THE LANDAU-DE GENNES THEORY OF NEMATIC LIQUID CRYSTALS: UNIAXIALITY VERSUS BIAXIALITY

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(Communicated by Xingbin Pan)

Abstract. We study small energy solutions within the Landau-de Gennes theory for nematic liquid crystals, subject to Dirichlet boundary conditions. We consider two-dimensional and three-dimensional domains separately. In the two-dimensional case, we establish the equivalence of the Landau-de Gennes and Ginzburg-Landau theory. In the three-dimensional case, we give a new definition of the defect set based on the normalized energy. In the three-dimensional uniaxial case, we demonstrate the equivalence between the defect set and the isotropic set and prove the $C^{1,\alpha}$-convergence of uniaxial small energy solutions to a limiting harmonic map, away from the defect set, for some $0 < \alpha < 1$, in the vanishing core limit. Generalizations for biaxial small energy solutions are also discussed, which include physically relevant estimates for the solution and its scalar order parameters. 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 [11]. 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 [16].

The simplest continuum theory for nematic liquid crystals is the Oseen Frank theory [11, 16]. It describes the state of a liquid crystal by a unit-vector field, $\mathbf{n}$, which describes the average local orientation of the molecules. The liquid crystal energy, within the one-constant approximation, reduces to the Dirichlet energy

$$I[\mathbf{n}] = \int_{\Omega} |\nabla \mathbf{n}|^2 \, dV$$

and the corresponding energy minimizers are examples of harmonic maps into the unit sphere [5]. The Oseen-Frank theory is limited in the sense that it is restricted to uniaxial materials (materials with a single preferred direction of molecular alignment) with a constant degree of orientational ordering.

The Landau-de Gennes theory is a more general continuum theory for nematic liquid crystals [11, 29]. 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 [17, 22]

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

(2)

where $s, r$ are scalar order parameters, $n, m$ are eigenvectors of $Q$ and $I$ is the $3 \times 3$ identity matrix. In the uniaxial phase, $Q$ takes the simpler form of

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

(3)

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

The Landau-de Gennes energy functional, $I_{LG}$, is a nonlinear integral functional of $Q$ and its spatial derivatives. In the absence of any surface energies or external fields and working within the one-constant approximation, $I_{LG}$ is given by [11, 22]

$$I_{LG}[Q] = \int_{\Omega} \frac{L_{el}}{2} |\nabla Q|^2 + f_B(Q) \, dV$$

(4)

where $\Omega$ is the domain, $f_B(Q)$ is the bulk energy density that dictates the preferred phase - isotropic, uniaxial or biaxial, $L_{el}$ is a positive material-dependent elastic constant and $|\nabla Q|^2$ 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.

This paper has two main aims - (1) to give a mathematical definition of a defect in the Landau-de Gennes framework and (2) to elucidate the analogies and differences between the Landau-de Gennes and Ginzburg-Landau theories [3, 4] and use Ginzburg-Landau techniques in the context of liquid crystals. Defects are widely observed in nematic systems and yet, global and local Landau-de Gennes minimizers have no analytic singularities. We define the defect set in terms of the normalized energy on balls, by analogy with similar definitions in the theory of harmonic maps [26] and obtain results on the defect locations and the Hausdorff dimension of the defect set. We demonstrate the equivalence between the Landau-de Gennes and Ginzburg-Landau theories on two-dimensional domains, by means of a direct calculation. There are however important technical differences for three-dimensional domains. We introduce the concept of a small energy solution; small energy solutions are classical solutions of the Euler-Lagrange equations associated with the energy functional (4) and they have small energy in the sense that

$$I_{LG}[Q^*] \leq I_{LG}[Q^0]$$

(5)

where $Q^*$ denotes a small energy solution and $Q^0$ is a limiting harmonic map [17]. Such small energy sequences include global energy minimizers. The second half of the paper focuses on uniaxial small energy solutions. This is the first step in the mathematical analysis of arbitrary solutions and this is a natural mathematical problem that has not been studied in the literature. It is also important to point out
that the study of uniaxial solutions can be viewed as a generalized Ginzburg-Landau theory from $\mathbb{R}^3$ to $\mathbb{R}^3$. The governing equations have an approximate Ginzburg-Landau structure away from the defect set and Ginzburg-Landau techniques can be exploited to obtain non-trivial results (see [20] for recent work on three-dimensional Ginzburg-Landau theory). In the biaxial case, we study maps from $\mathbb{R}^3$ to $\mathbb{R}^5$. This is technically much harder and the nonlinearities are more complex than in the uniaxial case. In particular, Ginzburg-Landau techniques cannot be readily transferred to the biaxial case and hence, the biaxial case is not a good paradigm for illustrating the applicability of Ginzburg-Landau methods in liquid crystal problems.

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 [17] in a three-dimensional (3D) framework that are crucial for the development of this paper. We work in the vanishing core limit, which is expressed in terms of a dimensionless variable $L$. The variable $L$ is proportional to the ratio of the nematic correlation length [24, 21] to the domain size and the vanishing core limit is the limit $L \to 0^+$. This limit is particularly relevant for macroscopic domains that are much larger than the correlation length. The results in [17] are for global Landau-de Gennes energy minimizers. We demonstrate that these results are also valid for small energy sequences (5) and this is a non-trivial observation, since results for global energy minimizers don’t necessarily carry over to special sequences of solutions. We define the defect set to be the set of points where there is an energy concentration within balls of radius on the order of the nematic correlation length. This is a physically intuitive definition and we can demonstrate that this definition includes regions of localised abrupt changes in the eigenvalue structure or discontinuities in the solution eigenvectors. We also use the concept of a null lagrangian to obtain a new lower bound for the Landau-de Gennes energy in (4) in terms of the geometry and material parameters and there are analogous results in Oseen-Frank theory.

In Section 5, we study uniaxial small energy solutions on 3D domains in the low-temperature regime, in the vanishing core limit. We derive the governing equations for uniaxial solutions and the governing equations reduce to the harmonic map equations in the limit of constant scalar order parameter. The isotropic set, $S = \{x \in \Omega; Q(x) = 0\}$, is a natural candidate for the defect set (see (3)) and we demonstrate the equivalence between our definition of the defect set and the isotropic set. We exploit the Ginzburg-Landau structure of the governing equations to study the far-field properties because there are important technical differences near singularities. We adapt results from [8, 9] to prove the $C^{1,\alpha}$-convergence of small energy uniaxial solutions to a limiting harmonic map, everywhere 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 the completely general biaxial case. Finally, in Section 7, we discuss certain directions for future research. 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-convex multi-well bulk potentials.
2. Preliminaries. Let $\bar{S}_d \subset M^{d \times d}$ denote the space of symmetric, traceless $d \times d$ matrices i.e.

$$\bar{S}_d \overset{def}{=} \{ Q \in M^{d \times d}; Q_{ij} = Q_{ji}, \ Q_{ii} = 0 \}$$

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

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

We take our domain $\Omega$ to be either a two-dimensional or three-dimensional i.e. $d = 2$ or $d = 3$, 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 [22]. 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. In 2D, $f_B$ attains its minimum on the set of $Q$-tensors defined by

$$Q_2 = \left\{ Q \in \bar{S}_2; Q = \sqrt{\frac{2a^2}{c^2}} \left( n \otimes n - \frac{1}{2} I_2 \right) \right\}$$

where $n \in S^1$ and $I_2$ is the $2 \times 2$ identity matrix. In 3D, $f_B$ attains its minimum on the set of uniaxial $Q$-tensors given by [18]

$$Q_{\min} = \left\{ Q \in \bar{S}_3, Q = s_+ \left( n \otimes n - \frac{1}{3} I \right) \right\}$$

with $n \in S^2$, $I$ is the $3 \times 3$ identity matrix and

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

We work with strong anchoring conditions or Dirichlet boundary conditions. The prescribed boundary condition $Q_b$ is given by

$$Q_b = s_{eq}(d) \left( n_b \otimes n_b - \frac{1}{d} I \right)$$

where $d$ is the domain dimension, $I$ is the corresponding identity matrix,

$$s_{eq}(d) = \begin{cases} \sqrt{\frac{2a^2}{c^2}}, & d = 2 \\ s_+, & d = 3. \end{cases}$$

$n_b$ is a unit-vector field ($n_b \in S^1$ in 2D and $n_b \in S^2$ in 3D) with non-zero topological degree. Clearly, $Q_b \in Q_2$ in 2D and $Q_b \in Q_{\min}$ in 3D. We define our admissible space to be

$$\mathcal{A}_Q = \{ Q \in W^{1,2}(\Omega; \bar{S}_d) : Q = Q_b \text{ on } \partial \Omega, \text{ with } Q_b \text{ as in (10)} \},$$

where $W^{1,2}(\Omega; \bar{S}_d)$ is the Sobolev space of square-integrable $Q$-tensors in $d$-dimensions ($d = 2$ or $d = 3$ in this paper) with square-integrable first derivatives [10]. The existence of global energy minimizers for $I_{CG}$ in the admissible space $\mathcal{A}_Q$ follows readily.
from the direct methods in the calculus of variations [17, 18]. 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” in 3D, $Q^0 : \Omega \rightarrow Q_{\min}$; $Q^0$ is defined to be

$$Q^0 = s_+ \left( n_0 \otimes n_0 - \frac{1}{3} I \right)$$

(13)

where $n_0$ is a minimizer of the Dirichlet energy

$$I_{OF}[n] = \int_{\Omega} |\nabla n|^2 \ dV$$

(14)

on $\Omega \subset \mathbb{R}^3$, in the admissible space

$$A_n = \{ n \in W^{1,2}(\Omega; S^2) : n = n_0 \text{ on } \partial \Omega \}.$$ (15)

The terminology limiting harmonic map stems from the fact that $n_0$ is a harmonic unit-vector field [26] 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], [16]. 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, especially in the context of far-field properties away from defects. Working within the one-constant approximation, the Oseen-Frank energy reduces to the Dirichlet energy in (14) 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. Then $Q \in S_2$ can be written as

$$Q = \lambda (n \otimes n - m \otimes m)$$

(16)

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 (16) 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 (16) as

$$Q = 2\lambda \left( n \otimes n - \frac{1}{2} I_2 \right)$$

(17)

where $I_2$ is the $2 \times 2$ identity matrix. We can also think of $Q \in S_2$ as being a symmetric, traceless $3 \times 3$ matrix: $Q = (\frac{1}{3} \lambda)n \otimes n + (\frac{1}{3} - \lambda)m \otimes m - \frac{1}{3} z \otimes z$, where $z$ is the unit-vector in the $z$-direction.

Straightforward calculations show that

$$|Q|^2 = 2\lambda^2$$

$$\text{tr}Q^3 = Q_{ij}Q_{jp}Q_{pi} = 0 \quad i, j, p = 1, 2.$$ (18)

Then the Landau-de Gennes energy functional in (4) simplifies to

$$I_{LG}[Q] = \int_{\Omega} \frac{L_{el}}{2} |\nabla Q|^2 + \left\{ -\frac{a^2}{2} \text{tr}Q^2 + \frac{c^2}{4} (\text{tr}Q^2)^2 \right\} \ dV$$

(19)

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

$$Q_{ij, kk} = \frac{1}{L_{el}} (-a^2 + c^2 |Q|^2) Q_{ij} \quad i, j = 1, 2$$

(20)
and using the scaling $\tilde{Q} = \sqrt{\frac{c}{\alpha}} Q$, we obtain the following system of partial differential equations -

$$
\tilde{Q}_{ij,kk} = \frac{a^2}{L_{el}} \left( |Q|^2 - 1 \right) \tilde{Q}_{ij} \quad i,j,k = 1,2
$$

$$
\tilde{Q} = \sqrt{2} \left( n_b \otimes n_b - \frac{1}{2} I \right) \quad \text{on } \partial \Omega.
$$

(21)

The system (21) is simply the Ginzburg-Landau system of equations for superconductors in two dimensions [27] and we are interested in the asymptotic properties of global energy minimizers either in the limit $a^2 \to \infty$ (low temperature regime) or $L_{el} \to 0^+$. The latter limit is relevant for macroscopic domains with characteristic length scale much larger than the nematic correlation length.

Let $Q^{L_{el}}$ be a global minimizer of $I_{LG}$ in (19), in the admissible space $\mathcal{A}_Q = \{ Q \in W^{1,2}(\Omega; S_2) ; Q = s_{eq} \left( n_b \otimes n_b - \frac{1}{2} I \right) \text{ on } \partial \Omega \}$ for a fixed $L_{el} > 0$, where $s_{eq}$ has been defined in (11). Then $Q^{L_{el}}$ is necessarily of the form

$$
Q^{L_{el}}(x) = s^{L_{el}}(x) \left( n^{L_{el}}(x) \otimes n^{L_{el}}(x) - \frac{1}{2} I_2 \right)
$$

for some scalar function $s^{L_{el}} : \bar{\Omega} \to \mathbb{R}$, $n^{L_{el}} \in S^1$ and $Q^{L_{el}}$ is a classical solution of (21). Let $\Theta_{L_{el}} = \{ x \in \Omega ; s^{L_{el}}(x) = 0 \}$ denote the isotropic set of $Q^{L_{el}}$. We have a topologically non-trivial boundary condition in (21), since $n_b$ has non-zero topological degree when viewed as a map from $\partial \Omega$ to $S^1$. Hence, the unit-vector field $n^{L_{el}}$ necessarily has interior discontinuities and let $S_n$ denote the defect set of $n^{L_{el}}$. Then

$$
S_n \subset \Theta_{L_{el}}
$$

(23)

since $Q^{L_{el}}$ is well-defined at all points inside $S_n$. 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 $\Theta_{L_{el}}$ ([3, 6]).** As $L_{el} \to 0$, the isotropic set $\Theta_{L_{el}}$ converges in Gromov-Hausdorff sense to a set $\Theta_0$ consisting of $|D|$ isolated points, $\{ a_1, \ldots, a_{|D|} \}$, where $D$ is the topological degree of the boundary condition $Q_b$ in (10).

