the development of a generalized Ginzburg-Landau theory from $\mathbb{R}^3$ to higher dimensions ($\mathbb{R}^5$ in this case), for non-standard non-convex multi-well bulk potentials.

2 Preliminaries

Let $\tilde{S} \subset M^{3 \times 3}$ denote the space of symmetric, traceless $3 \times 3$ matrices i.e.

$$\tilde{S} \overset{\text{def}}{=} \{ Q \in M^{3 \times 3}; Q_{ij} = Q_{ji}, \; Q_{ii} = 0 \}$$

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

$$|Q| \overset{\text{def}}{=} \sqrt{\text{tr} Q^2} = \sqrt{Q_{ij}Q_{ij}} \quad i, j = 1 \ldots 3.$$ 

We take our domain $\Omega$ to be either a two-dimensional or three-dimensional bounded, connected and simply-connected set with smooth boundary, $\partial \Omega$. We work with the simplest form of the bulk energy density, $f_B$, in [4] that allows for a first-order nematic-isotropic phase transition [20]. We focus on the low-temperature regime; the function $f_B$ is bounded from below and can be written as

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

where $a^2, b^2, c^2 \in \mathbb{R}^+$ are material-dependent and temperature-dependent positive constants and $C(a^2, b^2, c^2)$ is a positive constant that ensures $f_B(Q) \geq 0$ for all $Q$-tensors. We note that $C(a^2, b^2, c^2)$ plays no role in energy minimization, in either spatially homogeneous or inhomogeneous cases. The negative coefficient of $\text{tr} (Q^2)$ incorporates the fact that we are working below the nematic-isotropic transition temperature where $f_B$ attains its minimum on the set of uniaxial $Q$-tensors given by [16]

$$Q_{\text{min}} = \left\{ Q \in \tilde{S}; Q = s_+ \left( n \otimes n - \frac{1}{3} I \right) \right\}$$

with $n \in S^2$ and

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}.$$
We study uniaxial global minimizers of $I_{LG}$, with $f_B$ as in (4), with strong anchoring conditions or Dirichlet boundary conditions. The prescribed boundary condition $Q_b$ is given by
\[
Q_b = s_+ \left( n_b \otimes n_b - \frac{1}{3} I \right)
\] (7)
where $n_b \in W^{1,2}(\Omega; M)$ ($M = S^1$ in 2D and $M = S^2$ in 3D) is a unit-vector field with non-zero topological degree $d$, when viewed as a map from $\partial \Omega$ to $M$. Clearly, $Q_b \in Q_{\min}$ where $Q_{\min}$ has been defined in (5). We define our admissible space to be
\[
A_Q = \{ Q \in W^{1,1}(\Omega; \hat{S}) : Q = Q_b \text{ on } \partial \Omega, \text{ with } Q_b \text{ as in (7)} \},
\] (8)
where $W^{1,2}(\Omega; \hat{S})$ is the Sobolev space of square-integrable $Q$-tensors with square-integrable first derivatives. The existence of global energy minimizers for $I_{LG}$ in the admissible space $A_Q$ follows readily from the direct methods in the calculus of variations [16,15]. For completeness, we recall that the $W^{1,2}$-norm is given by $\|Q\|_{W^{1,2}(\Omega)} = (\int_{\Omega} |Q|^2 + |\nabla Q|^2 \, dx)^{1/2}$. In addition to the $W^{1,2}$-norm, we also use the $L^\infty$-norm in this paper, defined to be $\|Q\|_{L^\infty(\Omega)} = \text{ess \ sup}_{x \in \Omega} |Q(x)|$.

Finally, we introduce the concept of a “limiting uniaxial harmonic map” $Q^0 : \Omega \rightarrow Q_{\min}$; $Q^0$ is defined to be
\[
Q^0 = s_+ \left( n_0 \otimes n_0 - \frac{1}{3} I \right)
\] (9)
where $n_0$ is a minimizer of the Dirichlet energy
\[
I_{OF}[n] = \int_{\Omega} |\nabla n|^2 \, dV
\] (10)
in the admissible space
\[
A_n = \{ n \in W^{1,2}(\Omega; M) : n = n_b \text{ on } \partial \Omega \}
\] (11)
where $M = S^1$ in 2D and $M = S^2$ in 3D. The terminology limiting harmonic map stems from the fact that $n_0$ is a harmonic unit-vector field [21] and it can be shown that $Q^0$ is a global minimizer of $I_{LG}$ in the restricted class $A_Q \cap \{ Q_{\min} \}$ [5,13]. We use the limiting harmonic map $Q^0$ to study the inter-relationship between the Landau-de Gennes theory and the Oseen-Frank theory for nematic liquid crystals. The Oseen-Frank theory is the simplest continuum theory for nematic liquid crystals, restricted to uniaxial phases with constant scalar order parameter [10]. Working within the one-constant approximation, the Oseen-Frank energy reduces to the Dirichlet energy in (10) and $n_0$, and hence $Q^0$, is a global Oseen-Frank energy minimizer in the admissible space $A_n$.

3 The 2D case

Let $\Omega \subset \mathbb{R}^2$ be a bounded, connected and simply-connected domain with smooth boundary. Let $\hat{S}_2$ denote the space of symmetric, traceless $2 \times 2$ matrices. Then $Q \in \hat{S}_2$ can be written as
\[
Q = \lambda (n \otimes n - m \otimes m)
\] (12)
where $\lambda \in \mathbb{R}$ and $n,m$ are the two orthonormal eigenvectors of $Q$. We note that there are only two degrees of freedom in the representation [12] and hence we can think of $Q$ as being a map $Q : \Omega \rightarrow \mathbb{R}^2$. Using the identity, $\delta_{ij} = n_i n_j + m_i m_j$, we can re-write (12) as
\[
Q = 2\lambda \left( n \otimes n - \frac{1}{2} I \right)
\] (13)

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where \( I \) is the \( 2 \times 2 \) identity matrix. Thus, all admissible \( Q \)-tensors in two dimensions necessarily have a uniaxial structure as in [2].

Straightforward calculations show that

\[
|Q|^2 = 2\lambda^2 \\
\text{tr} Q^3 = Q_{ij} Q_{jp} Q_{pi} = 0 \quad i, j, p = 1, 2.
\]

Then the Landau-de Gennes energy functional in (3) simplifies to

\[
\mathcal{I}_{LG}[Q] = \int_\Omega \left( \frac{1}{2} |\nabla Q|^2 + \frac{1}{L} \left\{ -\frac{a^2}{2} \text{tr} Q^2 + \frac{c^2}{4} (\text{tr} Q^2)^2 \right\} \right) dV
\]

for two-dimensional domains. The corresponding Euler-Lagrange equations are

\[
Q_{ij,kk} = \frac{1}{L} \left( -a^2 + c^2 |Q|^2 \right) Q_{ij} \quad i, j = 1, 2
\]

and using the scaling \( \tilde{Q} = \sqrt{\frac{c^2}{a^2}} Q \), we obtain the following system of partial differential equations

\[
\tilde{Q}_{ij,kk} = \frac{a^2}{L} \left( |\tilde{Q}|^2 - 1 \right) \tilde{Q}_{ij} \quad i, j, k = 1, 2 \\
\tilde{Q} = 2 \left( n_b \otimes n_b - \frac{1}{2} I \right) \text{ on } \partial \Omega.
\]

This is identical to the Ginzburg-Landau equations for superconductors in two dimensions [26] and we are interested in the asymptotic properties of global energy minimizers either in the limit \( a^2 \to \infty \) or \( L \to 0^+ \).

Let \( Q^L \) be a global minimizer of \( \mathcal{I}_{LG} \) in (15), in the admissible space

\[
\mathcal{A}_Q = \{ Q \in W^{1,2} (\Omega; S_2) : Q = s_+ (n_b \otimes n_b - \frac{1}{2} I) \text{ on } \partial \Omega \} \text{ for a fixed } L > 0.
\]

Then \( Q^L \) is necessarily of the form

\[
Q^L(x) = s^L(x) \left( n^L(x) \otimes n^L(x) - \frac{1}{2} I \right)
\]

for some scalar function \( s^L : \tilde{\Omega} \to \mathbb{R} \) and \( n^L \in W^{1,2} (\Omega; S^1) \). Let \( \Theta_L = \{ x \in \Omega : s^L(x) = 0 \} \) denote the isotropic set of \( Q^L \). We have a topologically non-trivial boundary condition in (17), since \( n_b \) has non-zero topological degree when viewed as a map from \( \partial \Omega \) to \( S^1 \). Hence, the unit-vector field \( n^L \) necessarily has interior discontinuities and let \( S_n \) denote the defect set of \( n^L \). Then

\[
S_n \subset \Theta_L
\]

and in what follows, we use existing results in the mathematical literature for Ginzburg-Landau theory in two dimensions, to make predictions about the structure and location of the isotropic set and the far-field properties of global energy minimizers.

**Dimension of \( \Theta_L \)** [2] [4]: The isotropic set \( \Theta_L \) consists of \( |d| \) isolated points, \( \{ a_1, \ldots, a_{|d|} \} \), where \( d \) is the topological degree of the boundary condition \( Q_b \) in (7).

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\(^1\)We can also think of \( Q \in S_2 \) as being a symmetric, traceless \( 3 \times 3 \) matrix:

\[ Q = (\lambda + \frac{\mu}{\rho}) n \otimes n + (\frac{\mu}{\rho} - \lambda) m \otimes m - \frac{\mu}{\rho} z \otimes z \in \tilde{S} \]

where \( z \) is the unit-vector in the \( z \)-direction and \( \tilde{S} \) is the space of symmetric, traceless \( 3 \times 3 \) matrices.
Defect locations [3, 26]: The configuration \( (a_1, \ldots, a_{|d|}) \) minimizes the renormalized energy \( W \) over \( (b_1, \ldots, b_{|d|}) \in \Omega^{|d|}, \) which is defined by

\[
W(b_1, \ldots, b_{|d|}) = -2\pi \sum_{i \neq j} \log |b_i - b_j| - 2\pi \sum_{i, j} R(b_i, b_j)
\]  

where \( R(x, y) = \Psi(x, y) - \log |x - y|, x, y \in \mathbb{R}^2 \) and \( \Psi(x, y) \) is given by the solution of an explicit boundary-value problem.