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

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

(24)

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 [3, 27].

**Far-field behaviour** [3, 27]: Let $\left\{ Q^{L_{el}} \right\}$ denote a sequence of global energy minimizers for (19), where $L_{el} \to 0^+$ as $k \to \infty$. Then (up to a subsequence),

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

for some $Q^* \in \cap_{1 \leq p < 2} W^{1,p}(\Omega; Q_2)$. 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, 27] for the proofs.
4. The 3D-case.

4.1. Preliminaries. Let $\Omega \subset \mathbb{R}^3$ be a bounded, connected and simply-connected domain with smooth boundary. An arbitrary $Q$-tensor field, $Q : \Omega \to \bar{S}_3$, 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 in contrast to the 2D case, $\text{tr} Q^3 \neq 0$ in general.

We study the Landau-de Gennes energy functional, $I_{LG}$ in (4), in the admissible space $A_Q = \{ Q \in W^{1,2}_\Omega, \bar{S}_3 ; Q = Q_b \text{ on } \partial \Omega \}$ where $Q_b$ has been defined in (10) and (11). The corresponding Euler-Lagrange equations are

$$L_{el} \Delta Q_{ij} = -a^2 Q_{ij} - b^2 \left( Q_{ik} Q_{kj} - \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right) + c^2 Q_{ij} \text{tr}(Q^2) \quad i, j = 1, 2, 3, \quad (25)$$

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 all solutions are actually classical solutions of (25) and they are smooth and real analytic on $\Omega$ [17].

The equations (25) can be non-dimensionalized as follows. Define a characteristic length scale $R = \frac{|\Omega|}{|\partial \Omega|}$ where $|\Omega|$ denotes the volume of $\Omega$ and $|\partial \Omega|$ denotes the surface area of $\partial \Omega$; introduce the following scaled variables:

$$\bar{r} = \frac{r}{R}; \quad \bar{a}^2 = \frac{a^2}{a_{NI}^2}, \quad \bar{b}^2 = \frac{b^2}{a_{NI}^2}, \quad \bar{c}^2 = \frac{c^2}{a_{NI}^2} \quad (26)$$

where $a_{NI}^2 = \frac{b^4}{27c^2}$. In terms of these re-scaled variables, the equations (25) reduce to

$$\frac{L_{el}}{a_{NI}^2 R^2} \frac{\partial^2 Q_{ij}}{\partial r_k \partial r_k} = -\bar{a}^2 Q_{ij} - \bar{b}^2 \left( Q_{ik} Q_{kj} - \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right) + \bar{c}^2 Q_{ij} \text{tr}(Q^2) \quad i, j = 1, 2, 3. \quad (27)$$

We define the dimensionless parameter

$$L = \frac{L_{el}}{a_{NI}^2 R^2} \quad (28)$$

where $\xi_u = \sqrt{\frac{L_{el}}{a_{NI}^2}}$ is a uniaxial correlation length related to defect core size [21]. We note that the system (27) has an associated dimensionless free energy

$$\overline{I_{LG}}[Q] = \int_{\Omega} \frac{1}{2} |\nabla Q|^2 + \overline{f_B}(Q) d\bar{V} \quad (29)$$

where $L$ is defined in (28), $\overline{I_{LG}} = \frac{I_{LG}}{a_{NI}^2 R^2}$, $\overline{f_B} = \frac{f_B}{a_{NI}^2}$ and $f_B$ has been defined in (6), $\overline{\Omega}$ and $d\bar{V}$ are the re-scaled domain and volume element respectively. The re-scaled bulk energy density $\overline{f_B}$ attains its minimum on the set $Q_{min}$ as before

$$Q_{min} = \left\{ Q \in \bar{S}_3, Q = s_+ \left( n \otimes n - \frac{1}{3} I \right) \right\} \quad (30)$$

where $s_+$ has been defined in (9). We are guaranteed the existence of a global $\overline{I_{LG}}$-minimizer in the admissible space, $A_Q$, for each $L > 0$. It is intuitively clear that as
$L \to 0^+$, the global energy minimizers are approximate bulk energy minimizers with the elastic energy density being dominant in the vicinity of defects or interfaces. In what follows, we drop the bars from the re-scaled variables for convenience and all subsequent results should be interpreted in terms of the dimensionless quantities above.

We briefly comment on limiting harmonic maps in a 3D setting:

\[ Q^0 = s_+ \left( n_0 \otimes n_0 - \frac{1}{3} I \right) \]

where \( n_0 \) is an energy minimizing harmonic map in the admissible space \( A_n = \{ n \in W^{1,2}(\Omega; S^2) : \text{n = n}_b \text{ on } \partial \Omega \} \). We note that \( Q^0 \in A_Q \), where the admissible space \( A_Q \) has been defined in (12). Let \( S_0 \) denote the singular set of \( n_0 \) (and hence, of \( Q^0 \)). Then \( S_0 \) is a discrete set consisting of isolated, interior point singularities [5, 26].

We, henceforth, work in the vanishing core limit \( L \to 0^+ \). Let \( Q^{L_k} \) be a sequence of solutions for the re-scaled system (27), where \( L_k \to 0^+ \) as \( k \to \infty \). Then we refer to \( \{ Q^{L_k} \} \) as a small energy sequence if

\[ \mathcal{I}_{LG}[Q^{L_k}] \leq \mathcal{I}_{LG}[Q^0] \quad \forall L > 0. \tag{31} \]

The limit \( L \to 0^+ \) is referred to as the vanishing core limit in the rest of the paper since it is relevant for macroscopic domains with \( R >> \xi_n \) [24]. We, next, quote important results from [17, 18] that are crucial for the analysis of small energy solutions, away from the singular set, \( S_0 \), of the limiting harmonic map, in the vanishing core limit. The results in [17] are for global energy minimizers and they transfer to small energy sequences because of the energy bound (5).

**Maximum principle** [18]: Let \( Q \) be an arbitrary solution of the Euler-Lagrange equations (27) in the space \( A_Q \). Then

\[ \| \mathcal{Q} \|_{L^\infty(\Omega)} \leq \sqrt{\frac{2}{3}} s_+ \tag{32} \]

where \( s_+ \) has been defined in (9).

**Strong convergence to** \( Q^0 \): Let \( \Omega \subset \mathbb{R}^3 \) be a bounded, connected and simply-connected domain with smooth boundary. Let \( \{ Q^{L_k} \} \) be a small energy sequence in the admissible space \( A_Q \) (\( A_Q \) has been defined in (12)) where \( L_k \to 0 \) as \( k \to \infty \). There exists a minimizing harmonic map extension \( n_0 : \Omega \to S^2 \) of \( n_b \) such that after passing to a subsequence, \( Q^{L_k} \to Q^0 = s_+ (n_0 \otimes n_0 - \frac{I}{3}) \) strongly in \( W^{1,2}(\Omega; S_3) \) as \( k \to \infty \).

**Proof.** This has been demonstrated in [17] for sequences of global Landau-de Gennes energy minimizers \( \{ Q^{L_k} \} \), where \( L_k \to 0 \) as \( k \to \infty \). The same arguments also apply to small energy sequences (5).

Let \( \{ Q^{L_k} \} \) be a small energy sequence in the admissible space \( A_Q \). We recall that the limiting harmonic map \( Q^0 \in A_Q \). From the inequality (5) and the energy definition (4), we have that

\[ \int_{\Omega} \frac{1}{2} |\nabla Q^{L_k}|^2 \, dV \leq \int_{\Omega} \frac{1}{2} |\nabla Q^{L_k}|^2 + \frac{f_B(Q^{L_k})}{L_k} \, dV \leq \int_{\Omega} \frac{1}{2} |\nabla Q^0|^2 \, dV = C(\Omega)s_+^2 \tag{33} \]

since \( f_B(Q^0) = 0 \). The sequence of inequalities (33) shows that the \( W^{1,2} \)-norms of the \( Q^{L_k} \)'s are bounded uniformly in \( L \). Hence, we can extract a weakly convergent subsequence (also denoted by \( \{ Q^{L_k} \} \)) such that \( Q^{L_k} \) converges weakly to \( Q^1 \) in
W^{1,2}$, for some $Q^1 \in A_Q$ as $L_k \to 0$. Using the lower semicontinuity of the $W^{1,2}$-norm with respect to the weak convergence, we have that
\[
\int_{\Omega} |\nabla Q|^2 \, dV \leq \int_{\Omega} |\nabla Q^0|^2 \, dV. \tag{34}
\]
On the other hand, as $L_k \to 0$, we have $f_B(Q^{L_k}(x)) \to 0$ for almost all $x \in \Omega$ (see (33)). Therefore, the weak limit $Q^1 \in Q_{\text{min}}$ and is of the form
\[
Q^1(x) = s_+\left(n^1 \otimes n^1 - \frac{1}{3} I\right), \quad n^1 \in S^2, \text{a.e. } x \in \Omega \tag{35}
\]
where $s_+$ has been defined in (9). We note that $|\nabla Q^1|^2 = 2s_+^2|\nabla n^1|^2$ and $|\nabla Q^0|^2 = 2s_+^2|\nabla n^0|^2$ and recall that $Q^0$ is a global Landau-de Gennes energy minimizer in the restricted space $A_Q \cap Q_{\text{min}}$ to deduce that $\int_{\Omega} |\nabla Q^1|^2 \, dV = \int_{\Omega} |\nabla Q^0|^2 \, dV$ and hence,
\[
\int_{\Omega} |\nabla Q^0|^2 \, dV \leq \liminf_{L_k \to 0} \int_{\Omega} |\nabla Q^{L_k}|^2 \, dV \leq \limsup_{L_k \to 0} \int_{\Omega} |\nabla Q^{L_k}|^2 \, dV \leq \int_{\Omega} |\nabla Q^0|^2 \, dV \tag{36}
\]
from which the strong convergence result, $Q^{L_k} \to Q^0$ in $W^{1,2}$, follows.

Next, we present monotonicity lemmas from [17] for any solution of the Euler-Lagrange equations (27); these lemmas are true for an arbitrary solution of (27) and hence, there is no need to outline the proof for small energy sequences. The proofs of (37) and (38) follow a standard pattern using the Pohozaev identity; complete details can be found in [17].

**Interior and boundary monotonicity lemmas** [17]: Let $Q$ be an arbitrary solution of the Euler-Lagrange equations (27). Define the normalized energy on balls $B(x, r) \subset \Omega = \{y \in \Omega : |x - y| \leq r\}$:
\[
\mathcal{F}(Q, x, r) = \frac{1}{r} \int_{B(x, r)} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV.
\]
Then we have the following interior monotonicity lemma:
\[
\mathcal{F}(Q, x, r) \leq \mathcal{F}(Q, x, R) \quad \forall x \in \Omega; \quad r \leq R \text{ and } B(x, R) \subset \Omega. \tag{37}
\]
Similarly, for $x_0 \in \partial \Omega$, we define the region $\Omega_r = \overline{\Omega} \cap B(x_0, r)$ with $r > 0$, and the corresponding normalized energy to be
\[
\mathcal{E}(Q, x_0, r) = \frac{1}{r} \int_{\Omega_r} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV.
\]
Then there exists $r_0 > 0$ so that
\[
\frac{d}{dr} \mathcal{E} \geq -C (a^2, b^2, c^2, Q_b, r_0, \Omega) \quad 0 < r < r_0 \tag{38}
\]
where the positive constant $C$ is independent of $L$.

An immediate consequence of the strong convergence and the monotonicity lemmas is the following:

**Convergence of bulk energy density away from $S_0$** [17]: Let $\{Q^{L_k}\}$ be a small energy sequence in the admissible space $A_Q$, where $L_k \to 0$ as $k \to \infty$. Then there exists a subsequence $\{Q^{L_k}\}$ such that $Q^{L_k} \to Q^0$ in $W^{1,2}(\Omega, S_3)$ as $k \to \infty$, where $Q^0$ has been defined in (13).
For any compact set $K \subset \bar{\Omega}$ such that $K$ contains no singularity of $Q^0$, we have that
\[
\lim_{L_k \to 0} f_B(Q^{L_k}(x)) = 0 \quad x \in K
\] (39) and the limit is uniform on $K$.

**Outline of Proof:** The proof for global energy minimizers carries over directly to small energy sequences. We briefly present the details in the interior case $K \subset \Omega$, where $K$ does not contain any singularities of $Q^0$. The boundary case follows from analogous arguments, using the boundary monotonicity lemma in (38).

From the strong convergence result in the limit $L \to 0^+$, we have that the strong limit is $Q^0 = s_+ (n_0 \otimes n_0 - \frac{1}{3})$ where $n_0$ is a global energy minimizer of the harmonic map problem in (14), subject to the topologically non-trivial boundary condition $n = n_b$ on $\partial \Omega$.