Far-field behaviour [3, 26]: Let \( \{ Q^{L_k} \} \) denote a sequence of global energy minimizers for \( (15) \), where \( L_k \to 0^+ \) as \( k \to \infty \). Then (up to a subsequence),

\[
Q^{L_k} \to Q^* \text{ in } C^{1,\alpha} (\bar{\Omega} \setminus \Theta_{L_k}), \quad \forall \alpha < 1 \text{ and in } W^{1,p}(\Omega), \quad \forall p \in [1, 2)
\]

for some \( Q^* \in \cap_{1 \leq p < 2} W^{1,p}(\Omega; S^1) \). The limit \( Q^* \) is the canonical harmonic map associated with \( a_1, \ldots, a_{|d|} \) and the degrees \( \text{sgn } d, \ldots, \text{sgn } d \).

The interested reader is referred to [3, 26] for the proofs.

4 Uniaxial minimizers and their defect sets in 3D

Let \( \Omega \subset \mathbb{R}^3 \) be a bounded, connected and simply-connected domain with smooth boundary. An arbitrary \( Q \)-tensor field, \( Q : \Omega \to S \) can be written as

\[
Q = \sum_{i=1}^{3} \lambda_i e_i \otimes e_i \quad \sum_i \lambda_i = 0
\]

where \( e_i \) are the orthonormal eigenvectors, \( \lambda_i \) are the corresponding eigenvalues and \( \text{tr} Q^2 \neq 0 \) in general.

We study uniaxial global minimizers of the Landau-de Gennes energy functional, \( I_{LG} \) in (3), in the admissible space \( \mathcal{A}_Q = \{ Q \in W^{1,2}(\Omega; S) ; Q = Q_b \text{ on } \partial \Omega \} \). The corresponding Euler-Lagrange equations are

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

where the term \( b^2 \frac{\delta_{ij}}{3} \text{tr}(Q^2) \) is a Lagrange multiplier associated with the tracelessness constraint. It follows from standard arguments in elliptic regularity that a global minimizer \( Q^* \) is actually a classical solution of (21) and \( Q^* \) is smooth and real analytic on \( \Omega \), up to the boundary [15].

We assume that a uniaxial global minimizer exists for each \( L > 0 \). For \( Q \) uniaxial (of the form \( Q = s(n \otimes n - \frac{1}{3} I) \) where \( s : \Omega \to \mathbb{R} \) and \( n \in W^{1,2}(\Omega; S^2) \), see [2]), a direct calculation shows that

\[
\left( Q_{ik} Q_{kj} - \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right) = \frac{s}{3} Q_{ij}
\]

and hence, the Euler-Lagrange equations (21) simplify to

\[
L Q_{ij, kk} = \frac{1}{3} \left( 2c^2 s^2 - b^2 s - 3a^2 \right) Q_{ij}, \quad i, j = 1 \ldots 3.
\]
Let $Q^L$ denote a uniaxial global Landau-de Gennes minimizer for a fixed $L > 0$. Then $Q^L$ is a classical solution of (21) and we are interested in the qualitative properties of $Q^L$ in the limit $L \to 0$.

We briefly comment on limiting harmonic maps in a 3D setting: $Q^0 = s_+ (n_0 \otimes n_0 - \frac{1}{3} I)$ where $n_0$ is an energy minimizing harmonic map in the admissible space $A_n = \{ n \in W^{1,2}(\Omega; S^2); n = n_0 \text{ on } \partial \Omega \}$. Let $S_0$ denote the singular set of $n_0$ (and hence, of $Q^0$). Then $S_0$ consists of precisely $|d|$ isolated point singularities [15, 24].

We, next, quote important results from [15, 16] that are crucial for the analysis in this paper.

**Maximum principle** [16]: Let $Q$ be an arbitrary solution (not necessarily uniaxial) of the Euler-Lagrange equations (21) in the space $A_Q$. Then

\[ \|Q\|_{L^\infty(\Omega)} \leq \sqrt{\frac{2}{3}} s_+ \]  

where $s_+$ has been defined in [3].

**Strong convergence to $Q^0$** [15]: Let $\Omega \subset \mathbb{R}^3$ be a bounded, connected and simply-connected domain with smooth boundary. Let $\{Q^{L_k}\}$ be a sequence of uniaxial global minimizers of $I_{LG}$ in the admissible space $A_Q$ ($I_{LG}$ and $A_Q$ have been defined in [3] and [8] respectively) where $L_k \to 0$ as $k \to \infty$. Then $Q^{L_k} \to Q^0$ strongly in $W^{1,2}(\Omega; S)$ (upto a subsequence), where $Q^0$ has been defined in [9].

**Interior and boundary monotonicity lemmas** [15]: Let $Q$ be an arbitrary solution of the Euler-Lagrange equations (21). Define the normalized energy on balls $B(x, r) \subset \Omega = \{ y \in \Omega : |x - y| \leq r \}$:

\[ F(Q, x, r) = \frac{1}{r} \int_{B(x, r)} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV. \]

Then we have the following interior monotonicity lemma:

\[ F(Q, x, r) \leq F(Q, x, R) \quad \forall x \in \Omega; \ r \leq R \text{ and } B(x, R) \subset \Omega. \tag{24} \]

Similarly, for $x_0 \in \partial \Omega$, we define the region $\Omega_r = \Omega \cap B(x_0, r)$ with $r > 0$, and the corresponding normalized energy to be

\[ E(Q, x_0, r) = \frac{1}{r} \int_{\Omega_r} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV. \]

Then there exists $r_0 > 0$ so that

\[ \frac{d}{dr} E \geq -C \left( a^2, b^2, c^2, Q_b, r_0, \Omega \right) \quad 0 < r < r_0 \tag{25} \]

where the positive constant $C$ is independent of $L$.

The proofs of (24) and (25) follow a standard pattern using the Pohozaev identity; complete details can be found in [15]. An immediate consequence of the strong convergence and the monotonicity lemmas is the following:

**Convergence of bulk energy density away from $S_0$** [15]: Let $\{Q^{L_k}\}$ be a sequence of global Landau-de Gennes energy minimizers in the admissible space $A_Q$, where $L_k \to 0$ as $k \to \infty$. Assume that we have a sequence $Q^{L_k}$ with $L_k \to 0$ as $k \to \infty$, such that $Q^{L_k} \to Q^0$ in $W^{1,2}(\Omega, S)$, as $k \to \infty$, where $Q^0$ has been defined in [9].

For any compact set $K \subset \bar{\Omega}$ such that $K$ contains no singularity of $Q^0$, we have that

\[ \lim_{L_k \to 0} f_B(Q^{L_k}(x)) = 0 \quad x \in K \tag{26} \]
and the limit is uniform on $K$.

Consider a sequence of uniaxial global Landau-de Gennes energy minimizers $Q^{L_k}$ such that $L_k \to 0$ as $k \to \infty$. Then $Q^{L_k}$ can be written in the form

$$Q^{L_k} = s^{L_k} \left( n^{L_k} \otimes n^{L_k} - \frac{1}{3} I \right)$$

(27)

for $s^k : \Omega \to \mathbb{R}$ and $n^k \in W^{1,2}(\Omega; S^2)$. Then (26) implies that (up to subsequence), $s^k$ converges uniformly to $s_+$ everywhere away from $S_0$ i.e. we have

$$\left| s^k(x) - s_+ \right| \leq \epsilon(L_k, x) \quad x \in \bar{\Omega} \setminus B_\delta(S_0)$$

(28)

where $\epsilon \to 0^+$ as $k \to \infty$, $B_\delta(S_0)$ is a small $\delta$-neighbourhood of the singular set $S_0$ and $0 < \delta < 1$ is an arbitrary small constant independent of $L$.

**Uniform convergence in the interior** [15]: Let $\{Q^{L_k}\}$ be a sequence of global Landau-de Gennes minimizers in $A_Q$ such that $L_k \to 0$ as $k \to \infty$. Then (up to a subsequence) $Q^{L_k} \to Q^0$ strongly in $W^{1,2}(\Omega, \mathbb{S})$.

Let $K \subset \Omega$ be a compact set which does not contain any singularities of $Q^0$. We define

$$\epsilon_L(Q^L) = \frac{1}{2} |\nabla Q^L|^2 + \frac{f_B(Q)}{L}.$$  

Then

(i) there exists a constant $C > 0$ independent of $L$ such that

$$- \Delta \epsilon_L(Q^L)(x) \leq C \epsilon_L^2(Q^L)(x) \quad x \in K$$

(29)

for $L$ sufficiently small;

(ii) we have a uniform bound for $\epsilon_L(Q^L)$ in the interior of $\Omega$, away from $S_0$ in the limit $L \to 0^+$ i.e.

$$\epsilon_L(Q^L)(x) \leq C'(a^2, b^2, c^2, \Omega) \quad x \in K$$

(30)

for all $L$ sufficiently small and a positive constant $C'$ independent of $L$;

(iii) $Q^{L_k}$ converges uniformly to $Q^0$ everywhere in the interior of $\Omega$, away from $S_0$.

$$\lim_{k \to \infty} Q^{L_k}(x) = Q^0(x) \text{ uniformly for } x \in K.$$  

(31)

We emphasize that (30) and (31) only hold in the interior of $\Omega$. In Section 5 we extend these uniform convergence results up to the boundary for the uniaxial case.