Let $\alpha = f_B(Q^{L_k})(x_0)$ for some arbitrary point $x_0 \in K$. From [3, 17], we have that for any solution $Q$ of the system (27),
\[
\|\nabla Q\|_{L^\infty(\bar{\Omega})} \leq \frac{C}{\sqrt{L}}
\] and that $f_B$ is a Lipschitz function of $Q$, so that
\[
\|\nabla f_B\|_{L^\infty(\bar{\Omega})} \leq \frac{\bar{C}}{\sqrt{L}}
\] where $C$ and $\bar{C}$ are positive constants independent of $L$.

For $R_0$ small enough such that $B(x_0, R_0) \subset K$ for all $x_0 \in K$, we have
\[
\frac{1}{R_0} \int_{B(x_0, R_0)} |\nabla Q^0|^2 \, dV \leq C_K R_0^2 \leq \epsilon \quad \forall x_0 \in K
\] since $B(x_0, R_0)$ does not contain any singularities. From the strong convergence result, for $L_k$ sufficiently small, we have
\[
\frac{1}{R_0} \int_{B(x_0, R_0)} |\nabla Q^{L_k}|^2 \, dV \leq \frac{1}{R_0} \int_{B(x_0, R_0)} |\nabla Q^0|^2 \, dV + \epsilon \quad \forall x_0 \in K.
\] Using the interior monotonicity lemma (37), we now have for $\rho_k < R_0$
\[
\int_{B(x_0, \rho_k)} \frac{f_B(Q^{L_k})}{L_k} \, dV \leq \frac{\rho_k}{R_0} \int_{B(x_0, R_0)} \frac{1}{2} |\nabla Q^{L_k}|^2 \, dV + \frac{f_B(Q^{L_k})}{L_k} \, dV \leq 3\epsilon
\] (41) since $\int_{\Omega} \frac{f_B(Q^{L_k})}{L_k} \, dV = o(1)$ as $L_k \to 0$ from the strong convergence result. Finally, we use (40) in (41) and let $\rho_k = \frac{\alpha R_0}{D}$ for some suitably chosen positive constant $D$ independent of $L_k$, to deduce that
\[
\alpha^3 \leq D' \epsilon
\] for some constant $D'$ independent of $L_k$. As $\epsilon > 0$ is arbitrary (and can be made as small as possible by our choice of $R_0$) and these estimates are independent of our choice of $x_0$, (39) follows in the interior case. \qed
If \( \{Q^{L_k}\} \) is a uniaxial small energy sequence, then \( Q^{L_k} \) can be written in the form

\[
Q^{L_k} = s_k \left( n_k \otimes n_k - \frac{1}{3} I \right)
\]

for \( s_k : \Omega \rightarrow \mathbb{R} \) and \( n_k \in W^{1,2}(\Omega; \mathbb{S}^2) \). Then (39) implies that (up to subsequence), \( s_k \) converges uniformly to \( s_+ \) everywhere away from \( S_0 \) i.e. we have

\[
|s_k(x) - s_+| \leq \epsilon(L_k, x) \quad x \in \Omega \setminus B_\delta(S_0)
\]

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

\[
\left\{ Q^{L_k} = s_k \left( n_k \otimes n_k - \frac{1}{3} I \right) + r_k \left( m_k \otimes m_k - \frac{1}{3} I \right) \right\}
\]

is a biaxial small energy sequence, then (39) implies that

\[
|s_+ - s_k| \leq \epsilon_{1,k}, \quad |r_k| \leq \epsilon_{2,k}
\]

everywhere away from \( S_0 \), where \( \epsilon_{1,k}, \epsilon_{2,k} \rightarrow 0^+ \) as \( k \rightarrow \infty \).

**Uniform convergence in the interior** [17]: Let \( \{Q^{L_k}\} \) be a small energy sequence in \( A_\Omega \) such that \( L_k \rightarrow 0 \) as \( k \rightarrow \infty \). Then (up to a subsequence) \( Q^{L_k} \rightarrow Q^0 \) strongly in \( W^{1,2}(\Omega, S_3) \) as \( k \rightarrow \infty \).

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

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

(i) There exists a constant \( C > 0 \) independent of \( L \) such that

\[
- \Delta e_L(Q^L)(x) \leq C e_L^2(Q^L)(x) \quad x \in K
\]

for \( L \) sufficiently small, provided there exists a ball \( B(x, \rho_x) \subset K' \) where \( K' \) is a compact neighbourhood of \( K \) that does not contain any singularities of \( Q^0 \).

(ii) There exist constants \( C_1, C_2, L_0 > 0 \) (all constants independent of \( L_k \)) so that if for \( a \in K, 0 < r < \text{dist}(a, \partial K) \), we have

\[
\frac{1}{r} \int_{B(a, r)} e_L(Q^L)(x) \, dV \leq C_1,
\]

then

\[
e_L(Q^{L_k})(x) \leq C_2 \quad x \in B(a, r/2)
\]

for all \( L < L_0 \).

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

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

**Outline of Proof**: We briefly comment on why the aforesaid results for global energy minimizers carry over to small energy sequences with no changes in the proof. The Bochner inequality (45) follows from the uniform convergence of the bulk energy density in (39), the global upper bound in (32) and the structure of the Euler-Lagrange equations in (27) (see [17] for the proof). All of these prerequisites hold for small energy sequences and hence (45) holds for small energy sequences away from the singular set, \( S_0 \), of the limiting harmonic map.

The energy density bound in (47) follows from the uniform convergence of the bulk energy density in (39), the structure of the Euler-Lagrange equations in (27)
and the monotonicity lemmas in (37) and (38). The uniform convergence result in (48) is a consequence of the strong convergence of a small energy sequence to a limiting harmonic map as $L \to 0^+$, the uniform convergence of the bulk energy density in (39) and the energy density bound (47). The interested reader is referred to [17] for details. □

We emphasize that (47) and (48) only hold in the interior of $\Omega$. In Sections 5 and 6, we refine these convergence results in the interior and up to the boundary.

4.2. Lower bound for Landau-de Gennes energy. In the Oseen-Frank theory for nematic liquid crystals, the state variable is a unit-vector field $n : \Omega \to S^2$. It has been demonstrated in [11, 14, 16] that

$$(\text{div } n)^2 - \text{tr} (\nabla n)^2 = n_{i,j} n_{j,i} - n_{i,j} n_{j,i} = \partial_i [n_i n_{i,j} - n_{i,j} n_j] \quad i,j = 1 \ldots 3 \quad (49)$$

where $n_{i,j} = \frac{\partial n_i}{\partial x_j}$ etc. and for any $n \in \mathcal{A}(n_0) = \{ n \in W^{1,2}(\Omega; S^2); n_0 = \text{trace of } n \text{ on } \partial \Omega \}$, there exists a number $\mathcal{L}(n_0)$ such that

$$\mathcal{L}(n_0) = \int_\Omega \left( (\text{div } n)^2 - \text{tr} (\nabla n)^2 \right) dV.$$ 

The contribution $\left( (\text{div } n)^2 - \text{tr} (\nabla n)^2 \right)$ is an example of a Null Lagrangian [1]. In [16], the authors use this null lagrangian to demonstrate that the unit-vector field $n = \frac{x}{|x|}$ is a global minimizer of the Dirichlet energy in (14) on a unit ball in three dimensions, subject to the boundary condition $n = x$ on $S^2$.

Consider the quantity

$$(\text{div } Q)^2 - \text{tr} (\nabla Q)^2 = Q_{i,j} Q_{k,k} - Q_{i,j,k} Q_{i,j} \quad i,j,k = 1 \ldots 3$$

for an arbitrary symmetric, traceless $3 \times 3$ matrix $Q \in S_3$. One can directly verify that the above is a full divergence i.e.

$$(\text{div } Q)^2 - \text{tr} (\nabla Q)^2 = \partial_j [Q_{i,j} Q_{k,k} - Q_{i,k} Q_{i,j}] \quad (50)$$

where $Q_{i,j,k} = \frac{\partial Q_{i,j}}{\partial x_k}$. We can show that the quantity $(\text{div } Q)^2 - \text{tr} (\nabla Q)^2$ is a null lagrangian by reproducing the arguments in Lemma 1.2 in [14] and in the next lemma, we derive an elementary inequality involving $|\nabla Q|^2$ and this null lagrangian.

Lemma 4.1.

$$2|\nabla Q|^2 \geq (\text{div } Q)^2 - \text{tr} (\nabla Q)^2.$$ \quad (51)

Proof. In Einstein convention, (51) is equivalent to

$$2Q_{i,j,k} Q_{i,j,k} \geq Q_{i,j} Q_{k,k} - Q_{i,j,k} Q_{i,j} \quad i,j,k = 1 \ldots 3. \quad (52)$$

We prove inequality (52) for each $i = 1 \ldots 3$. Then

$$|\nabla Q|^2 = Q_{i,1}^2 + Q_{i,2}^2 + Q_{i,3}^2 + Q_{i,2,1}^2 + Q_{i,3,1}^2 + Q_{i,3,2}^2 + Q_{i,3,3}^2$$

and

$$Q_{i,j,k} Q_{k,k} - Q_{i,j,k} Q_{i,j} = 2(Q_{i,1} Q_{i,2,2} + Q_{i,2,2} Q_{i,3,3} + Q_{i,1,1} Q_{i,3,3} - Q_{i,1,2} Q_{i,2,1} - Q_{i,1,3} Q_{i,3,1} - Q_{i,2,3} Q_{i,3,2})$$

and (51) follows directly. □
Lemma 4.2. Let $Q \in A_Q$ where $A_Q$ has been defined in (12). Then

$$I_{LG}[Q] \geq \frac{1}{4} \int_{\partial \Omega} [Q_{bij} Q_{bik,k} - Q_{bik} Q_{bij,k}] \nu_j \, dS$$

(53)

where $Q_{bij}$ is the $ij$-th component of the boundary condition $Q_b$ and $\nu$ is the unit outer normal to $\partial \Omega$.

Proof. Lemma 4.2 follows directly from Lemma 4.1. From Lemma 4.1, we have that

$$I_{LG}[Q] = \int_\Omega \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV \geq \frac{1}{4} \int_\Omega Q_{ij,j} Q_{ik,k} - Q_{ij,k} Q_{ik,j} \, dV$$

(54)

where we use the inequality $f_B \geq 0$ for all $Q \in \hat{S}_3$, the relations (50) and (51) and the fact that $Q_{ij,j} Q_{ik,k} - Q_{ij,k} Q_{ik,j}$ is a null lagrangian so that its integral only depends on the boundary condition $Q_b$. Equation (53) gives us a lower bound for the energy that only depends on the boundary data and the domain.

We can apply Lemma 4.2 directly to compute a lower bound for the Landau-de Gennes energy in the case $\Omega = B(0, R)$ with unit normal $\nu_j = x_j/R$ and Dirichlet boundary condition

$$Q_b = s_+ \left( \frac{x}{R} \otimes \frac{x}{R} - \frac{I}{3} \right) \quad x \in \partial B(0, R).$$

One can check from Lemma 4.2 that

$$I_{LG}[Q] \geq \frac{4\pi s_+^2 R}{6}$$

for any $Q$ in the corresponding admissible space.

4.3. The defect set. We have already seen that solutions of the Landau-de Gennes Euler-Lagrange equations (see (27)) have no analytic singularities. However, experimentally observed singularities should be associated with some energy concentration. Singular sets have been defined in terms of the normalized energy, within the harmonic map theoretical framework and the Oseen-Frank framework i.e. the singular set $S$ is defined to be [9, 26, 14]

$$S = \left\{ x \in \Omega; \lim_{r \to 0} \frac{1}{r} \int_{B(x,r)} E(n) \, dx \neq 0 \right\}$$

(55)

where $n$ is the corresponding state variable and $E(n)$ is the corresponding energy density.

This definition won’t work in the Landau-de Gennes framework since

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

on $\Omega$ (from the $L^\infty$-bound on the gradient, $|\nabla Q| \leq \frac{C}{\sqrt{L}}$, and $|f_B(Q)| \leq C''(a^2, b^2, c^2)$ for positive constants $C'$ and $C''$ independent of $L$). Therefore,

$$\frac{1}{r} \int_{B(x,r)} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV \leq \frac{C''}{L} r^2 \to 0 \quad as \, r \to 0$$

for all $x \in \Omega$ and a positive constant $C''$ independent of $L$. However, we expect that there should be energy concentration within balls centered at singularities with
radius comparable to the nematic correlation length i.e. we seek a characteristic length \( r_*(L) \) such that

\[
e_0 \leq \frac{1}{r_*} \int_{B(x_*, r_*)} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV \leq C' r_*^2 \quad \forall L > 0
\]  

(56)

for singular points \( x_* \in \Omega \) and \( e_0 > 0 \) independent of \( L \) and

\[
\frac{1}{r_*} \int_{B(x_*, r_*)} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV \leq \alpha L \quad \text{as } L \to 0^+
\]

for a positive constant \( \alpha \) independent of \( L \) otherwise. From (56), we deduce that

\[
r_* = \lambda_0 \sqrt{L}
\]  

(57)

where \( \lambda_0 > 0 \) is independent of \( L \). Numerical simulations show that the nematic correlation length is \( O(\sqrt{L}) \) [21]. Guided by such estimates for the nematic correlation length and (57), we propose a definition for the Landau-de Gennes defect set, \( S_{LG} \), for sufficiently small values of \( L \) as shown below:

**Definition 4.3.** For each \( L > 0 \), let \( Q^L \) be a corresponding small energy solution. We define \( \bar{L}_o > 0 \) to be such that

\[
f_B(Q^L)(x) \leq \epsilon \quad \forall x \in K,
\]  

(58)

for all \( L < \bar{L}_o \), where \( 0 < c_0 < 1 \) is a small fixed constant and \( K \subset \Omega \) is an arbitrary compact subset that does not contain any singularities of the limiting harmonic map \( Q^0 \). We define a point \( x_* \in \Omega \) to be a singular point if there exist positive constants \( \lambda_0 \) and \( \sigma \) independent of \( L \) such that \( B(x_*, \lambda_0 \sqrt{L}) \subset \Omega \) for \( L < \bar{L}_o \) and

\[
\frac{1}{\lambda_0 \sqrt{L}} \int_{B(x_*, \lambda_0 \sqrt{L})} \frac{1}{2} |\nabla Q|^2 + \frac{f_B(Q)}{L} \, dV > \sigma(\epsilon_1^2, b^2, c^2)
\]  

(59)

i.e. the normalized energy in balls of radius \( O(\sqrt{L}) \) does not tend to zero as \( L \to 0^+ \). The defect set \( S_{LG}(Q^L) \) is defined to be the set of all such singular points, for \( L < \bar{L}_o \).

**Remark 1.** For each \( L > 0 \), we are guaranteed the existence of a global energy minimizer in our admissible space and a global energy minimizer is an example of a small energy solution. We know that \( \bar{L}_o \) exists from the uniform convergence of the bulk energy density to its minimum value everywhere away from the singularities of the limiting harmonic map in the \( L \to 0 \) limit.

**Lemma 4.4.** The 1-dimensional Hausdorff measure of \( S_{LG}(Q^L) \), where \( Q^L \) is a small energy solution for \( 0 < L < \bar{L}_o \), is bounded by \( \mathcal{I}_{LG}(Q^0) \), where \( Q^0 \) is the limiting harmonic map defined in (13) i.e.

\[
\mathcal{H}^1 [S_{LG}(Q^L)] \leq c \mathcal{I}_{LG}(Q^0) = C(\Omega) s_+^2
\]  

(60)

where \( \mathcal{H}^1 \) is the one-dimensional Hausdorff measure, \( c \) and \( C \) are positive constants independent of \( L \) and \( s_+ \) has been defined in (9). (See [12] for definition of Hausdorff measure.)

**Proof.** The proof of Lemma 4.4 follows the proof of an analogous result for Ginzburg-Landau theory in [7]. Fix \( 0 < L < \bar{L}_o \) and work with the defect set

\[
S_{LG}(Q^L) = \left\{ x_\in \Omega : \frac{1}{\lambda_1 \sqrt{L}} \int_{B(x_*, \lambda_1 \sqrt{L})} \frac{1}{2} |\nabla Q^L|^2 + \frac{f_B(Q^L)}{L} \, dV > \sigma_1(\epsilon_1^2, b^2, c^2) \right\}
\]  

(61)
for some positive constants $\lambda_i, \sigma_i$. Apply Vitali’s covering theorem [27] to the cover 
$\{ B(x_i, \lambda_i \sqrt{L}) : x_i \in S_{LG}(Q^L) \}$ and get a countable subset 
$\{ x_i : i \in J \}$ such that

$$B(x_i, \lambda_i \sqrt{L}) \cap B(x_j, \lambda_j \sqrt{L}) = \emptyset \quad i \neq j \quad (62)$$

and

$$S_{LG}(Q^L) \subset \cup_{i \in J} B(x_i, 5\lambda_i \sqrt{L}) \subset \Omega. \quad (63)$$

From the definition of $S_{LG}(Q^L)$ in (61), we have

$$\int_{B(x_i, \lambda_i \sqrt{L})} \frac{1}{2} |\nabla Q^L|^2 + \frac{f_B(Q^L)}{L} \, dV > \sigma_i \lambda_i \sqrt{L}. \quad (64)$$

Summing (64) over $i \in J$, using the inclusion $\cup_{i \in J} B(x_i, 5\lambda_i \sqrt{L}) \subset \Omega$ and the 
definition of a small energy solution in (5), we obtain the following sequence of inequalities

$$\sum_{i \in J} \sigma_i \lambda_i \sqrt{L} \leq \int_{\cup_{i \in J} B(x_i, 5\lambda_i \sqrt{L})} \frac{1}{2} |\nabla Q^L|^2 + \frac{f_B(Q^L)}{L} \, dV \leq J_{LG}(Q^L) \leq J_{LG}(Q^0) \quad (65)$$

and from the definition of the one-dimensional Hausdorff measure [12], we have

$$\mathcal{H}^1 [S_{LG}(Q^L)] \leq c J_{LG}(Q^0) \quad (66)$$

for a positive constant $c$ independent of $L$. Lemma 4.4 now follows.

The definition of the singular set in (59) is a natural definition. Qualitatively speaking, it identifies points $x \in \Omega$ where the energy density

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

cannot be bounded independently of $L$ in the limit $L \to 0$, as singular points. This would include points where $f_B(Q)$ deviates significantly from its minimum value (e.g. isotropic points), points of discontinuities in the eigenvectors or points close to the singular set of the limiting harmonic map $Q^0$ in (13). These concepts will be made more precise for the uniaxial case where we establish the equivalence between the singular set defined in (59), the singular set of the limiting harmonic map and the isotropic set.

5. Uniaxial solutions in 3D, their isotropic set and far-field behaviour.

This section focuses on uniaxial small energy solutions of (27). Uniaxial small energy solutions are known to exist in some prototype examples and one such uniaxial small energy solution, the radial-hedgehog solution on a three-dimensional ball with radial boundary conditions, has been studied in detail in [19]. The existence of purely uniaxial global energy minimizers is an open problem but as pointed out in Section 1, a detailed mathematical analysis of uniaxiality is the first natural mathematical step in the study of arbitrary solutions.

Let $Q$ be a uniaxial solution of (27) for a fixed $L > 0$. 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 (3)), direct calculations show that

$$|Q|^2 = \frac{2}{3} s^2, \quad \text{tr} Q^3 = \frac{2}{9} s^3, \quad \left( Q_{ik} Q_{kj} - \frac{\delta_{ij}}{3} \text{tr}(Q^2) \right) = \frac{s}{3} Q_{ij}.$$
and hence, the Euler-Lagrange equations (27) simplify to

$$LQ_{ij, kk} = \frac{1}{3} (2c_2 s^2 - b^2 s - 3a^2) Q_{ij}, \quad i, j = 1 \ldots 3.$$  \hspace{1cm} (67)

A uniaxial small energy solution $Q^L$ is analytic on $\Omega$ and 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 $\Omega$ [28]. From [18], we have that

$$s^L(x) \leq s_+ \quad x \in \Omega$$  \hspace{1cm} (68)

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 $Q_0$ in (10) and hence, every interior extension of $Q_0$ 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 $|\nabla n^L|^2(x) \to \infty$ as $x \to x_n$ but both $Q^L$ and

$$|\nabla Q^L|^2 = \frac{2}{3} |\nabla s^L|^2 + 2 (s^L)^2 |\nabla n^L|^2$$

are well-defined on $\widehat{\Omega}$. Therefore, $Q^L(x_n) = 0$ and consequently $s^L(x_n) = 0$. We deduce that $S^L_n \subset \Theta_L$ and from [23], we have that $n^L$ (eigenvectors) has the same degree of regularity as $Q^L$ as long as the number of distinct eigenvalues does not change. Hence, $n^L$ is analytic everywhere away from $\Theta_L$. We first make an elementary observation about the defect locations, in the vanishing core limit $L \to 0^+$.

**Lemma 5.1.** Let $\{ Q^{Lk} = s^{Lk} (n^{Lk} \otimes n^{Lk} - \frac{1}{3} I) \}$ be a small energy uniaxial sequence in the admissible space $A_{Q_0}$, where $L_k \to 0$ as $k \to \infty$. There exists a minimizing harmonic map extension $n_0 : \Omega \to S^2$ of $n_0$ such that after passing to a subsequence, $Q^{Lk} \to Q^0 = s_+ (n_0 \otimes n_0 - \frac{1}{3} I)$ strongly in $W^{1, 2}(\Omega; S_3)$ as $k \to \infty$.

Let $S_0$ denote the singular set of the limiting harmonic map $Q^0$ and let $S^L_n$ denote the defect set of the leading eigenvector $n^{Lk}$. Let $x_n \in S^L_n$. Then

$$\text{dist}(x_n, S_0) \leq \epsilon(L)$$

where $\epsilon(L_k) \to 0$ as $L_k \to 0^+$.

**Proof.** Let $x_n \in S^L_n$. As mentioned above, $s^{Lk}(x_n) = 0$ and $x_n \in \Theta_{L_k}$, where $\Theta_{L_k}$ has been defined above. However, for a small energy solution, the bulk energy density $f_B(Q^{Lk})$ converges uniformly to its minimum value, everywhere away from $S_0$, in the interior and up to the boundary, as $L_k \to 0$. Recalling (43), we deduce that $\text{dist}(x_n, S_0) \to 0$ as $L_k \to 0^+$. Lemma 5.1 now follows. \hfill \Box

Lemma 5.1 is also equivalent to the statement $\text{dist}(\Theta_{L_k}, S_0) \to 0$ as $L_k \to 0^+$ i.e. the isotropic set of a uniaxial small energy sequence converges uniformly to the singular set of a limiting harmonic map in the vanishing core limit.

**Theorem 5.2.** Let $Q^L$ be a uniaxial small energy solution in the admissible space $A_{Q_0}$, for a fixed $L > 0$. Then $Q^L = s^L (n^L \otimes n^L - \frac{1}{3} I)$ for some real-valued function $s^L : \overline{\Omega} \to \mathbb{R}$ and $n^L \in W^{1, 2}(\Omega; S^2)$. The following equations hold everywhere in $\Omega$, away from the isotropic set $\Theta_L$:

$$\Delta s^L - 3s^L|\nabla n^L|^2 = \frac{s^L}{3L} (2c_2 (s^L)^2 - b^2 s^L - 3a^2)$$  \hspace{1cm} (69)

$$\Delta n^L_j + |\nabla n^L|^2 n^L_j + 2 \frac{\partial_k s^L}{s^L} n^L_{j,k} = 0 \quad j, k = 1, 2, 3.$$  \hspace{1cm} (70)
Here $\mathbf{n}^L_{j,k}$ denotes the partial derivative $\frac{\partial \mathbf{n}^L_j}{\partial x_k}$. Alternatively, $\mathbf{n}^L = (\sin \theta^L \cos \phi^L, \sin \theta^L \sin \phi^L, \cos \theta^L)$, 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:

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

(71)

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

(72)

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

**Proof.** In what follows, we drop the superscript $L$ from $\mathbf{Q}^L$ for brevity. Since $\mathbf{Q}$ is a classical solution of (67), we have that $\mathbf{n}$ and $s = \frac{1}{2} \mathbf{Q}_{ij} (\mathbf{n}_i n_j - \frac{1}{3} \delta_{ij})$ are analytic away from $\Theta_L$. Hence, we have

$$\mathbf{Q}_{ij,k} = \partial_k s \left( \mathbf{n}_i n_j - \frac{1}{3} \delta_{ij} \right) + s \left( \mathbf{n}_i n_{j,k} + n_j n_{i,k} \right)$$

$$\mathbf{Q}_{ij,kk} = \Delta s \left( \mathbf{n}_i n_j - \frac{1}{3} \delta_{ij} \right) + 2 \partial_k s \left( \mathbf{n}_i n_{j,k} + n_j n_{i,k} \right) + s \left( \mathbf{n}_i n_{j,kk} + n_j n_{i,kk} + 2 n_{i,k} n_{j,k} \right)$$

(73)

where $i, j, k = 1 \ldots 3$, $\mathbf{Q}_{ij,k} = \frac{\partial \mathbf{Q}_{ij}}{\partial x_k}$ etc.

Consider the decoupled equations (67)

$$L \mathbf{Q}_{ij,kk} = \frac{1}{3} (2c^2 s^2 - b^2 s - 3a^2) \mathbf{Q}_{ij}$$

and multiply both sides by $\mathbf{n}_i$ to get the following vector equation

$$\frac{2}{3} \mathbf{n}_j \Delta s + 2 \partial_k s \mathbf{n}_{j,k} + s (\mathbf{n}_{j,kk} - |\nabla \mathbf{n}|^2 \mathbf{n}_j) = \frac{2s}{9L} (2c^2 s^2 - b^2 s - 3a^2) \mathbf{n}_j.$$  

(74)

Multiplying both sides of (74) by $\mathbf{n}_j$, we obtain the following scalar partial differential equation for $s$-

$$\frac{2}{3} \Delta s - 2s |\nabla \mathbf{n}|^2 = \frac{2s}{9L} (2c^2 s^2 - b^2 s - 3a^2)$$  

(75)

and (69) now follows. In (74) and (75), we use (73) and the relations $\mathbf{n}_i, \mathbf{n}_i = 1, \mathbf{n}_i n_{i,k} = 0$ and $\mathbf{n}_i n_{i,kk} = -|\nabla \mathbf{n}|^2$.