A uniaxial global Landau-de Gennes minimizer $Q^L$ is fully characterized by its scalar order parameter $s^L$ and distinguished eigenvector $n^L$. The scalar order parameter, $s^L$, is a locally Lipschitz function of $Q^L$ and hence, is continuous on $\Omega$ [27]. From [10], we have that

$$0 \leq s^L(x) \leq s_+ \quad x \in \bar{\Omega}$$

(32)

and let $\Theta_L = \{x \in \Omega; s^L(x) = 0\}$ denote the isotropic set of $Q^L$. We have a topologically non-trivial boundary condition $Q_b$ in [7] and hence, every interior extension of $Q_b$ must have discontinuities. We interpret the defect set of $Q^L$ as being the defect set of $n^L$. Let $S^L_n$ denote the defect set of $n^L$ and let $x_n \in S^L_n$. Then $Q^L(x_n) = 0$, since $Q^L$ is well-defined on $\bar{\Omega}$ and consequently $s^L(x_n) = 0$. We deduce that $S^L_n \subset \Theta_L$ and from [21], we have that $n^L$ is analytic everywhere away from $\Theta_L$. We first make an elementary observation about the defect locations as $L \to 0^+$.
**Lemma 1** Let $S_0$ denote the singular set of the limiting harmonic map $Q^0$ defined in $(\ref{2})$. Let $x_n \in S^L_n$. Then

$$\text{dist} \left(x_n, S_0\right) \leq \varepsilon(L)$$

where $\varepsilon(L) \to 0$ as $L \to 0^+$. 

**Proof:** Let $x_n \in S^L_n$. As mentioned above, $s^L(x_n) = 0$ and $x_n \in \Theta_L$, where $\Theta_L$ has been defined above. However, the bulk energy density $f_B(Q^L)$ converges uniformly to its minimum value, everywhere away from $S_0$, in the interior and up to the boundary, as $L \to 0$. Recalling (28), we deduce that $\text{dist}(x_n, S_0) \to 0$ as $L \to 0^+$. Lemma 1 now follows. □

Lemma 1 is also equivalent to the statement $\text{dist}(\Theta_L, S_0) \to 0$ as $L \to 0^+$ i.e. the isotropic set of a uniaxial global Landau-de Gennes energy minimizer converges to the singular set of a limiting harmonic map in the limit of vanishing elastic constant.

**Proposition 1** Let $Q^L$ be an uniaxial global minimizer of $\mathcal{I}_\Theta(Q)$ in the admissible space $\mathcal{A}_Q$, for a fixed $L > 0$. Then $Q^L = s^L (n^L \otimes n^L - \frac{1}{3}I)$ for some non-negative function $s : \overline{\Omega} \to \mathbb{R}^+$ and $n \in W^{1,2}(\Omega; S^2)$. The following equations hold everywhere in $\Omega$, away from the isotropic set $\Theta_L$:

$$\Delta s^L - 3s^L |\nabla n^L|^2 = \frac{s^L}{3L} \left(2c^2(s^L)^2 - b^2s^L - 3a^2\right)$$

$$\Delta n^L_j + |\nabla n^L|^2 n^L_j + 2 \frac{\partial s^L}{\partial x^j} n^L_{j,k} = 0 \quad j,k = 1,2,3. \tag{34}$$

Here $n^L_{j,k}$ denotes the partial derivative $\frac{\partial n^L_j}{\partial x^k}$. Alternatively, $n^L = (\sin \theta^L \cos \phi^L, \sin \theta^L \sin \phi^L, \cos \theta^L)$, where $\theta^L, \phi^L$ are functions of spherical polar coordinates $(r, \theta, \phi)$ centered at the origin. Then $\theta^L$ and $\phi^L$ satisfy the following coupled nonlinear partial differential equations

$$\nabla \cdot ((s^L)^2 \nabla \theta^L) = (s^L)^2 \sin \theta^L \cos \theta^L |\nabla \phi^L|^2$$

$$\nabla \cdot ((s^L)^2 \sin^2 \theta^L \nabla \phi^L) = 0. \tag{35}$$

**Remark:** In general, $Q \in W^{1,2}$ implies that the tensor $n \otimes n \in W^{1,2}$. However, for simply-connected three-dimensional domains, $n \otimes n \in W^{1,2}(\Omega) \implies n \in W^{1,2}(\Omega; S^2)$. [1]

**Proof:** In what follows, we drop the superscript $L$ from $Q^L$ for brevity. Since $Q$ is a classical solution of (22), we have that

$$Q_{ij,k} = \frac{\partial s}{\partial x^j} n_i n_j + \frac{1}{3} \partial_{ij} + s(n_{i,j,k} + n_{j,i,k})$$

$$Q_{ij, kk} = \Delta s \left(n_i n_j - \frac{1}{3} \delta_{ij}\right) + 2 \partial_{k}s \left(n_{i,j,k} + n_{j,i,k}\right) + s(n_{i,j,k} + n_{j,i,k} + 2n_{i,k} n_{j,k}) \tag{37}$$

where $i, j, k = 1 \ldots 3, Q_{ij,k} = \frac{\partial Q_{ij}}{\partial x^k}$ etc.

Consider the decoupled equations (22)

$$LQ_{ij, kk} = \frac{1}{3} \left(2c^2 s^2 - b^2 s - 3a^2\right) Q_{ij}$$

and multiply both sides by $n_i$ to get the following vector equation

$$\frac{2}{3} n_j \Delta s + 2 \partial_{k} s n_{j,k} + s(n_{j,k,k} + n_{j,k} + 2n_{i,k} n_{j,k}) = \frac{2s}{2L} \left(2c^2 s^2 - b^2 s - 3a^2\right) n_j. \tag{38}$$
Multiplying both sides of (38) by \( n_j \), we obtain the following scalar equation for \( s \):

\[
\frac{2}{3} \Delta s - 2s |\nabla n|^2 = \frac{2s}{9L} \left( 2c^2 s^2 - b^2 s - 3d^2 \right) \tag{39}
\]

and (33) now follows. In (38) and (39), we use (37) and the relations \( n_i n_i = 1 \), \( n_i n_{i,k} = 0 \) and \( n_i n_{i,kk} = -|\nabla n|^2 \).

For (34), we multiply both sides of the vector equation (38) by \( n_j \) for \( p = 1, 2, 3 \) to get the following system of three equations -

\[
2 \partial_k s n_{j,p} n_{j,k} + s n_{j,p} n_{j,kk} = 0 \quad p = 1, 2, 3. \tag{40}
\]

Multiplying both sides by the scalar order parameter \( s \), (40) simplifies to

\[
\partial_k \left( s^2 n_{j,k} \right) = \lambda_1 n_j + \lambda_2 e_j \tag{41}
\]

where

\[
\lambda_1 = n_j \partial_k \left( s^2 n_{j,k} \right) = -s^2 |\nabla n|^2.
\]

We substitute (42) into (38) to get

\[
\frac{2s}{3} n_j \Delta s - 2s^2 |\nabla n|^2 n_j + \lambda_2 e_j = \frac{2s}{9L} \left( 2c^2 s^2 - b^2 s - 3d^2 \right) n_j
\]

from which we deduce that \( \lambda_2 = 0 \). Hence

\[
\partial_k \left( s^2 n_{j,k} \right) + s^2 |\nabla n|^2 n_j = 0 \quad j = 1 \ldots 3 \tag{43}
\]

from which (34) follows.

An alternative formulation of (41) can be obtained by writing the unit-vector field \( n \) in terms of its spherical angles, \( \theta^L(r, \theta, \phi) \) and \( \phi^L(r, \theta, \phi) \), where \( (r, \theta, \phi) \) are spherical polar coordinates centered at the origin i.e.

\[
n = \left( \sin \theta^L \cos \phi^L, \sin \theta^L \sin \phi^L, \cos \theta^L \right). \tag{44}
\]

Straightforward computations show that

\[
\frac{\partial n}{\partial x_k} = \partial_k \theta^L \left( \cos \theta^L \cos \phi^L, \cos \theta^L \sin \phi^L, -\sin \theta^L \right) + \sin \theta^L \partial_k \phi^L \left( -\sin \phi^L, \cos \phi^L, 0 \right)
\]

\[
\frac{\partial^2 n}{\partial x_k \partial x_k} = \partial_{kk} \theta^L \left( \cos \theta^L \cos \phi^L, \cos \theta^L \sin \phi^L, -\sin \theta^L \right) - \left( \partial_k \theta^L \right)^2 \left( \sin \theta^L \cos \phi^L, \sin \theta^L \sin \phi^L, \cos \theta^L \right) + 2 \cos \theta^L \partial_k \theta^L \partial_k \phi^L \left( -\sin \phi^L, \cos \phi^L, 0 \right) + \sin \theta^L \partial_{kk} \phi^L \left( -\sin \phi^L, \cos \phi^L, 0 \right) - \sin \theta^L \left( \partial_k \phi^L \right)^2 \left( \cos \phi^L, \sin \phi^L \right)
\]

Substituting (45) into (38) and taking the dot product of both sides with \( \left( \cos \theta^L \cos \phi^L, \cos \theta^L \sin \phi^L, -\sin \theta^L \right) \), we obtain

\[
2 \partial_k \theta^L + s \partial_{kk} \theta^L - s \sin \theta^L \cos \theta^L |\nabla \phi^L|^2 = 0. \tag{46}
\]
We multiply both sides of (46) by $s$ and equation (53) now follows. Similarly, we take the scalar product of (53) with the unit-vector $(-\sin \phi^L, \cos \phi^L, 0)$ to obtain

$$s \sin \theta^L \partial_k \phi^L + 2s \cos \theta^L \partial_k \theta^L \partial_k \phi^L + 2 \sin \theta^L \partial_k \theta^L \partial_k \phi^L = 0.$$  \hfill (47)

As above, we multiply both sides of (47) by $s \sin \theta$ and (56) then follows. The proof of Proposition 1 is now complete. \hfill □

Comment: We note that for $s$ constant, (56) is equivalent to the harmonic map equations $\Delta n_0 + |\nabla n_0|^2 n_0 = 0$ \cite{23}.

Next, we use asymptotic methods to predict the minimizer profile near isolated isotropic points in $\Theta_L$ and establish a $1 - 1$ correspondence between isolated isotropic points and isolated point defects.

**Proposition 2** Let $Q^L$ be an uniaxial global minimizer of $I_{LG}$ in the admissible space $A_Q$, for a fixed $L > 0$. Then $Q^L(x) = s^L(x) \left( n^L(x) \otimes n^L(x) - \frac{1}{3} I \right)$. Let $Gn \subset \Theta$ denote the set of isolated point defects in $n^L$ and let $\Gamma_L \subset \Omega$ denote the set of isolated isotropic points of $Q^L$.

(i) Let $x_L \in \Gamma_L$ be an isolated interior isotropic point. Let $(r, \theta, \phi)$ denote a local spherical co-ordinate system centered at $x_L$; then

$$\left| \nabla n^L \right|^2 \sim \frac{\alpha(\theta, \phi)}{r^2} \text{ as } r \to 0$$ \hfill (48)

where $\alpha$ only depends on $\theta, \phi$ and is independent of the radial coordinate $r$. Then $x_L \in \Gamma_n$ too.

(ii) Let $x_n \in \Gamma_n$ be an isolated point defect. Then $x_n \in \Gamma_L$ and hence, $\Gamma_n = \Gamma_L$.

**Proof:** (i) Consider the coupled equation (33):

$$\Delta s - 3s |\nabla n|^2 = \frac{s}{3L} \left( 2c^2 s^2 - b^2 s - 3a^2 \right)$$ \hfill (49)

Let $x_L \in \Gamma_L$ be an isolated isotropic point. Since $s^L(x) = \frac{2}{3} Q^L(x) \left( n^L(x) \otimes n^L(x) - \frac{1}{3} I \right)$ is the product of two analytic matrices away from $x_L$, we deduce that $s^L(x)$ is analytic for $0 < r < r_0$, for some $r_0 > 0$. We are interested in the leading-order behaviour of $|\nabla n^L|^2$ as $r \to 0$.

From the local analyticity of $s^L$, we have the following power series expansion

$$s^L(x) = r^n g(\theta, \phi) + h(r, \theta, \phi) \quad 0 < r < r_0 < r_1, \ n \geq 1,$$ \hfill (50)

where $(r, \theta, \phi)$ is a local spherical coordinate system centered at $x_L$, $\frac{h(r)}{r^2} = o(1)$ as $r \to 0$ and $r_0$ is the radius of convergence of the series \cite{30}. Further, $g \neq 0$ for $r \neq 0$ and $\{g, h\}$ are analytic functions with bounded derivatives in a sufficiently small neighbourhood of $x_L$. Substituting (50) into (49) and expressing $\Delta s^L$ in spherical polar coordinates

$$\Delta s^L = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial s^L}{\partial r} \right) + \frac{1}{r^2 \sin^2 \phi} \frac{\partial^2 s^L}{\partial \theta^2} + \frac{1}{r^2 \sin \phi} \frac{\partial}{\partial \phi} \left( \sin \phi \frac{\partial s^L}{\partial \phi} \right),$$ \hfill (51)

we have that

$$r^{-2} \left[ n(n + 1) g + \frac{g_{\theta \theta}}{\sin^2 \phi} + g_{\phi \phi} + \cot \phi g_{\phi} \right] +$$

$$+ \frac{2h_r}{r} + h_{rr} + \frac{h_{\theta \theta}}{r^2 \sin^2 \phi} + \frac{h_{\phi \phi}}{r^2} + \cot \phi \frac{h_{\phi}}{r^2} -$$

$$- 3|\nabla n^L|^2 \left( r^n g(\theta, \phi) + h(r, \theta, \phi) \right) =$$

$$= \left( r^n g + h \right) \left( \frac{1}{3L} \left[ 2c^2 (r^n g + h)^2 - b^2 (r^n g + h) - 3a^2 \right] \right) \text{ as } r \to 0.$$ \hfill (52)
All the terms on the right-hand side are $O(r^n)$ whereas the leading order term on the left-hand side of (52) is $O(r^{n-2})$. Since $h$ is an analytic function and $\frac{h}{r^n} = o(1)$ as $r \to 0$, we have that $h_r/r, h_{rr} = o(r^{n-2})$ as $r \to 0$. Therefore, for (52) to hold as $r \to 0$, we must have

$$|\nabla n|^2 \sim \frac{1}{3r^2} \left[ n(n+1) + \frac{g_{\theta\theta}}{g \sin^2 \phi} + \frac{g_{\phi\phi}}{g} + \cot \phi \frac{g_{\phi}}{g} \right] \text{ as } r \to 0 \quad (53)$$

and (48) now follows. It follows that $|\nabla n|^2$ is not defined as $r \to 0$ and hence, the isolated isotropic point $x_L \in \Gamma_n$ too.

(ii) Let $x_n \in \Gamma_n$. Then $Q^L(x_n) = 0$, since $Q^L$ is well-defined on $\bar{\Omega}$. Therefore, we must have $s^L(x_n) = 0$ and by definition, $x_n \in \Gamma_L$. Combining (i) and (ii), we conclude that $\Gamma_L = \Gamma_n$. □

Comment: By analogy with [18], one might expect that uniaxial global minimizers can only account for isolated point defects and all higher-dimensional defects are intrinsically biaxial. We hypothesize that $n = 2$ in (50) i.e. we have a quadratic decay of the scalar order parameter as we approach point defects, by analogy with the study of vortices in Ginzburg-Landau theory [17].

Comment: The estimate (48) is analogous to a similar result on singularity profiles within the Oseen-Frank theory of uniaxial nematic liquid crystals with a constant scalar order parameter $s$ [5]. In [5], the authors show that near every singularity $x_p \in \Omega$, we have

$$n \sim R \frac{x - x_p}{|x - x_p|} \quad (54)$$

for some rotation $R \in SO(3)$. Therefore,

$$|\nabla n|^2 \sim \frac{2}{|x - x_p|^2} \text{ as } x \to x_p.$$

The estimate (48) suggests that we have a similar radial hedgehog-type of profile (54) near the isolated zero $x_L \in \Omega$, for uniaxial global minimizers within the Landau-de Gennes theory.

5 Far-field results

In this section, we study the qualitative properties of uniaxial global minimizers $\{Q^L\}$ away from the isotropic set $\Theta_L$, in the limit $L \to 0$. This is equivalent to studying the qualitative properties of $\{Q^L\}$ away from the singular set $S_0$ of the limiting harmonic map $Q^0$ defined in [9], as $L \to 0^+$. Let $Q^L = s^L (n^L \otimes n^L - \frac{1}{3} I)$ be a uniaxial global minimizer for fixed $L > 0$. Recall that for $L$ sufficiently small,

$$0 \leq s_+ - s^L(x) \leq \epsilon_1(L) \quad (55)$$

or equivalently

$$|Q^L|^2 - \frac{2}{3} s_+^2 \leq \epsilon_2(L) \quad (56)$$

where $\epsilon_1(L), \epsilon_2(L) \to 0$ as $L \to 0^+$, everywhere away from $S_0$.

Our first result is an inequality for

$$A^L = \frac{1}{2} Q^L_{ij,k} Q^L_{ij,k}$$

that holds everywhere away from $S_0$ on $\Omega$. We do not use Lemma 2 in the subsequent sections but keep it as an interesting technical result.
Lemma 2. Let \( A^L = \frac{1}{2} Q_{ij,k}^L Q_{ij,k}^L \) by definition. Then we have the following inequality on \( \Omega \setminus B_\delta(S_0) \) for \( L \) sufficiently small

\[-\Delta A^L + |D^2 Q^L|^2 \leq \frac{1}{\alpha^2} |D^2 Q^L|^2 + \alpha^4 \frac{A^L}{|Q|^2}\]  

(57)

where \( \alpha > 1 \) is a positive constant independent of \( L \) that can be worked out explicitly, \( B_\delta(S_0) \) is a small \( \delta \)-neighbourhood of \( S_0 \) and \( \delta > 0 \) is independent of \( L \).

Proof: The derivation of (57) closely follows the methods in [4]. In what follows, we drop the superscript \( L \) for brevity. First, consider the decoupled equations (22); setting \( f(s) = \left(2c^2 s^2 - b^2 s - 3a^2\right) \)

and differentiating both sides of (22) with respect to \( x_p \), we obtain

\[ Q_{ij,kp} = Q_{ij,p}^3 L f(s) + f'(s) \frac{Q_{ij} Q_{rs} Q_{rs,p}}{\sqrt{6}L} |Q| \text{ for } p = 1, 2, 3. \]  

(58)

From (56) and the global upper bound (23), we have that \(|Q|\) is bounded away from zero on \( \Omega \setminus B_\delta(S_0) \) and

\[ f(s) \leq 0, \quad f'(s) > 0, \quad f''(s) > 0, \]  

(59)

on the set \( \Omega \setminus B_\delta(S_0) \), where \( f'(s) = \frac{df}{ds}, f''(s) = \frac{d^2f}{ds^2} \) etc. A straightforward computation shows that

\[ \Delta A = |D^2 Q|^2 + Q_{ij,k} Q_{ij,ppk} \]  

(60)

and using (58), we obtain

\[ \Delta A = |D^2 Q|^2 + |\nabla Q|^2 \frac{f(s)}{3L} + \frac{f'(s)}{\sqrt{6}L} \frac{|Q| \cdot \nabla Q|^2}{|Q|}. \]  

(61)

From (59) and (22), we have the following inequality

\[-\Delta A + |D^2 Q|^2 \leq |\nabla Q|^2 \frac{|\Delta Q|}{|Q|}. \]  

(62)

Finally, we use the inequality

\[ |\Delta Q| \leq \alpha |D^2 Q| \]

where \( \alpha > 1 \) is a positive constant that can be worked out explicitly. Substituting the above into (62),

\[-\Delta A + |D^2 Q|^2 \leq 2\alpha A |D^2 Q| \leq \frac{1}{\alpha^2} |D^2 Q|^2 + \alpha^4 \frac{A^2}{|Q|^2} \]  

(63)

and (57) now follows. □

We recall the uniform convergence result in (31) and (30), whereby we establish a uniform bound for \(|\nabla Q|^L|\), independent of \( L \), everywhere away from \( S_0 \) in the interior of \( \Omega \). The next step is to extend this uniform convergence result up to the boundary. To do so, we adapt the small energy
regularity theorem in [7] to the Landau-de Gennes framework to obtain a uniform bound for $|\nabla Q^L|$ independent of $L$, everywhere away from $S_0$ up to the boundary.