For (70), we multiply both sides of the vector equation (74) by the derivative $\mathbf{n}_{j,p}$ for $p = 1, 2, 3$ to get the following system of three equations -

$$2 \partial_k s \mathbf{n}_{j,p} n_{j,k} + s \mathbf{n}_{j,p} n_{j,k} = 0 \quad p = 1, 2, 3.$$  

(76)

Multiplying both sides by the scalar order parameter $s$, (76) simplifies to

$$\mathbf{n}_{j,p} \partial_k (s^2 \mathbf{n}_{j,k}) = 0 \quad p = 1, 2, 3.$$  

(77)

Next, we note that for a fixed $p$, $(\mathbf{n}_j, \mathbf{n}_{j,p}, \mathbf{e}_j)$ form an orthogonal basis at each point $x \in \Omega$ (where $\mathbf{e}_j = \mathbf{n}_j \times \mathbf{n}_{j,p}$) away from the isotropic set $\Theta_L$ so that

$$\partial_k (s^2 \mathbf{n}_{j,k}) = \lambda_1 \mathbf{n}_j + \lambda_2 \mathbf{e}_j$$  

(78)

where

$$\lambda_1 = \mathbf{n}_j \partial_k (s^2 \mathbf{n}_{j,k}) = -s^2 |\nabla \mathbf{n}|^2.$$
We substitute (78) into (74) to get
\[
\frac{2s}{3} n_j \Delta s - 2s^2 |\nabla n|^2 n_j + \lambda_2 e_j = \frac{2s^2}{9L} (2c^2 s^2 - b^2 s - 3a^2) n_j
\]
from which we deduce that \( \lambda_2 = 0 \). Hence
\[
\partial_k \left( s^2 n_{j,k} \right) + s^2 |\nabla n|^2 n_j = 0 \quad j = 1 \ldots 3
\]  
(79)
from which (70) follows.

An alternative formulation of (77) 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.
\[
n = (\sin \theta^L \cos \phi^L, \sin \theta^L \sin \phi^L, \cos \theta^L) .
\]  
(80)
Straightforward computations show that
\[
\frac{\partial n}{\partial x_k} = \partial_k \theta^L (\cos \theta^L \cos \phi^L, \cos \theta^L \sin \phi^L, -\sin \theta^L) + \sin \theta^L \partial_k \phi^L (-\sin \phi^L, \cos \phi^L, 0)
\]
\[
\frac{\partial^2 n}{\partial x_k \partial x_k} = \partial_{kk} \theta^L (\cos \theta^L \cos \phi^L, \cos \theta^L \sin \phi^L, -\sin \theta^L)
\]
\[
- (\partial_k \theta^L)^2 (\sin \theta^L \cos \phi^L, \sin \theta^L \sin \phi^L, \cos \theta^L)
\]
\[
+ 2 \cos \theta^L \partial_k \theta^L \partial_k \phi^L (-\sin \phi^L, \cos \phi^L, 0) + \sin \theta^L \partial_{kk} \phi^L (-\sin \phi^L, \cos \phi^L, 0)
\]
\[
- \sin \theta^L (\partial_k \phi^L)^2 (\cos \phi^L, \sin \phi^L, 0) .
\]  
(81)
Substituting (81) into (74) and taking the dot product of both sides with \((\cos \theta^L \cos \phi^L, \cos \theta^L \sin \phi^L, -\sin \theta^L)\), we obtain
\[
2 \partial_k s \partial_k \theta^L + s \partial_{kk} \theta^L - s \sin \theta^L \cos \theta^L |\nabla \phi^L|^2 = 0.
\]  
(82)
We multiply both sides of (83) by \( s \) and equation (71) now follows. Similarly, we take the scalar product of (74) with the unit-vector \((-\sin \phi^L, \cos \phi^L, 0)\) to obtain
\[
s \sin \theta^L \partial_k s \theta^L + 2s \cos \theta^L \partial_k \theta^L \partial_k \phi^L + 2 \sin \theta^L \partial_k s \partial_k \phi^L = 0.
\]  
(83)
As above, we multiply both sides of (84) by \( s \sin \theta^L \) and (72) then follows. The proof of theorem 5.2 is now complete.

**Remark 3.** We note that for \( s \) constant, (70) is equivalent to the harmonic map equations \( \Delta n_0 + |\nabla n_0|^2 n_0 = 0 \) [5].

5.1. **Far-field results.** In this section, we study the qualitative properties of uniaxial small energy solutions \( \{Q^L\} \) away from the isotropic set \( \Theta_L \), in the vanishing core limit, \( L \to 0 \). From Lemma 5.1, 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 (13), as \( L \to 0^+ \).

Let \( Q^L = s^L (n^L \otimes n^L - \frac{1}{3} I) \) be a uniaxial small energy solution of (27), for fixed \( L > 0 \). Recall from (39) that for \( L \) sufficiently small,
\[
0 \leq s_+ - s^L(x) \leq \epsilon_1(L)
\]  
(85)
or equivalently
\[
|Q^L|^2 - \frac{2}{3} s_+^2 |Q^L|^2 \leq \epsilon_2(L)
\]  
(86)
where \( \epsilon_1(L), \epsilon_2(L) \to 0 \) as \( L \to 0^+ \), everywhere away from \( S_0 \). The inequalities (85) and (86) give the governing equations a Ginzburg-Landau like structure that can be exploited to prove far-field properties.

Our first result is an inequality for

\[
A^L = \frac{1}{2} Q_{ij,k}^L Q_{ij,k}^L
\]

that holds everywhere away from \( S_0 \) on \( \bar{\Omega} \). We do not use Lemma 5.3 in the subsequent sections but keep it as an interesting technical result and as an example of a Ginzburg-Landau type of result away from singularities (see [4] for an analogous inequality in Ginzburg-Landau theory for 2D domains).

**Lemma 5.3.** 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

\[
- \Delta A^L + \left( 1 - \frac{1}{\alpha^2} \right) |\nabla^2 Q^L|^2 \leq \alpha^4 \frac{A^L}{|Q^L|^2}
\]

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 (87) closely follows the methods in [4]. In what follows, we drop the superscript \( L \) for brevity. First, consider the decoupled equations (67); setting 

\[
f(s) = (2c^2 s^2 - b^2 s - 3a^2)
\]

and differentiating both sides of (67) with respect to \( x_p \), we obtain

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

From (86) and the global upper bound (32), we have that \( |Q| \) is bounded away from zero on \( \Omega \setminus B_\delta(S_0) \) and

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

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

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

where \( |\nabla^2 Q|^2 = Q_{ij,kp} Q_{ij,kp} \) and using (88), we obtain

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

Note that \( (Q_{ij} Q_{ij,k})^2 = (Q \cdot \nabla Q)^2 = \frac{1}{4} |\nabla |Q|^2|^2 \), \( i,j,k = 1 \ldots 3 \). From (89) and (67), we have the following inequality

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

Finally, we use the inequality

\[
|\Delta Q| \leq \alpha |\nabla^2 Q|
\]
where \( \alpha > 1 \) is a positive constant that can be worked out explicitly. Substituting the above into (92),

\[
- \Delta A + |\nabla^2 Q|^2 \leq 2\alpha A \frac{|\nabla^2 Q|}{Q} \leq \frac{1}{10^2} |\nabla^2 Q|^2 + \alpha^4 \frac{A^2}{|Q|^2}
\]

(93) and (87) now follows.

We recall the uniform convergence result in (48) and (47), whereby we establish a uniform bound for \( |\nabla Q|^2 \), independent of \( L \), everywhere away from \( S_0 \) in the interior of \( \Omega \), in the vanishing core limit. 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 \([8, 9]\) to the Landau-de Gennes framework, as demonstrated in theorem 5.4.

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 \( \Omega_\rho(x_0) = \{x \in \Omega; |x| \leq \rho; x_3 \geq 0\} \).

**Theorem 5.4.** Let \( \{Q^{L_k}\} \) be a uniaxial small energy sequence 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 \( W^{1,2}(\Omega; \mathbb{S}_3) \) 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 exist \( C_1 > 0, C_2 > 0, L_0 > 0 \) (all constants independent of \( L_k \) and \( x_0 \)) so that if for some \( 0 < r < \rho \), we have

\[
\frac{1}{r^2} \int_{\Omega_r(x_0)} \frac{1}{2} |\nabla Q^{L_k}|^2 + \frac{f_B(Q^{L_k})}{L_k} \, dx \leq C_1
\]

then

\[
r^2 \sup_{\Omega_{r/2}(x_0)} e_{L_k}(Q^{L_k}) \leq C_2 \text{ for all } L_k < \tilde{L}_0
\]

where

\[
e_{L_k}(Q^{L_k}) = \frac{1}{2} |\nabla Q^{L_k}|^2 + \frac{f_B(Q^{L_k})}{L_k}.
\]

**Proof.** The first half of the proof of theorem 5.4 closely follows the scaling arguments for the interior uniform convergence result (47) in [17] and the details are reproduced here for completeness. The second half closely follows the arguments in Theorem 3.1 in [7] for harmonic maps from a \( m \)-dimensional domain to a \( n \)-dimensional target space, and Theorem 2.1 in [9] for Ginzburg-Landau functionals defined for maps from \( \mathbb{R}^m \) to \( \mathbb{R}^n \).

We first recall from (39) and the definition of \( Q_{\text{min}} \) in (8) that since \( \Omega_r(x_0) \) contains no singularity of \( Q^0 \), \( \exists m^k(x) \in \mathbb{S}^2 \) such that

\[
|Q^{L_k}(x) - s_+ \left( m^k(x) \otimes m^k(x) - \frac{1}{3}I \right) | < \epsilon_0 \ll 1 \quad x \in \Omega_r(x_0)
\]

for \( L < \tilde{L}_0 \) (Such a \( \tilde{L}_0 \) exists by virtue of the uniform convergence of \( f_B \) to its minimum value away from the singular set of \( Q^0 \) as \( L \to 0 \). To see (96), we recall theorem 10 from [17], where we show that for uniaxial \( Q \)-tensors i.e. \( Q = s (m \otimes m - \frac{1}{3}I) \) for some \( m \in \mathbb{S}^2 \), \( f_B(Q) \geq C(a^2, b^2, c^2) (s - s_+)^2 \) for some positive constant \( C \).) We also note that \( Q^0 \) has a finite number of interior isolated point defects \( \{x_1, \ldots, x_N\} \) (from standard results in the theory of harmonic maps [5]) and set \( d_{\text{min}} = \min_{i=1,\ldots,N} \text{dist} (x_i, \partial \Omega) \). Therefore, for every \( x_0 \in \partial \Omega \), we can define \( \Omega_r(x_0) \) for some \( r < d_{\text{min}} \) such that \( \Omega_r(x_0) \) contains no singularity of \( Q^0 \).
Let $\hat{r}$ of $r$ implies the conclusion (95). We prove this claim by contradiction. Assume that

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

(97)

Define $e_{1k} = \max_{x \in \Omega_r(x_0)} e_{L_k}(Q^{L_k}) = e_{L_k}(Q^{L_k})(x_1)$. Then

$$\max_{x \in \Omega_{2/3r-1}(x_1)} e_{L_k}(Q^{L_k}) \leq 4e_{1k}$$

(98)

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 (97).

Define $r_2(k) = \frac{2/3r-1}{2} \sqrt{e_{1k}}$ and let

$$R^{L_k}(x) = Q^{L_k} \left( x_1 + \frac{x}{\sqrt{e_{1k}}} \right).$$

(99)

Let $\hat{L}_k = e_{1k}L_k$. Then $R^{L_k}$ has the following properties on $\Omega_r(0)$:

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

(100)

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

(101)

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

(102)

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

We next claim that $r_2(k) \leq 1$ for sufficiently large $k$. It is obvious that $r_2(k) \leq 1$ implies the conclusion (95). We prove this claim by contradiction. Assume that $r_2(k) > 1$; then using the same arguments as in [8], one is led to the existence of a sequence of solutions $\{R^{L_k}\}$ of (102) on $\Omega_1(0)$, with the following properties:

$$-\Delta R^{L_k}_{ij} + \frac{1}{3L_k} \left( 2c^2s^2 - b^2s - 3a^2 \right) R^{L_k}_{ij} = 0 \text{ in } \Omega_1(0)$$

$$\max_{x \in \Omega_1(0)} e_{L_k}(R^{L_k}) \leq 4 \ e_{L_k}(R^{L_k})(0) = 1$$

$$R^{L_k}|_{x'} = Q_b \left( x_1 + \frac{x'}{\sqrt{e_{1k}}} \right) \text{ when } x_1 + \frac{x'}{\sqrt{e_{1k}}} \in \partial \Omega$$

where

$$\left| \nabla Q_b \left( x_1 + \frac{x'}{\sqrt{e_{1k}}} \right) \right| \leq \epsilon_k \| \nabla Q_b \|_{L^\infty(\partial \Omega)},$$

$$\left| \nabla^2 Q_b \left( x_1 + \frac{x'}{\sqrt{e_{1k}}} \right) \right| \leq \epsilon_k^2 \| \nabla^2 Q_b \|_{L^\infty(\partial \Omega)}$$

(103)

where the last two inequalities follow from scaling and $\epsilon_k \to 0$ as $k \to \infty$. 

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From (45) and (101), we deduce that $R^{L_k}$ satisfies the following Bochner-type inequality on $\Omega_1(0)$:

$$- \Delta e_{L_k}(R^{L_k}) \leq C' e_{L_k}(R^{L_k}) \quad x \in \Omega_1(0)$$

(104)

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:

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

(105)

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

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

from (96), for $k$ sufficiently large. From theorem 5.2, we have that $s_k$ and $n^k$ satisfy the following equations in $\Omega_1(0)$:

$$\Delta s_k - 3s_k|\nabla n^k|^2 = \frac{s_k}{3L_k}(2c^2 s^2_k - b^2 s_k - 3a^2)$$

(106)

$$\Delta n^k_j + |\nabla n^k|^2 n^k_j + 2 \frac{\partial_p s_k}{s_k} n^k_{j,p} = 0$$

(107)

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

(108)

Equation (108) implies that

$$|\nabla n^k| \leq \frac{2}{s_+}, \quad \left| \frac{2\nabla s_k}{s_k} \right| \leq \frac{6}{s_+} \text{ on } \Omega_1(0)$$

(109)

for $k$ sufficiently large.