Consider a boundary point $x_0 \in \partial \Omega$ and define the region $\Omega_r(x_0) = \Omega \cap B_r(x_0)$, where $B_r(x_0)$ is a ball of radius $r$ centered at $x_0$. Let $\rho$ be a suitably small positive constant such that for any $x_0 \in \partial \Omega$, we may choose a coordinate system $\{x_\alpha\}$ so that $x_0$ is at the origin and $\Omega_\rho(x_0)$ corresponds to $B^*_\rho(x_0) = \{x \in \Omega; |x| \leq \rho; x_3 \geq 0\}$.

**Proposition 3** Let $\{Q^{L_k}\}$ be a sequence of uniaxial global minimizers for $I_{LG}$ in the admissible space $\mathcal{A}_Q$, where $L_k \to 0$ as $k \to \infty$. We can extract a subsequence such that $Q^{L_k} \to Q^0$ strongly in $W^{1,2}(\Omega; S)$ as $k \to \infty$. Let $x_0 \in \partial \Omega$ be such that $\Omega_r(x_0)$ contains no singularity of the limiting harmonic map $Q^0$. Then there exists $C_1 > 0, C_2 > 0, r_0 > 0, L_0 > 0$ (all constants independent of $L_k$) so that if

$$\int_{\Omega_r(x_0)} \frac{1}{2} |\nabla Q^L|^2 + \frac{f_B(Q^L)}{L} \, dx \leq C_1 \quad r < \min \{r_0, \rho\}$$

then

$$r^2 \sup_{\Omega_{r/2}(x_0)} e_L(Q^L) \leq C_2 \quad \text{for all } L_k < L_0$$

where

$$e_L(Q^L) = \frac{1}{2} |\nabla Q^L|^2 + \frac{f_B(Q^L)}{L}.$$

**Proof:** The first half of the proof of Proposition 3 closely follows the scaling arguments for the interior uniform convergence result (30) in [15] and the second half closely follows the arguments in Theorem 2.1 in [7].

We first recall from (26) that since $\Omega_r(x_0)$ contains no singularity of $Q^0$, $\exists m(x) \in S^2$ such that

$$|Q^L(x) - s_+ \left( m(x) \otimes m(x) - \frac{1}{3} I \right)| < \epsilon_0 << 1 \quad x \in \Omega_r(x_0)$$

for $L$ sufficiently small.

We continue reasoning similarly to [15]. We fix an arbitrary $L_k < L_0$. We let $0 < r_1 < \frac{2r}{3} < \min \left\{ \frac{2r_0}{3}, \frac{2\rho}{3} \right\}$ and $x_1 \in \Omega_{r_1}(x_0)$ be such that

$$\max_{0 \leq s \leq \frac{2r}{3}} \left( \frac{2r}{3} - s \right)^2 \max_{\Omega_{r_1}(x_0)} e_{L_k}(Q^{L_k}) = \left( \frac{2r}{3} - r_1 \right)^2 e_{L_k}(Q^{L_k})(x_1).$$

Define $e^{L_k}_1 = \max_{x \in \Omega_{r_1}(x_0)} e_{L_k}(Q^{L_k}) = e_{L_k}(Q^{L_k})(x_1)$. Then

$$\max_{\Omega_{2/3r_1}(x_1)} e_{L_k}(Q^{L_k}) \leq 4e^{L_k}_1$$

where we use the inclusion $\Omega_{2/3r_1}(x_1) \subset \Omega_{2/3r_1}(x_0)$, $\frac{2/3r_1}{2} \leq \frac{2r}{3}$ by definition of $r_1$ and the inequalities (67).

Define $r_2 = \frac{2/3r_1}{2} \sqrt{e^{L_k}_1}$ and let

$$R^{L_k}(x) = Q^{L_k} \left( x_1 + \frac{x}{\sqrt{e^{L_k}_1}} \right).$$

(69)
Let $L_k = e_1^{L_k} L_k$. Then $R^{L_k}$ has the following properties on $\Omega_{r_2}(0)$:

$$e_{L_k}(R^{L_k}) = \frac{1}{e_1^{L_k}} e_{L_k}(Q^{L_k})$$

(70)

$$\max_{x \in \Omega_{r_2}(0)} e_{L_k}(R^{L_k}) \leq 4 \quad e_{L_k}(R^{L_k})(0) = 1$$

(71)

$$R^{L_k}_{ij,kk} = \frac{1}{L_k} (2e^2 s^2 - b^2 s - 3a^2) R^{L_k}_{ij}$$

(72)

where $s^2 = \frac{3}{2} |Q^{L_k}|^2$.

We next claim that $r_2 \leq 1$. It is obvious that $r_2 \leq 1$ implies the conclusion (65). We prove this claim by contradiction. Assume that $r_2 > 1$; then using the same arguments as in (73), one is led to the existence of a sequence of solutions $\{R^{L_k}\}$ of (72) on $\Omega_1(0) = B^+_1(0)$, with the following properties:

$$-\Delta R^{L_k}_{ij} + \frac{1}{L_k} (2e^2 s^2 - b^2 s - 3a^2) R^{L_k}_{ij} = 0 \text{ in } B^+_1(0)$$

$$\max_{x \in B^+_1(0)} e_{L_k}(R^{L_k}) \leq 4 \quad e_{L_k}(R^{L_k})(0) = 1$$

$$R^{L_k}|_{x_3 = 0} = Q_b \left( x + \frac{x_3}{\sqrt{e_1^{L_k}}} \right) \text{ with}$$

$$|\nabla R^{L_k}|_{x_3 = 0} \leq \epsilon_k |\nabla Q_b|_{L^\infty(\partial \Omega)}, \quad |\nabla^2 R^{L_k}|_{x_3 = 0} \leq \epsilon_k^2 |\nabla^2 Q_b|_{L^\infty(\partial \Omega)} \text{ with } \epsilon_k \to 0 \text{ as } k \to \infty$$

$$\int_{B^+_1(0)} e_{L_k}(R^{L_k}) \, dx \leq \delta_k \to 0^+ \text{ as } k \to \infty.$$  

(73)

From (29) and (71), we deduce that $R^{L_k}$ satisfies the following Bochner-type inequality on $B^+_1(0)$:

$$-\Delta e_{L_k}(R^{L_k}) \leq C' e_{L_k}(R^{L_k}) \quad x \in B^+_1(0)$$

(74)

where $C'$ is a constant independent of $L_k$.

Next, we write $R^{L_k}$ explicitly in terms of its scalar order parameter and leading eigenvector -

$$R^{L_k}_{ij} = s_k \left( n_k^n n_j^n - \frac{1}{3} \delta_{ij} \right) \quad n_k^n \in W^{1,2}(\Omega; S^2)$$

(75)

where $|R^{L_k}|^2 = \frac{2}{3} s_k^2$ and

$$|s_k - s_+| \leq \frac{s_+}{100}$$

from (66), for $k$ sufficiently large. From Proposition II we have that $s_k$ and $n_k^n$ satisfy the following equations in $B^+_1(0)$:

$$\Delta s_k - 3s_k |\nabla n_k^n|^2 = \frac{s_k}{3L_k} (2e^2 s_k^2 - b^2 s_k - 3a^2)$$

(76)

$$\Delta n_k^n + |\nabla n_k^n|^2 + \frac{2}{s_k} \frac{\partial_p s_k}{s_k} n_{kp}^k = 0$$

(77)

$$|\nabla R^{L_k}|^2 = \frac{2}{3} |\nabla s_k|^2 + 2s_k^2 |\nabla n_k^n|^2 \leq 4.$$  

(78)
From (66) and (78), we deduce that
\[ |\nabla n_k| \leq \frac{2}{s_+}, \quad \left| \frac{2\nabla s_k}{s_k} \right| \leq \frac{6}{s_+} \quad \text{on } B_1^+(0). \] (79)

We combine (79) and (77) to deduce that
\[ \sup_{B_2^{4/3}(0)} |\nabla n_k|^2 \leq c_0 \delta_k^{4/3} \rightarrow 0 \quad k \rightarrow \infty \] (80)

where \( c \) is a constant independent of \( k \). In particular, this implies that \( ||\nabla n_k||_{L^\infty(\partial\Omega)} \leq c_0 \delta_k^{4/3} \rightarrow 0 \) as \( k \rightarrow \infty \). The proof of (80) is identical to the proof of Theorem 2.1 in [7] and the details are omitted for brevity.

Next, look at the equation (33) and introduce the function
\[ \bar{s}_k = s_+ - s_k. \]

Then \( \bar{s}_k \) is a solution of the following problem on \( B_1^+(0) \):
\[ -\Delta \bar{s}_k = 3s_k |\nabla n_k|^2 - \frac{2c_2 s_k \bar{s}_k (s_k - s_-)}{3L_k}, \]
\[ \bar{s}_k(x) = 0 \quad x \in \{ B_1^+(0) \cap x_3 = 0 \} \] (81)

where \( s_- < 0 \) is a constant. Repeating the same arguments as in [7], we obtain the following estimates:
\[ \bar{s}_k(x) \leq c_1 x_3 \delta_k^{1/3} \quad x \in B_{1/2}^+(0) \]
\[ ||\nabla \bar{s}_k||_{L^\infty(\partial\Omega)} = ||\nabla s_k||_{L^\infty(\partial\Omega)} \leq c_0 \delta_k^{4/3} \rightarrow 0 \quad k \rightarrow \infty \] (82)

where \( c_0 \) and \( c_1 \) are positive constants independent of \( L \).