These conclusions immediately imply that there exists a constant $C > 0$ such that

$$1 \leq C \int_{\Omega_1(0)} \frac{1}{2} |\nabla R^{L_k}|^2 + \frac{f_B(R^{L_k})}{L_k} \ dV$$

$$= C \int_{\Omega_1(0)} \frac{1}{3} |\nabla s_k|^2 + s^2_k|\nabla n^k|^2 + \frac{f_B(R^{L_k})}{L_k} \ dV \text{ as } k \to \infty.$$  

(110)

In fact, if the constant $C$ does not exist, then $\exists$ a sequence $\{R^k\}$ ($\{s_k\}, \{n^k\}$) which satisfies (103), (104), (106)-(109) such that

$$\int_{\Omega_1(0)} \frac{1}{2} |\nabla R^k|^2 \ dV \to 0 \text{ as } k \to \infty$$

or equivalently

$$\int_{\Omega_1(0)} |\nabla s_k|^2 \ dV \to 0 \text{ as } k \to \infty$$

and

$$\int_{\Omega_1(0)} |\nabla n^k|^2 \ dV \to 0 \text{ as } k \to \infty.$$  

We look at the equations for $s_k$ and $n^k$ separately. The methods now closely follow the arguments in [9]. Using (107) and (109), we repeat the arguments in [9]
to deduce that (also see [15])
\[
\left| \nabla n^k \right|^2 (x) \leq C \left[ \int_{\Omega_1(0)} |\nabla n^k|^2 dV + \left\| \nabla n^k \right\|_{L^2(\Omega_1(0))}^2 + \left\| \nabla Q_b \left( x_1 + \frac{x'}{\sqrt{\epsilon_k^3}} \right) \right\|_{C^1(\partial \Omega)} \right]
\]
\[
\leq \delta_k \to 0 \text{ as } k \to \infty
\]
for \( x \in \Omega_{2/3}(0) \), where we have used the inequalities above and the inequalities in (103).

We introduce the function \( \bar{s}_k = s_+ - s_k \) and then from (106), we have that \( \bar{s}_k \) satisfies
\[
-\Delta \bar{s}_k = 3s_k |\nabla n|^2 - \frac{2c^2 s_k (s_k - s_-)}{3L_k}
\]
We have \( 0 \leq \bar{s}_k \leq s_+ \) from (32) and \( \bar{s}_k = 0 \) on \( \partial \Omega \) because of our choice of the boundary condition \( Q_b \) in (10). Repeating the same arguments as in [9], then
\[
-\Delta \bar{s}_k (x) \leq C \delta_k \quad x \in \Omega_{2/3}(0)
\]
\( \bar{s}_k = 0 \quad x_3 = 0 \)
(112)
since \( x_3 = 0 \) on the boundary \( \partial \Omega_{2/3}(0) \), \( C > 0 \) is independent of \( k \) and we have used (111). Hence for \( x \in \Omega_{1/2}(0) \), we have
\[
\bar{s}_k (x) \leq Cx_3 \delta_k \to 0 \text{ as } k \to \infty \text{ for } x \in \Omega_{1/2}(0)
\]
and
\[
|\nabla \bar{s}_k| (x) \leq C \delta_k \to 0 \text{ as } k \to \infty
\]
for \( x \in \Omega_{1/2}(0) \). (Alternatively, one could apply Lemma 3.3 of Chapter II and Theorem 9.1 of Chapter IV in [15] to the equation for \( \bar{s}_k \) to obtain
\[
\left\| \nabla \bar{s}_k \right\|_{C^\alpha (\Omega_{3/4}(0))} \leq C \left\| \bar{s}_k \right\|_{W^{2,q}(\Omega_{3/4}(0))}
\]
\[
\leq C \left\| \nabla \bar{s}_k \right\|_{L^q(\Omega_1(0))} + C \left\| \bar{s}_k \right\|_{W^{2, \frac{n+2}{q}}(\partial \Omega)} \leq C
\]
where all constants \( C \) are independent of \( k \) and depend only on \( \Omega \) and \( Q_b \), \( q > n + 2 \) with \( n = 3 \) in our case and \( \alpha = 1 - \frac{n+2}{q} \). This estimate coupled with \( \int_{\Omega_1(0)} |\nabla s_k|^2 \, dV \to 0 \) as \( k \to \infty \) would also yield the uniform bound (114). The same comments apply to the equation for \( n^k \).

We next return to the Bochner inequality in (104) and define
\[
\hat{\epsilon}_k = \max \left\{ 0, \epsilon_{L_k} (R_{L_k}^2) - (1 + 2s_+^2) \delta_k^2 \right\}
\]
where \( s_+ \) is a constant defined in (9) (recall that \( f_B (R_{L_k}^2) = 0 \) on \( \partial \Omega \) because of the boundary condition \( Q_b \) in (12)). Then \( \hat{\epsilon}_k \) satisfies
\[
-\Delta \hat{\epsilon}_k (x) \leq C \hat{\epsilon}_k'' (x) \quad \text{for } x \in \Omega_{1/2}(0)
\]
\[
\hat{\epsilon}_k (x) = 0 \text{ for } x \in \partial \Omega.
\]
(116)
Finally, we can use the same arguments as in [9] (Moser’s estimate) to show that (116) implies the following
\[
\sup_{x \in \Omega_{1/4}(0)} \hat{\epsilon}_k (x) \to 0 \text{ as } k \to \infty,
\]
contradicting \( \hat{\epsilon}_k (0) = 1 - (1 + 2s_+^2) \delta_k^2 > \frac{1}{2} \) for \( k \) sufficiently large.
Therefore, there exists a positive constant $C > 0$ such that (110) holds. We next use the boundary version of the monotonicity lemma (38) and the inequality $r_2 \geq 1$ to obtain the following sequence of inequalities:

$$\int_{\Omega_{1/2}(0)} e_{L_k}(R^{L_k}) \, dV \leq \frac{1}{r_2} \int_{\Omega_{r_2}(0)} e_{L_k}(R^{L_k}) \, dV + C(r_2 - 1)$$

$$\leq \frac{2}{r^2 - 1} \int_{\Omega_{2/r-1}(x_1)} e_{L_k}(Q^{L_k})(x) \, dV + \frac{C}{\sqrt{\epsilon_1}} (r_2 - 1)$$

$$\leq \frac{3}{r} \int_{\Omega_2(x_1)} e_{L_k}(Q^{L_k})(x) \, dV + C \left( \frac{r}{3} - \frac{1}{\sqrt{\epsilon_1}} \right) \leq C_1 + C'r. \quad (118)$$

If we choose $C_1$ and $r$ small enough, then we get a contradiction to the claim in (110). Therefore, $r_2(k) \leq 1$ for $k$ sufficiently large and from the definition of $r_2$ in (99), we deduce the uniform energy density bound in (95), everywhere away from the singular set of the limiting harmonic map, up to the boundary.

For the reader’s convenience, we quote Lemma 2 from [4] which is used in theorem 5.6.

**Lemma 5.5 ([4])**. Let $\omega(r)$ be a solution of

$$-\epsilon^2 \Delta \omega + \omega = 0 \text{ on } B(0, R)$$

$$\omega = 1 \text{ on } \partial B(0, R). \quad (119)$$

Then for $\epsilon < \frac{3R}{4}$, $\omega(r) \leq e^{\frac{1}{\epsilon} \left( r^2 - r^2 \right)}$ on $B(0, R)$.

**Theorem 5.6.** Let $\{Q^{L_k}\}$ be a uniaxial small energy sequence of solutions of (27) in admissible space $A_Q$, where $L_k \to 0^+$ as $k \to \infty$. Then as $k \to \infty$, we can extract a suitable subsequence such that $Q^{L_k} \to Q^0$ 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 (13) and $\delta$ is independent of $L_k$.

**Proof.** The proof follows the methods in [4] and the key ingredient is to establish a global bound for $s_+ - \epsilon L_k$, everywhere away from $S_0$, for $L_k$ sufficiently small.

We drop the superscript $L_k$ in what follows for convenience. Consider the equation (69) on $\Omega \setminus B_\delta(S_0)$ and introduce the function

$$\psi = \frac{s_+ - s}{L_k}, \quad (120)$$

$s_+$ has been defined in (30) and $s_- = (b^2 - \sqrt{b^2 + 24a^2c^2})/4e^2 < 0$. Then (69) can be re-written as

$$\Delta s - 3s|\nabla \psi|^2 = -\frac{2c^2}{3} \psi (s - s_-) \quad (121)$$

From (32) and (43) (the uniform convergence of the bulk energy density to its minimum value everywhere away from the singular set of $Q^0$), we have that $\frac{2}{3}s_+^2 \geq |Q^0| \geq \frac{2}{3}s_+^2 - \epsilon L$ or equivalently $s_+ - \epsilon L \leq s \leq s_+$ where $\epsilon L \to 0$ as $L \to 0$, on $\Omega \setminus B_\delta(S_0)$. Therefore,

$$\frac{2c^2}{3} (s - s_-) \geq \frac{1}{\beta}$$

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

Let $x_0 \in \overline{\Omega} \setminus B_3(S_0)$ be an arbitrary point and let $K' \supseteq \overline{\Omega} \setminus B_3(S_0)$ be a neighbourhood that does not contain any defects of $Q^0$. Choose $d$ sufficiently small so that $\overline{\Omega} \cap B(x_0, d) \subseteq K'$. We note that $|\nabla Q|^2 = \frac{2}{3} |\nabla s|^2 + 2s^2 |\nabla n|^2$ where $Q = s (n \otimes n - \frac{1}{3} I)$ and recall the global uniform bound (95) everywhere away from $S_0$ (for $L$ sufficiently small) to deduce that

$$|\nabla n|^2(x) \leq C(a^2, b^2, c^2, \Omega)$$
onumber

on $\overline{\Omega} \cap B(x_0, d)$. Combining the above, we have that $\psi$ satisfies the following inequality on $\overline{\Omega} \cap B(x_0, d)$

$$- \beta L \Delta \psi + \psi \leq \gamma |\nabla n|^2 \leq D(a^2, b^2, c^2, \Omega)$$

(122)

where $\gamma$ and $D$ are positive constants independent of $L$. Applying standard maximum principle arguments and Lemma 2 from [4], we conclude that

$$\|\psi\|_{L^\infty(\overline{\Omega} \cap B(x_0, d))} \leq D'(a^2, b^2, c^2, \Omega)$$

(123)

where $D'$ is a positive constant independent of $L$.

Consider the governing equations (67) for a uniaxial small energy solution $Q$; they can be written in terms of the function $\psi$ as shown below -

$$\Delta Q = \frac{1}{3L} \left( 2c^2 s^2 - b^2 s - 3a^2 \right) Q \leq -\alpha \psi Q$$

(124)

\((124)\) means that $\frac{1}{3L} \left( 2c^2 s^2 - b^2 s - 3a^2 \right) Q_{ij} \leq -\alpha \psi Q_{ij}$ for $i, j = 1 \ldots 3$) where $\alpha > 0$ is a constant independent of $L$, we have used the definition of $\psi$ in (120) and the uniform convergence of bulk energy density everywhere away from $S_0$ (refer to (39)). Finally, we combine the global upper bound (32) and the $L^\infty$-estimate (123) to conclude that

$$\|\Delta Q\|_{L^\infty(\overline{\Omega} \cap B(x_0, d))} \leq D''(a^2, b^2, c^2, \Omega)$$

(125)

where $D''$ is a positive constant independent of $L$ i.e. $|\Delta Q|$ can be bounded independently of $L$ on $\overline{\Omega} \cap B(x_0, d)$. The choice of $x_0 \in \overline{\Omega} \setminus B_3(S_0)$ is arbitrary. We use (125) and Sobolev estimates to establish $\{Q^{L^k}\} \rightarrow Q^0$ in $C^{1,\alpha}(\Omega \setminus B_3(S_0))$ as $k \rightarrow \infty$, for some $0 < \alpha < 1$. The proof of theorem 5.6 is now complete. \qed

Remark 4. One immediate consequence of (123) is that $s_+ - s^L \leq CL$, where $C$ is a positive constant independent of $L$, everywhere away from $S_0$ in the limit $L \rightarrow 0$. This explicitly estimates the rate of convergence in (43) and improves upon a previous estimate in [17] where an analysis of the bulk energy density $f_B$ in (6) shows that $s_+ - s \leq C_1 \sqrt{L}$ with $C_1$ being a positive constant independent of $L$.

Lemma 5.7. Let $Q^L = s^L (n^L \otimes n^L - \frac{1}{3} I)$ be a uniaxial small energy solution of (27) in $A_Q$, for $L$ sufficiently small so that Theorems 5.4 and 5.6 hold. Then for $x \in \Omega \setminus B_3(S_0)$, we have

$$|\nabla s^L(x)| \leq \epsilon_1(x)$$

(126)

$$\|\nabla n^L(x)\|^2 - |\nabla n_0|^2 \leq \epsilon_2(x)$$

where $n_0$ and $Q^0$ are defined in (13) and $\epsilon_1, \epsilon_2 \rightarrow 0^+$ as $L \rightarrow 0^+$.