Finally, we define \( \tilde{e}_k = \max \left\{ 0, e_{L_k}(R \delta_k) - (c + c_0) \delta_k^{4/3} \right\} \). (Recall that \( f_B(R \delta_k) = 0 \) on \( x_3 = 0 \) because of the choice of the boundary condition \( Q_b \).) Then from (23), (80) and (82), we have that
\[ -\Delta \tilde{e}_k(x) \leq C'' \tilde{e}_k(x) \quad x \in B_{1/2}^+(0) \]
\[ \tilde{e}_k(x)|_{x_3=0} = 0 \] (83)

for a constant \( C'' \) independent of \( L \). Using standard arguments as in [7], (83) implies that
\[ \sup_{x \in B_{1/4}^+(0)} \tilde{e}_k(x) \leq c_3 \delta_k \rightarrow 0 \quad \text{as } k \rightarrow \infty \]

contradicting (71). The proof of Proposition 3 is now complete. \[ \square \]

For the reader’s convenience, we quote Lemma 2 from [4] which is used in Proposition 4:

Lemma 2 from [4]: Let \( \omega(r) \) be a solution of
\[ -\epsilon^2 \Delta \omega + \omega = 0 \quad \text{on } B(0, R) \]
\[ \omega = 1 \quad \text{on } \partial B(0, R). \] (84)

Then for \( \epsilon < \frac{3R}{2}, \omega(r) \leq e^{\frac{1}{2\pi} \left( r^2 - R^2 \right)} \) on \( B(0, R) \).
Proposition 4 Let \( \{Q^k\} \) be a sequence of uniaxial global Landau-de Gennes minimizers in the admissible space \( \mathcal{A}_Q \), where \( L_k \to 0^+ \) as \( k \to \infty \). Then as \( k \to \infty \), we can extract a suitable subsequence such that \( Q^k \to Q^0 \) in \( C^{1,\alpha}(\Omega \setminus B_\delta(S_0)) \) for some \( 0 < \alpha < 1 \) and \( B_\delta(S_0) \) is a small \( \delta \)-neighbourhood of the singular set, \( S_0 \), of the limiting harmonic map, \( Q^0 \), where \( Q^0 \) has been defined in (4) and \( \delta \) is independent of \( L_k \).

Proof: The proof follows the methods in [41] and the key ingredient is to establish a global bound for \( \frac{s_+ - s_-^2}{L^2} \), everywhere away from \( S_0 \), for \( L_k \) sufficiently small.

We drop the superscript \( L_k \) in what follows for convenience. Consider the equation (33) on \( \Omega \setminus B_\delta(S_0) \) and introduce the function

\[
\psi = \frac{s_+ - s}{L}, \tag{85}
\]

s_+ has been defined in (14) and \( s_- = \left( \frac{b^2}{2} - \sqrt{b^2 + 24a^2c^2} \right) \). Then (33) can be re-written as

\[
\Delta s - 3s|\nabla n|^2 = -\frac{2\epsilon^2s}{3}\psi(s - s_-) \tag{86}
\]

From (23) and (28), we have that \( \frac{2}{3} s_+^2 \geq |Q|^2 \geq \frac{2}{3} s_-^2 - \epsilon_L \) where \( \epsilon_L \to 0 \) as \( L \to 0 \), on \( \Omega \setminus B_\delta(S_0) \). Therefore,

\[
\frac{2\epsilon^2s}{3}(s - s_-) \geq \frac{1}{\beta}
\]

on \( \Omega \setminus B_\delta(S_0) \), where \( \beta \) is a positive constant independent of \( L \).

We note that \( |\nabla Q|^2 = \frac{2}{3}|\nabla s|^2 + 2s^2|\nabla n|^2 \) where \( Q = s(n \otimes n - \frac{1}{3}I) \). We recall the global uniform bound (65) everywhere away from \( S_0 \) to deduce that

\[
|\nabla n|^2 \leq C(a^2, b^2, c^2, \Omega)
\]

on \( \Omega \setminus B_\delta(S_0) \). Combining the above, we have that \( \psi \) satisfies the following inequality on \( \Omega \setminus B_\delta(S_0) \)

\[
-\beta L\Delta\psi + \psi \leq \gamma|\nabla n|^2 \leq D(a^2, b^2, c^2, \Omega) \tag{87}
\]

where \( \gamma \) and \( D \) are positive constants independent of \( L \). Applying standard maximum principle arguments, we conclude that

\[
\|\psi\|_{L^\infty(\Omega \setminus B_\delta(S_0))} \leq D'(a^2, b^2, c^2, \Omega) \tag{88}
\]

where \( D' \) is a positive constant independent of \( L \).

Consider the governing equations (22) for a uniaxial global minimizer \( Q \); they can be written in terms of the function \( \psi \) as shown below -

\[
\Delta Q = \frac{1}{3L} \left( 2\epsilon^2s^2 - b^2s - 3a^2 \right) Q \leq -\alpha\psi Q \tag{89}
\]

where \( \alpha > 0 \) is a constant independent of \( L \), we have used the definition of \( \psi \) in (55) and the uniform convergence of bulk energy density everywhere away from \( S_0 \) (refer to (24)). Finally, we combine the global upper bound (23) and the \( L^\infty \)-estimate (85) to conclude that

\[
\|\Delta Q\|_{L^\infty(\Omega \setminus B_\delta(S_0))} \leq D''(a^2, b^2, c^2, \Omega) \tag{90}
\]
where $D''$ is a positive constant independent of $L$ i.e. $|\Delta Q|$ can be bounded independently of $L_k$ everywhere away from $S_0$. Finally, we use (11) and Sobolev estimates to establish \{Q^{L_k}\} \to Q^0 in $C^{1,\alpha}(\Omega \setminus B_\delta(S_0))$ as $k \to \infty$, for some $0 < \alpha < 1$. The proof of Proposition 4 is now complete. □

Comment: One immediate consequence of (18) is that $s_+ - s^L \leq C L$, where $C$ is a positive constant independent of $L$, everywhere away from $S_0$ in the limit $L \to 0$. This explicitly estimates the rate of convergence in (18) and improves upon a previous estimate in [15] where an analysis of the bulk energy density $f_B$ in (1) shows that $s_+ - s \leq C_1 \sqrt{L}$ where $C_1$ is a positive constant independent of $L$.

Lemma 3 Let $Q^L = s^L (n^L \otimes n^L - \frac{1}{3} I)$ be a uniaxial global minimizer of $\mathcal{I}_{C^G}$ in $\mathcal{A}_Q$, for $L$ sufficiently small. Then for $x \in \Omega \setminus B_\delta(S_0)$, we have

\[
\begin{align*}
|\nabla s^L| & \leq \epsilon_1(x) \\
||\nabla n^L(x)| - |\nabla n_0|| & \leq \epsilon_2(x) \\
\end{align*}
\]  

(91)

where $n_0$ and $Q^0$ are defined in (10) and $\epsilon_1, \epsilon_2 \to 0^+$ as $L \to 0^+$.

Proof: Lemma 2 is a direct consequence of Proposition 4. Let $x \in \Omega \setminus B_\delta(S_0)$. Then from Proposition 4 we have that

\[
\begin{align*}
|Q^L_{ij}(x) - Q^0_{ij}(x)| & \leq \epsilon_3(x) \\
|Q^L_{ij,k}(x) - Q^0_{ij,k}(x)| & \leq \epsilon_4(x) \\
\end{align*}
\]  

(92)

where $Q^0$ is the limiting harmonic map in (9), $Q_{ij,k} = \frac{\partial Q}{\partial x_k}$ and $\epsilon_3, \epsilon_4 << 1$. One can directly compute

\[
|\nabla Q^0|^2 = 2s_+^2 |\nabla n_0|^2 .
\]  

(93)

On the other hand,

\[
|Q^L|^2 = \frac{2}{3} s^L \partial_k s^L 
\]  

(94)

and therefore,

\[
Q^L_{ij} Q^L_{ij,k} = \frac{2}{3} s^L \partial_k s^L 
\]  

(95)

where $|s^L(x) - s_+| < \epsilon_5(x) << 1$ for $x \in \Omega \setminus B_\delta(S_0)$, from (18).

One can re-write $Q^L_{ij} Q^L_{ij,k}$ as shown below -

\[
Q^L_{ij} Q^L_{ij,k} = (Q^L_{ij}(x) - Q^0_{ij}(x))Q^L_{ij,k}(x) + Q^0_{ij}(x) (Q^L_{ij,k}(x) - Q^0_{ij,k}(x)) 
\]  

(96)

since $Q^0_{ij} Q^0_{ij,k} = 0$ from $|Q^0|^2 = \frac{2}{3} s_+^2$. Using the inequalities (92), the global bound (15) and the triangle inequality, we have that

\[
|Q^L_{ij}(x) Q^L_{ij,k}(x)| \leq \epsilon_6(x) << 1
\]  

(97)

for $x \in \Omega \setminus B_\delta(S_0)$ and from (14) and (18), this necessarily implies that

\[
|\nabla s^L| \leq \epsilon_7(L)
\]  

(98)

away from $S_0$, where $\epsilon_7 \to 0^+$ as $L \to 0^+$.
On the other hand, from Proposition 4, $Q^L \to Q^0$ in $C^{1, \alpha}(\Omega; S)$ as $L \to 0$ (up to a subsequence), everywhere away from $S_0$. Therefore, for $x \in \Omega \setminus B_\delta(S_0)$,

$$||\nabla Q^L||^2 - ||\nabla Q^0||^2| \leq \epsilon_8(x)$$

(98)

where $\epsilon_8 \to 0^+$ as $L \to 0^+$. A direct computation shows that

$$||\nabla Q^L||^2 = \frac{2}{3}||\nabla s^L||^2 + 2(s^L)|\nabla n^L|^2.$$ Combining (28), (97), (98) and (93), we have that $|\nabla n^L|^2 \to |\nabla n_0|^2$ as $L \to 0^+$. Lemma 3 now follows. □

Proposition 5 Let $Q^L = s^L (n^L \otimes n^L - \frac{1}{3} I)$ be a uniaxial global minimizer of $I_{\mathcal{L}G}$ in $A_Q$, for $L$ sufficiently small. Then for $x \in \Omega \setminus B_\delta(S_0)$, we have that

$$\left| \frac{\abs{s^L - s^L}}{L} - \frac{9 \abs{\nabla n_0}^2}{\sqrt{b^4 + 24a^2c^2}} \right| \leq \epsilon_9(x)$$

(99)

where $\epsilon_9 \to 0^+$ as $L \to 0^+$.