Proof. Lemma 5.7 is a direct consequence of theorem 5.6. Let $x \in \Omega \setminus B_3(S_0)$. Then from theorem 5.6, we have that

$$|Q^L_{ij}(x) - Q^0_{ij}(x)| \leq \epsilon_3(x)$$

$$|Q^L_{ij,k}(x) - Q^0_{ij,k}(x)| \leq \epsilon_4(x)$$

(127)
where $Q^0$ is the limiting harmonic map in (13), $Q_{ij,k} = \frac{\partial Q_{ij}}{\partial x_k}$ and $\epsilon_3, \epsilon_4 << 1$. One can directly compute

$$|\nabla Q^0|^2 = 2s_+^2 |\nabla n_0|^2. \quad (128)$$

On the other hand,

$$|Q^L|^2 = \frac{2}{3} (s^L)^2$$

and therefore,

$$Q^L_{ij} Q^L_{ij,k} = \frac{2}{3} s^L \partial_k s^L \quad (129)$$

where $|s^L(x) - s_+| < \epsilon_5(x) << 1$ for $x \in \Omega \setminus B_{\delta}(S_0)$, from (43).

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

$$Q^L_{ij} Q^L_{ij,k} = (Q^L_{ij}(x) - Q^0_{ij}(x)) Q^L_{ij,k}(x) + Q^0_{ij}(x) (Q^L_{ij,k}(x) - Q^0_{ij,k}(x)) \quad (130)$$

since $Q^0_{ij}, Q^0_{ij,k} = 0$ from $|Q^0|^2 = \frac{2}{3} s^2$. Using the inequalities (127), the global bound (95) and the triangle inequality, we have that

$$|Q^L_{ij}(x) Q^L_{ij,k}(x)| \leq \epsilon_6(x) << 1 \quad (131)$$

for $x \in \Omega \setminus B_{\delta}(S_0)$ and from (129) and (43), this necessarily implies that

$$|\nabla s^L| \leq \epsilon_7(L) \quad (132)$$

away from $S_0$, where $\epsilon_7 \to 0^+$ as $L \to 0^+$.

On the other hand, from Theorem 5.6, $Q^L \to Q^0$ in $C^{1,\alpha}(\Omega; S_3)$ as $L \to 0$ (up to a subsequence), everywhere away from $S_0$. Therefore, for $x \in \Omega \setminus B_{\delta}(S_0)$,

$$||\nabla Q^L|^2(x) - |\nabla Q^0|^2(x)| \leq \epsilon_8(x) \quad (133)$$

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

$$|\nabla Q^L|^2 = \frac{2}{3} \nabla s^L|^2 + 2(s^L)^2|\nabla n|^2.$$

Combining (43), (132), (133) and (128), we have that $|\nabla n|^2 \to |\nabla n_0|^2$ uniformly as $L \to 0^+$. Lemma 5.7 now follows.

Theorem 5.8. Let $Q^L = s^L (n^L \otimes n^L - \frac{1}{3} I)$ be a uniaxial small energy solution of (27) in $A_Q$, for $L$ sufficiently small, so that Theorems 5.4 and 5.6 hold. Then for $x \in \Omega \setminus B_{\delta}(S_0)$, we have that

$$ \left| \frac{s_+ - s^L(x)}{L} - \frac{9 |\nabla n_0|^2}{\sqrt{b^2 + 24\alpha^2 c^2}} \right| \leq \epsilon_9(x, L) \quad (134)$$

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

Proof. Let $x_0 \in \Omega \setminus B_{\delta}(S_0)$ be an arbitrary point and let $K' \supset \Omega \setminus B_{\delta}(S_0)$ be a compact neighbourhood that does not contain any defects of $Q^0$. Choose $d$ sufficiently small so that $\Omega \cap B(x_0, d) \subset K'$. Consider the function $\psi^L = \frac{s_+ - s^L}{L}$ in (120) and the equation (69) on $\Omega \cap B(x_0, d)$

$$\Delta s^L - 3s^L |\nabla n|^2 = -2e^2 \frac{s^L}{3} (s^L - s_-)\psi^L \quad (135)$$
Proof. Let \( S = \Theta_x(x_0) \). Equation (135) can be re-arranged to give

\[
-L\Delta \left( \psi_L - \frac{9|\nabla n_0|^2}{\sqrt{b^4 + 24a^2c^2}} \right) + 2c^2 s^L(s^L - s) + \frac{9|\nabla n_0|^2}{\sqrt{b^4 + 24a^2c^2}} \leq \frac{9|\nabla n_0|^2}{\sqrt{b^4 + 24a^2c^2}}.
\]

Then

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

We note that \( \Delta |\nabla n_0|^2 = O(1) \) away from \( S_0 \) and the right-hand side of (136) can be written as

\[
3s^L|\nabla n_0|^2 - 3s_+ |\nabla n_0|^2 + 3s_+ |\nabla n_0|^2 - \frac{6c^2 s^L(s^L - s)}{\sqrt{b^4 + 24a^2c^2}} |\nabla n_0|^2 + O(L).
\]

Finally, we use (43) and (126) to deduce that

\[
3s^L|\nabla n_0|^2 - 3s_+ |\nabla n_0|^2 \leq \epsilon_{10}
\]

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

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

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

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

where \( \beta \) is a positive constant independent of \( L \) and \( \epsilon_{11} \to 0^+ \) as \( L \to 0^+ \). The choice of \( x_0 \in \Omega \setminus B_\delta(S_0) \) is arbitrary and hence, theorem 5.8 now follows from the maximum principle and Lemma 2 of [4]. \( \square \)

5.2. The defect set and the isotropic set. Recall our definition of the defect set in Section 4.3 i.e.

\[
S_{LG}(Q) = \left\{ x \in \Omega : \frac{1}{\lambda_0 \sqrt{L}} \int_{B(x, \lambda_0 \sqrt{L})} e_L(Q)(x) \, dV > \sigma \right\}
\]

for positive constants \( \lambda_0 \) and \( \sigma \) independent of \( L \), \( 0 < L < \bar{L} \) where \( \bar{L} \) has been defined in (58) and for a boundary point \( x \in \partial \Omega \), we replace \( B(x, \lambda_0 \sqrt{L}) \) by \( B(x, \lambda_0 \sqrt{L}) \cap \Omega \) in the definition of \( S_{LG} \) above.

Lemma 5.9. Let \( Q^L = s^L (n^L \otimes n^L - \mathbb{1}) \) be a uniaxial small energy solution of (27). Let \( \Theta_L = \{ x \in \Omega ; \psi_L(x) = 0 \} \) denote the isotropic set of \( Q^L \). Then \( \Theta_L \subseteq S_{LG}(Q^L) \).

Proof. Let \( x_0 \in \Theta_L \). Then \( Q^L(x_0) = 0 \) and

\[
f_B(Q^L)(x_0) \geq \beta(a^2, b^2, c^2)
\]

for a positive constant \( \beta \) independent of \( L \). From the global bound \( \| \nabla Q^L \|_{L=\infty(\Omega)} \leq \frac{C}{\sqrt{L}} \), [3] we have

\[
f_B(Q^L)(x) \geq \beta - \frac{C}{\sqrt{L}} \text{ on } B(x_0, r).
\]
We set \( r = \lambda_0 \sqrt{L} \) for some \( \lambda_0 \) independent of \( L \). Then, if we choose \( \lambda_0 \) suitably small, we have \( f_B(Q^L)(x) \geq \beta (a^2, b^2, c^2) \) for \( x \in B(x_0, \lambda_0 \sqrt{L}) \), where \( \beta \) is independent of \( L \). Therefore,

\[
\frac{1}{\lambda_0 \sqrt{L}} \int_{B(x_0, \lambda_0 \sqrt{T})} e_L(Q^L)(x) \, dV \\
\geq \frac{1}{\lambda_0 \sqrt{L}} \int_{B(x_0, \lambda_0 \sqrt{T})} \frac{f_B(Q^L)}{L} \, dV \geq \beta'' (a^2, b^2, c^2) > 0
\]  

(142)

where \( \beta'' \) is a positive constant independent of \( L \). Therefore, \( x_0 \in S_{LG}(Q^L) \) as required. Since \( x_0 \in \Theta_L \) is arbitrary, we deduce that \( \Theta_L \subseteq S_{LG}(Q^L) \) as claimed. \( \square \)

Next, we use an elementary covering argument to obtain an upper bound for the measure of the singular set, \( S_{LG}(Q^L) \), of a uniaxial small energy solution \( Q^L \).

Fix \( 0 < L \leq \bar{L}_0 \) and let \( Q^L \) be a corresponding uniaxial small energy solution. The corresponding singular set is

\[
S_{LG}(Q^L) = \left\{ x \in \Omega; \frac{1}{\lambda_0 \sqrt{L}} \int_{B(x_0, \lambda_0 \sqrt{T})} e_L(Q^L)(x) \, dV > \sigma \right\}
\]

for arbitrary positive constants \( \lambda_0 \) and \( \sigma \). We apply Vitali’s covering theorem to the cover \( \{ B(x, \lambda_0 \sqrt{L}); x \in S_{LG}(Q^L) \} \) to get a countable subset \( \{ x_i; i \in J \} \) such that (62) and (63) hold. We use the lower bound in (139) and the definition of a small energy solution in (5) to obtain the following sequence of inequalities:

\[
\sigma' \sqrt{L} |J| \leq \int_{\cup_{i=1}^{|J|} B(x_i, \lambda_0 \sqrt{L})} e_L(Q^L)(x) \, dV \leq cI_G[Q^0] \leq C (\Omega) s^2_+ \quad (143)
\]

where \( |J| \) denotes the cardinality of the set \( J \), \( c \) and \( \sigma' \) are positive constants independent of \( L \) and \( Q^0 \) is the limiting harmonic map defined in (13). Equation (143) shows that

\[
|J| \leq \frac{C}{\sqrt{L}} \quad (144)
\]

for a positive constant \( \tilde{C} \) independent of \( L \). We can obtain an upper bound for the measure of the singular set \( S_{LG}(Q^L) \) as shown below –

\[
|S_{LG}(Q^L)| \leq |J| \left| B(x_i, \lambda_0 \sqrt{L}) \right| \leq \tilde{C} L
\]  

(145)

for a positive constant \( \tilde{C} \) independent of \( L \).

Our next lemma establishes the equivalence between the singular set in (139) and the singular set of a limiting harmonic map in the limit \( L \to 0 \).

**Lemma 5.10.** Let \( Q^L \) be a uniaxial small energy solution of (27). Let \( \mathcal{R} = \Omega \setminus \bigcup_{i=1}^N B(x_i, \delta) \), where \( \{ x_1, \ldots, x_N \} \) are the \( N \) isolated point singularities of the limiting harmonic map \( Q^0 \) and \( 0 < \delta < 1 \) is a constant independent of \( L \). Then for \( L \) sufficiently small (\( L \leq \min \{ \bar{L}_0, L_0 \} \)) where \( \bar{L}_0 \) has been defined in (58) and \( L_0 \) has been defined in theorem 5.4, we have

\[
\mathcal{R} \cap S_{LG}(Q^L) = \phi \quad \text{as} \quad L \to 0.
\]  

(146)

**Proof.** Let \( \bar{\Omega} \supseteq \mathcal{R}' \supseteq \mathcal{R} \) be a compact neighbourhood of \( \mathcal{R} \) that contains no singularity of \( Q^0 \). From theorem 5.4, we have the following inequality

\[
e_L(Q^L)(x) = \frac{1}{2} |\nabla Q^L|^2(x) + \frac{f_B(Q^L)(x)}{L} \leq \alpha(a^2, b^2, c^2) \quad \forall x \in \mathcal{R}'
\]  

(147)
for $L$ sufficiently small. For each $x_0 \in R$ and $L$ sufficiently small, we can find a ball $B(x_0, \lambda_0 \sqrt{L})$ (with $\lambda_0$ is independent of $L$) such that $B(x_0, \lambda_0 \sqrt{L}) \cap \Omega \subset R$ and (147) holds everywhere on $B(x_0, \lambda_0 \sqrt{L}) \cap \Omega$. Then
\[
\frac{1}{\lambda_0 \sqrt{L}} \int_{B(x_0, \lambda_0 \sqrt{L})} e_L(Q^L)(x) \, dV \leq \alpha' L
\]  
(148)
for a positive constant $\alpha'$ independent of $L$. From (148), we have that
\[
\lim_{L \to 0} \frac{1}{\lambda_0 \sqrt{L}} \int_{B(x_0, \lambda_0 \sqrt{T})} e_L(Q^L)(x) \, dV = 0
\]
and hence, $x_0 \notin S_{LG}(Q^L)$. Since the point $x_0 \in R$ is arbitrary, we deduce that $R \cap S_{LG}(Q^L) = \emptyset$ for $L$ sufficiently small.

From Lemma 5.1, we have that the singular set, $S_0$, of a limiting harmonic map converges uniformly to the isotropic set of a uniaxial small energy solution $Q^L$ as $L \to 0$ and from Lemma 5.10, we have that $S_{LG}(Q^L)$ converges uniformly to $S_0$ as $L \to 0$. We, therefore, deduce that $S_{LG}(Q^L)$ converges uniformly to the isotropic set of $Q^L$ as $L \to 0$.

6. Biaxial case in 3D: Interior estimates. Consider a biaxial small energy sequence of solutions of (27), $\{Q^{L_k}\}$, in the admissible space $A_Q$ where $L_k \to 0^+$ as $k \to \infty$. From Section 4, $\{Q^{L_k}\}$ converges strongly to a limiting harmonic map $Q^0$ (as in (13)) in $W^{1,2}(\Omega, S_3)$ (up to a subsequence) [17], for $L_k \to 0^+$ as $k \to \infty$. From (39), we have that
\[
f_B(Q^{L_k}) \to 0
\]  
(149)
uniformly everywhere away from the singular set, $S_0$, of the limiting harmonic map or equivalently (see representation formula (2))
\[
s \to s_+, \quad r \to 0^+
\]  
(150)
uniformly away from $S_0$, as $k \to \infty$ [17].