Proof: Consider the function $\psi^L = \frac{s^L - s^L}{L}$ in (95) and the equation (93) on $\Omega \setminus B_\delta(S_0)$

$$\Delta s^L - 3s^L|\nabla n^L|^2 = -2s^L s^L - \frac{9}{3}(s^L - s^-)\psi$$

(100)

where $s_{\pm} = \frac{L^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}$. Equation (100) can be re-arranged to give

$$-L\Delta \left( \psi^L - \frac{9|\nabla n_0|^2}{\sqrt{b^4 + 24a^2c^2}} \right) + 2c^2 \frac{L^2 - s^-}{3} \left( \psi^L - \frac{9|\nabla n_0|^2}{\sqrt{b^4 + 24a^2c^2}} \right) =$$

$$= 3s^L|\nabla n|^2 + \frac{9L}{\sqrt{b^4 + 24a^2c^2}} \Delta |\nabla n_0|^2 - \frac{6c^2 s^L (s^L - s^-)}{\sqrt{b^4 + 24a^2c^2}} |\nabla n_0|^2. \quad (101)$$

We note that $\Delta |\nabla n_0|^2 = O(1)$ away from $S_0$ and the right-hand side of (101) can be written as

$$3s^L|\nabla n|^2 + \frac{9L}{\sqrt{b^4 + 24a^2c^2}} \Delta |\nabla n_0|^2 - \frac{6c^2 s^L (s^L - s^-)}{\sqrt{b^4 + 24a^2c^2}} |\nabla n_0|^2 =$$

$$= 3s^L|\nabla n|^2 - 3s^L |\nabla n_0|^2 + 3s^L |\nabla n_0|^2 - \frac{6c^2 s^L (s^L - s^-)}{\sqrt{b^4 + 24a^2c^2}} |\nabla n_0|^2 + O(L). \quad (102)$$

Finally, we use (28) and (91) to deduce that

$$3s^L|\nabla n|^2 - 3s^L |\nabla n_0|^2 \leq \epsilon_{10}$$

where $\epsilon_{10} \to 0^+$ as $L \to 0^+$ and

$$\frac{6c^2 s^L (s^L - s^-)}{\sqrt{b^4 + 24a^2c^2}} |\nabla n_0|^2 \to 3s^L |\nabla n_0|^2$$

as $L \to 0^+$, since $s^L - s^- \to (s^L - s^-) = \sqrt{b^4 + 24a^2c^2}/2c^2$ as $L \to 0^+$. Combining the above, we have that

$$-L\Delta \left( \psi^L - \frac{9|\nabla n_0|^2}{\sqrt{b^4 + 24a^2c^2}} \right) + \beta \left( \psi^L - \frac{9|\nabla n_0|^2}{\sqrt{b^4 + 24a^2c^2}} \right) \leq \epsilon_{11} \quad (104)$$

where $\beta$ is a positive constant independent of $L$ and $\epsilon_{11} \to 0^+$ as $L \to 0^+$. Proposition 4 now follows from the maximum principle and Lemma 2 of [4]. □
6 Generalizations

This paper focuses on qualitative properties of global minimizers of the Landau-de Gennes energy functional on 2D and 3D domains. In the 2D case, we show that the Landau-de Gennes theory is equivalent to Ginzburg-Landau theory for superconductors and make predictions about the dimension of the defect set, the defect locations and the asymptotic profile of global minimizers close to and far away from the defect set.

In 3D, we focus on uniaxial global minimizers of the Landau-de Gennes energy functional because this is the first step in a rigorous study of arbitrary minimizers. The topological defects are contained inside the isotropic set of the uniaxial global minimizers. We derive the governing equations for the scalar order parameter $s^L$ and the leading eigenvector $n^L$; these equations reflect the coupling between the two quantities. We show that the topological defects (or equivalently the isotropic set) are necessarily contained in a small neighbourhood of the singular set of a limiting harmonic map and establish the vortex-like or radial hedgehog-like profile of isolated point defects. We also study the qualitative properties of uniaxial global minimizers away from the isotropic set. In particular, we establish the $C^{1,\alpha}$-convergence of uniaxial global minimizers to a limiting harmonic map, everywhere away from the isotropic set. As mentioned in Section 2, a limiting harmonic map is an energy minimizer within the Oseen-Frank theory for uniaxial liquid crystals with constant order parameter. These convergence results suggest that Oseen-Frank theory and Landau-de Gennes theory give qualitatively similar information away from topological defects and the Landau-de Gennes theory can potentially give new information near topological defects.

As mentioned in Section 1, some of our results will also apply to uniaxial solutions with bounded energy in the limit $L \to 0^+$. In particular, the strong convergence result in Section 4 will hold for any sequence of solutions of (21) and (22) whose energy is bounded from above by the energy of the limiting harmonic map $Q^0$, in the limit $L \to 0^+$. The interior and boundary monotonicity lemmas in Section 4 hold for all solutions of (21) (and hence, of (22) which is a special case of (21)). In particular, (28) will be valid for all sequences of uniaxial solutions, $\{Q^L_k\}$ of (22), whose energies are bounded above by the energy of a limiting harmonic map $Q^0$, in the limit $L_k \to 0^+$. We will still have the $C^{1,\alpha}$-convergence of $\{Q^L_k\}$ to $Q^0$ as $L_k \to 0$, everywhere away from the singular set of the limiting harmonic map.

Such sequences of uniaxial solutions with bounded energy do exist, such as radial-hedgehog solutions on a unit ball with strong radial anchoring conditions [17]. Radial-hedgehog solutions are uniaxial, spherically-symmetric solutions of (22). They are analogous to degree +1 vortices in Ginzburg-Landau theory and in [17], we use Ginzburg-Landau techniques to study these radial-hedgehog solutions, their defect cores and stability properties in the limit $L \to 0^+$.

Extensions to biaxial case: Some of the arguments in this paper can be extended to general biaxial minimizers of the form (11). As an example, let $\{Q^L_k\}$ be a sequence of minimizers (biaxial or uniaxial) of the Landau-de Gennes energy functional $I_{LG}$, in the admissible space $A_Q$. Then $\{Q^L_k\}$ converges strongly to a limiting harmonic map $Q^0$ (as in (9)) in $W^{1,2}(\Omega, S)$ (up to a subsequence) [15], for $L_k \to 0^+$ as $k \to \infty$. Using the interior and boundary monotonicity lemmas (24) and (25), we can show that

$$f_B(Q^L_k) \to 0$$

(105)
uniformly everywhere away from the singular set, \( S_0 \), of the limiting harmonic map or equivalently

\[
s \to s_+, \quad r \to 0^+ \tag{106}
\]

uniformly away from \( S_0 \), as \( k \to \infty \).

In what follows, we derive the analogue of Lemma 2 in the biaxial case.

**Lemma 4** Let \( Q^L \) be a global minimizer of \( I_{CG} \), for \( L \) sufficiently small. Let

\[
A^L = \frac{1}{2} Q^L_{ij,k} Q^L_{ij,k}. 
\]

Then on \( \Omega \setminus B_\delta(S_0) \), we have the following inequality

\[
- \Delta A^L + |D^2 Q^L|^2 \leq \frac{1}{\alpha^4} |D^2 Q^L|^2 + \alpha^4 \frac{A^L}{|Q^L|^2} \tag{107}
\]

where \( B_\delta(S_0) \) is a small \( \delta \)-neighbourhood of \( S_0 \) and \( \alpha > 1 \) is a positive constant independent of \( L \).

**Proof:** We start with the relation (60)

\[
\Delta A^L = |D^2 Q^L|^2 + Q^L_{ij,k} Q^L_{ij,ppk}
\]

and drop the superscript \( L \) for brevity.

We need to estimate \( |Q^L_{ij,k} Q^L_{ij,ppk}| \) in terms of \( |\Delta Q| |\nabla Q|^2 / |Q| \). Straightforward but tedious calculations show that

\[
L^2 |Q^L_{ij,k} Q^L_{ij,ppk}|^2 = a^4 |\nabla Q|^4 + c^4 \left( \text{tr} Q^2 \right)^2 |\nabla Q|^4 + 4b^4 (Q_{ip} Q_{pj,q} Q_{ij,q})^2 + + 4a^2 b^2 (Q_{ip} Q_{pj,q} Q_{ij,q}) |\nabla Q|^2 - 4b^2 c^2 |Q|^2 |\nabla Q|^2 - 2a^4 c^2 |Q|^2 |\nabla Q|^4 + + 4c^4 (Q \cdot \nabla Q)^4 + 4c^4 (Q \cdot \nabla Q)^2 |Q|^2 |\nabla Q|^2 - 4a^2 c^2 |Q|^2 (Q \cdot \nabla Q)^2 - 8b^2 c^2 (Q \cdot \nabla Q)^2 Q_{ip} Q_{pj,q} Q_{ij,q} \leq \]

\[
\leq C(a^2, b^2, c^2) |\nabla Q|^4 \tag{108}
\]

where we have used the Euler-Lagrange equations (21) to compute the right-hand side of (108) and the uniform convergence of the bulk energy density to its minimum value away from the singular set of the limiting harmonic map. It can be shown that the right-hand side of (108) vanishes for \( Q \in Q_{min} \), where \( Q_{min} \) has been defined in (15). The details of these calculations are omitted here for brevity.

Secondly,

\[
L^2 \frac{|\nabla Q|^4}{|Q|^2} |\Delta Q|^2 = a^4 |\nabla Q|^4 + 2a^2 b^2 |\nabla Q|^4 |\text{tr} Q^3| - 2a^2 c^2 |Q|^2 |\nabla Q|^4 - + 2b^2 |\nabla Q|^4 + c^4 |Q|^4 |\nabla Q|^4 + 2b^4 \frac{4 + r^4 + 3s^2 r^2 - 2s^3 r - 2s^3 r^3}{27 |Q|^2} |\nabla Q|^4 \geq D(a^2, b^2, c^2) |\nabla Q|^4 \tag{109}
\]

where

\[
D(a^2, b^2, c^2) = 0
\]

---

\(^2\)We are not making any assumptions about \( Q \); a general global minimizer for \( I_{CG} \) in the admissible space \( A \) exists from the direct methods in the calculus of variations
if and only if $Q \in Q_{\min}$.

Combining (108) and (109), we get that

$$|Q_{ij,k}Q_{ij,ppk}| \leq D'(a^2, b^2, c^2)|\nabla Q|^2|\Delta Q|$$ (110)

where $D'$ is a positive constant independent of $L$. Substituting (110) into (60) and repeating the same steps as in Lemma 2, (107) follows. The proof of Lemma 4 is then complete. □

**Corollary:** Let $Q^L$ be a global minimizer of $I_{LG}$ (biaxial or uniaxial), in the admissible space $A_{Q^L}$, for $L$ sufficiently small. Then we have the following interior estimates, away from the singular set, $S_0$, of the limiting harmonic map $Q^0$ in (9) :-

$$\frac{1}{2}|\nabla Q^L|^2 + \frac{f_B(L)}{L} \leq H(a^2, b^2, c^2, \Omega) \quad (111)$$

$$|Q^0| - |Q^L| \leq C(a^2, b^2, c^2)L \quad \text{on } K \subset \Omega \setminus B_\delta(S_0). \quad (112)$$

In particular, the largest positive eigenvalue, $\lambda^L_1$, of $Q^L$, satisfies the following inequality on the interior compact subset $K \subset \Omega \setminus B_\delta(S_0)$

$$\frac{2s_+}{3} - \lambda^L_1 \leq D(a^2, b^2, c^2)L \quad (113)$$

where $s_+$ has been defined in (6) and the positive constants $H, C$ and $D$ are independent of $L$.

**Proof:** The inequality (111) is a mere repetition of (30); see [15] for a proof.

Consider the function $|Q^L| = (Q^L_{pq}Q^L_{pq})^{1/2}$, $p, q = 1, 2, 3$.

Then a direct computation shows that $|Q^L|$ satisfies the following partial differential equation

$$\Delta |Q^L| = \frac{|\nabla Q^L|^2}{|Q^L|} - \frac{(Q \cdot \nabla Q)^2}{|Q^L|^3} + \frac{Q_{rs} \Delta Q_{rs}}{|Q^L|} \quad r, s = 1 \ldots 3 \quad (114)$$

where we have dropped the superscript $L$ for brevity.

On the interior compact subset $K \subset \Omega \setminus B_\delta(S_0)$, we have the following inequalities

$$\frac{2s_+}{3} - \epsilon_1 \leq |Q|^2 \leq \frac{2s_+}{3}$$

$$|\nabla Q|^2 \leq C_1(a^2, b^2, c^2) \quad (115)$$

where we have used (23), (105) and (111). Therefore, the first two terms on the right-hand side of (114) can be bounded independently of $L$. We use the Euler-Lagrange equations (21) to compute the third term on the right-hand side of (114) i.e.

$$\frac{Q_{rs} \Delta Q_{rs}}{|Q|} = \frac{1}{|Q|L} \{-a^2|Q|^2 - b^2 \text{tr} Q^3 + c^2|Q|^4\} = \frac{|Q|}{L} \left\{c^2|Q|^2 - \frac{b^2|Q|}{\sqrt{6}} - a^2\right\} + \frac{b^2|Q|^2}{\sqrt{6}L} \left(1 - \sqrt{6} \text{tr} Q^3\right).$$

We recall from [15] that

$$\beta^2(Q) = 1 - 6 \left(\frac{\text{tr} Q^3}{|Q|^3}\right)^2 \in [0, 1]$$

22
is the biaxiality parameter and as a direct consequence of (111), we have
\[ \beta^2(Q) = 1 - 6 \left( \frac{\text{tr} Q^3}{|Q|^3} \right)^2 \leq C_2(a^2, b^2, c^2)L \]
on the compact interior subset \( K \subset \Omega \setminus B_\delta(S_0) \), for a positive constant \( C_2 \) independent of \( L \). Further, we have the following sequence of inequalities on \( K \subset \Omega \setminus B_\delta(S_0) \)
\[ C_3(a^2, b^2, c^2) \left( |Q| - |Q^0| \right) \leq \left\{ c^2|Q|^2 - \frac{b^2|Q|^2}{\sqrt{6}} - a^2 \right\} \leq C_4(a^2, b^2, c^2) \left( |Q| - |Q^0| \right) \]
for positive constants \( C_3, C_4 \) independent of \( L \) (see (105) and (56)).

From the preceding remarks, we deduce that
\[ \Delta |Q(x)| = \alpha(a^2, b^2, c^2) + C_4(a^2, b^2, c^2) \frac{|Q(x)| - |Q^0(x)|}{L}, \quad x \in \Omega \setminus B_\delta(S_0) \quad (116) \]
where \( \alpha \) is a positive constant independent of \( L \). Define the function
\[ \psi = \frac{|Q^0| - |Q|}{L}. \]
Then using (116), we see that \( \psi \) satisfies the following inequality on \( K \subset \Omega \setminus B_\delta(S_0) \)
\[ -L \Delta \psi + \beta(a^2, b^2, c^2) \psi \leq \alpha'(a^2, b^2, c^2). \quad (117) \]
Finally, we apply the maximum principle and Lemma 2 in [4] to deduce that
\[ |\psi(x)| \leq \gamma(a^2, b^2, c^2) \quad x \in \Omega \setminus B_\delta(S_0), \quad (118) \]
for a positive constant \( \gamma \) independent of \( L \) and (112) follows. The inequality (112) improves upon a previous estimate in [15] where an analysis of the bulk energy density \( f_B \), coupled with (105), shows that \( |Q^0| - |Q| \leq A(a^2, b^2, c^2)\sqrt{L} \), for a positive constant \( A(a^2, b^2, c^2) \) independent of \( L \).

For (113), we use the following alternative representation formula to (1)
\[ Q^L = S_L \left( n \otimes n - \frac{1}{3} I \right) + R_L \left( m \otimes m - p \otimes p \right) \quad (119) \]
where \( n, m \) and \( p \) are the orthonormal eigenvectors and
\[ 0 \leq s_+ - S_L \leq C_6 \sqrt{L}; \quad R^2_L \leq C_5 L \quad (120) \]
on the interior compact subset \( K \subset \Omega \setminus B_\delta(S_0) \), for positive constants \( C_6, C_5 \) independent of \( L \) (see (105) and Proposition 7 in [15]). We note that
\[ |Q|^2 = \frac{2}{3} S^2_L + 2R^2_L \]
and hence the inequality (112) necessarily implies that
\[ s_+ - S_L \left( 1 + \frac{3R^2_L}{S^2_L} \right)^{1/2} \leq C_7 L, \]

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for a positive constant $C_7$ independent of $L$. This combined with (120) i.e. $R^2_L \leq C_5L$ yields the improved estimate
\[
0 \leq s_+ - S_L(x) \leq C_8L \quad x \in \Omega \setminus B_\delta(S_0)
\] (121)
where $C_8 > 0$ is independent of $L$. Finally, it suffices to note from (119) that the largest positive eigenvalue of $Q^L$ is given by
\[
\lambda^L_1 = \frac{2}{3} S_L
\]
and (113) directly follows from (121). □

One might expect that the techniques in this paper can be generalized to obtain the analogue of Proposition 4 and Proposition 5 in the biaxial case. However, this can be accomplished only if we have a better understanding of the full Euler-Lagrange equations (21). One strategy is to decompose the system (21) as follows -
\[
L \Delta Q_{ij} = -a^2 Q_{ij} - b^2 \left( Q_{ik} Q_{kj} - \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right) + c^2 Q_{ij} \text{tr}(Q^2) = -a^2 - b^2 \left( \frac{Q}{\sqrt{6}} \right) + c^2 |Q|^2
\]
where we can think of the first term as being a uniaxial component and the second term as being a biaxial component. We need to understand the coupling between the uniaxial and the biaxial components and to establish quantitative estimates on the magnitude of the biaxial component, in order to derive rigorous results for the structure of global Landau-de Gennes energy minimizers and their relation to the limiting harmonic map $Q^0$ in [8]. Other future directions are to characterize defects in Landau-de Gennes global minimizers (uniaxial versus biaxial cases), to study qualitative properties of Landau-de Gennes minimizers for different choices of the boundary conditions i.e. when $Q_b \neq Q_{\text{min}}$ where $Q_{\text{min}}$ has been defined in [5] and to study Landau-de Gennes minimizers in different temperature regimes. We plan to report on these problems in future work.

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