In what follows, we derive the analogue of Lemma 5.3 in the biaxial case.

**Lemma 6.1.** Let $\{Q^{L_k}\}$ be an arbitrary (uniaxial or biaxial) small energy sequence in the admissible space $A_Q$ ($A_Q$ has been defined in (12)) where $L_k \to 0$ as $k \to \infty$. Then there exists a minimizing harmonic map extension $n_0 : \Omega \to S^2$ of $n_b$ such that after passing to a subsequence, $Q^{L_k} \to Q^0 = s_+(n_0 \otimes n_0 - \frac{I}{2})$ strongly in $W^{1,2}(\Omega; \tilde{S}_3)$ as $k \to \infty$.

For $L \in \{L_k\}$ sufficiently small, define
\[
A^L = \frac{1}{2} Q^{L,k}_{ij,k} Q^{L,k}_{ij,k}.
\]
Then on $\Omega \setminus B_\delta(S_0)$, we have the following inequality
\[
- \Delta A^L + |\nabla^2 Q^L|^2 \leq \frac{1}{\alpha^2} |\nabla^2 Q^L|^2 + \alpha^4 \frac{A^{L^2}}{|Q^L|^2}
\]  
(151)
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 (90)
\[ \Delta A^L = |\nabla^2 Q^L|^2 + Q^L_{ij,k} Q^L_{ij,ppk} \]
and drop the superscript \( L \) for brevity.

We need to estimate \(|Q_{ij,k} Q_{ij,ppk}|\) in terms of \(|\Delta Q||\nabla Q|^2/|Q|\). Straightforward but tedious calculations show that
\[
L^2 |Q_{ij,k} Q_{ij,ppk}|^2 = a^4 |\nabla Q|^4 + c^4 (\text{tr} Q^2)^2 |\nabla Q|^4 + 4b^4 (Q_{ip} Q_{pj,q} Q_{ij,q})^2 \\
+ 4a^2 b^2 Q_{ip} Q_{pj,q} Q_{ij,q} |\nabla Q|^4 - 4b^2 c^2 |Q|^2 |\nabla Q|^2 Q_{ip} Q_{pj,q} Q_{ij,q} \\
- 2a^2 c^2 |Q|^2 |\nabla Q|^4 + 4c^4 (Q \cdot \nabla Q)^4 + 4c^4 (Q \cdot \nabla Q)^2 |Q|^2 |\nabla Q|^2 \\
- 4a^2 c^2 |\nabla Q|^2 (Q \cdot \nabla Q)^2 - 8b^2 c^2 (Q \cdot \nabla Q)^2 Q_{ip} Q_{pj,q} Q_{ij,q} \lesssim \\
\leq C(a^2, b^2, c^2)|\nabla Q|^4
\]
where we have used the Euler-Lagrange equations (27) to compute the right-hand side of (152) 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 (152) vanishes for \( Q \in Q_{\text{min}} \), where \( Q_{\text{min}} \) has been defined in (8). The details of these calculations are omitted here for brevity.

Secondly,
\[
L^2 \frac{|\nabla Q|^4}{|Q|^2} |\Delta Q|^2 = a^4 |\nabla Q|^4 + 2a^2 b^2 |\nabla Q|^4 (\text{tr} Q^2)^2 - 2a^2 c^2 |Q|^2 |\nabla Q|^4 \\
- 2b^2 c^2 (\text{tr} Q^3)^2 |\nabla Q|^4 + c^4 |Q|^4 |\nabla Q|^4 + 2b^2 \frac{s^4 + r^4 + 3s^2 r^2 - 2s^3 r - 2r^3}{27|Q|^2} |\nabla Q|^4
\]
\[
\geq D(a^2, b^2, c^2)|\nabla Q|^4
\]
where
\[
D(a^2, b^2, c^2) = 0
\]
if and only if \( Q \in Q_{\text{min}} \).

Combining (152) and (153), we get that
\[
|Q_{ij,k} Q_{ij,ppk}| \leq D'(a^2, b^2, c^2) \frac{|\nabla Q|^2}{|Q|} |\nabla Q| |\Delta Q|
\]
where \( D' \) is a positive constant independent of \( L \). Substituting (154) into (90) and repeating the same steps as in Lemma 5.3, (151) follows. The proof of Lemma 6.1 is then complete. \qed

Corollary 6.2. Let \( \{Q^{L_k}\} \) be an arbitrary (uniaxial or biaxial) small energy sequence in the admissible space \( A_Q \) (\( A_Q \) has been defined in (12)) where \( L_k \to 0 \) as \( k \to \infty \). Then there exists a minimizing harmonic map extension \( n_0 : \Omega \to S^2 \) of \( n_k \) such that after passing to a subsequence, \( Q^{L_k} \to Q^0 = s_+ (n_0 \otimes n_0 - \frac{1}{2}) \) strongly in \( W^{1,2} (\Omega; S_3) \) as \( k \to \infty \). If \( Q^{L_k} \) is biaxial for \( L_k \) sufficiently small, then we have the following interior estimates, away from the singular set, \( S_0 \), of the limiting harmonic map \( Q^0 \) in (13) :-
\[
\frac{1}{2} |\nabla Q^{L_k}|^2 + \frac{||B(Q^{L_k})||}{L_k} \leq H(a^2, b^2, c^2, \Omega)
\]
\[
|Q^0| - |Q^{L_k}| \leq C(a^2, b^2, c^2) L_k \quad \text{on} \quad K \subset \Omega \setminus B_\delta(S_0).
\]
In particular, the largest positive eigenvalue, $\lambda_{Lk}^{+}$, of $Q^{Lk}$, satisfies the following inequality on the interior compact subset $K \subset \Omega \setminus B_{k}(S_{0})$

$$\frac{2s_{+}}{3} - \lambda_{Lk}^{+} \leq D(a^{2},b^{2},c^{2})L_{k}$$

(157)

where $s_{+}$ has been defined in (9) and the positive constants $H,C$ and $D$ are independent of $L$.

Proof. The inequality (155) is a mere repetition of (47); see [17] for a proof. In what follows, we drop the subscript $k$ for brevity.

Consider the function

$$|Q^{L}| = (Q^{Lp}_{,q}Q^{L}_{,pq})^{1/2} \quad p,q = 1,2,3.$$ 

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

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

(158)

where $(Q_{,ij}Q_{,ij,k})^{2} = (Q \cdot \nabla Q)^{2} = \frac{1}{4} |\nabla Q|^{2}$. On the interior compact subset $K \subset \Omega \setminus B_{k}(S_{0})$, we have the following inequalities

$$\frac{2}{3} s_{+}^{2} - \epsilon_{1} \leq |Q^{L}|^{2} \leq \frac{2}{3} s_{+}^{2}$$

$$|\nabla Q^{L}|^{2} \leq C_{1}(a^{2},b^{2},c^{2})$$

(159)

where we have used (32), (149) and (155). Therefore, the first two terms on the right-hand side of (158) can be bounded independently of $L$. We use the Euler-Lagrange equations (27) to compute the third term on the right-hand side of (158) i.e.

$$\frac{Q^{L}_{,rs} \Delta Q^{L}_{,rs}}{|Q^{L}|} = \frac{1}{|Q^{L}|} \left\{-a^{2}|Q^{L}|^{2} - b^{2} \text{tr} Q^{L3} + c^{2} |Q^{L}|^{4} \right\}$$

$$= \frac{|Q^{L}|}{L} \left\{c^{2}|Q^{L}|^{2} - \frac{b^{2}|Q^{L}|}{\sqrt{6}} - a^{2}\right\} + \frac{b^{2}|Q^{L}|^{2}}{\sqrt{6}L} \left(1 - \sqrt{6} \frac{\text{tr} Q^{L3}}{|Q^{L}|^{3}}\right).$$

(160)

We recall from [17] that

$$\beta^{2}(Q^{L}) = 1 - 6 \left(\frac{\text{tr} Q^{L3}}{|Q^{L}|^{3}}\right)^{2} \in [0,1]$$

is the biaxiality parameter and as a direct consequence of (155), we have

$$\beta^{2}(Q^{L}) = 1 - 6 \left(\frac{\text{tr} Q^{L3}}{|Q^{L}|^{3}}\right)^{2} \leq C_{2}(a^{2},b^{2},c^{2})L$$

on the compact interior subset $K \subset \Omega \setminus B_{k}(S_{0})$, for a positive constant $C_{2}$ independent of $L$. Further, we have the following sequence of inequalities on $K \subset \Omega \setminus B_{k}(S_{0})$

$$C_{3}(a^{2},b^{2},c^{2}) \left(|Q^{L}| - |Q^{0}|\right) \leq \left\{c^{2}|Q^{L}|^{2} - \frac{b^{2}|Q^{L}|}{\sqrt{6}} - a^{2}\right\}$$

$$\leq C_{4}(a^{2},b^{2},c^{2}) \left(|Q^{L}| - |Q^{0}|\right)$$

for positive constants $C_{3}, C_{4}$ independent of $L$ (see (149) and (86)).
From the preceding remarks, we deduce that
\[
\Delta |Q^L|(x) \leq \alpha(a^2, b^2, c^2) + C_4(a^2, b^2, c^2)(\frac{|Q^L|(x) - |Q^0|(x)}{L}), \quad x \in \Omega \setminus B_{\delta}(S_0)
\] (161)
where \(\alpha\) is a positive constant independent of \(L\). Define the function
\[
\psi = \frac{(|Q^0| - |Q^L|)}{L}.
\]
Then using (161), we see that \(\psi\) satisfies the following inequality on \(K \subset \Omega \setminus B_{\delta}(S_0)\)
\[
-L\Delta \psi + \beta(a^2, b^2, c^2)\psi \leq \alpha'(a^2, b^2, c^2).
\] (162)
Finally, we apply the maximum principle and Lemma 2 in [4] to deduce that
\[
|\psi(x)| \leq \gamma(a^2, b^2, c^2) \quad x \in \Omega \setminus B_{\delta}(S_0),
\] (163)
for positive constants \(\alpha', \beta\) and \(\gamma\) independent of \(L\) and (156) follows. The inequality (156) improves upon a previous estimate in [17] where an analysis of the bulk energy density \(f_B\), coupled with (149) and (155), shows that
\[
|Q^0| - |Q^L| \leq A(a^2, b^2, c^2)\sqrt{L},
\]
for a positive constant \(A(a^2, b^2, c^2)\) independent of \(L\).

For (157), we use the following alternative representation formula to (2)
\[
Q^L = S_L \left( n \otimes n - \frac{1}{3} I \right) + R_L \left( m \otimes m - p \otimes p \right)
\] (164)
where \(n, m\) and \(p\) are the orthonormal eigenvectors and
\[
0 \leq s_+ - S_L \leq C_6\sqrt{L}; \quad R^2_L \leq C_5L \quad (165)
\]
on the interior compact subset \(K \subset \Omega \setminus B_{\delta}(S_0)\), for positive constants \(C_6, C_5\) independent of \(L\) (see (149) and Proposition 7 in [17]). We note that
\[
|Q^L|^2 = \frac{2}{3} S^2_L + 2R^2_L
\]
and hence the inequality (156) necessarily implies that
\[
s_+ - S_L \left( 1 + \frac{3R^2_L}{S^2_L} \right)^{1/2} \leq C_7L,
\]
for a positive constant \(C_7\) independent of \(L\). This combined with (165) i.e. \(R^2_L \leq C_5L\) yields the improved estimate
\[
0 \leq s_+ - S_L(x) \leq C_8L \quad x \in \Omega \setminus B_{\delta}(S_0) \quad (166)
\]
where \(C_8 > 0\) is independent of \(L\). Finally, it suffices to note from (164) that the largest positive eigenvalue of \(Q^L\) is given by
\[
\lambda^L_1 = \frac{2}{3} S_L
\]
and (157) directly follows from (166).

Let \(Q^L = S_L \left( n \otimes n - \frac{1}{3} I \right) + R_L \left( m \otimes m - p \otimes p \right)\) be an arbitrary Landau-de Gennes minimizer in the admissible space \(A_Q\), for \(L\) sufficiently small. In [17], we establish that an arbitrary Landau-de Gennes minimizer is either purely uniaxial everywhere or is biaxial everywhere except for possibly a set, \(\Psi_L\), of zero Lebesgue measure interfaces. Then the eigenvectors \(n, m\) are analytic everywhere away from \(\Psi_L\) [28] and \(S_L\) and \(R_L\) are constrained by the inequalities (166), everywhere.
away from $S_0$. The following equations hold on an interior compact set $K \subset \Omega$, that does not contain any singularities of $Q^0$ and does not intersect $\Psi_L$.

**Corollary 6.3.** Let $Q^L$ be an arbitrary Landau-de Gennes global minimizer in the admissible space $A_Q$, for $L$ sufficiently small. Let $K \subset \Omega \setminus \{B_\delta(S_0) \cup B_\sigma(\Psi_L)\}$ where $\delta$ and $\sigma$ are positive constants independent of $L$. Then the following equations hold everywhere on $K$:

\[
\Delta S_L - 3S_L|\nabla n|^2 + 3R_L \left[ (n \cdot \nabla m)^2 - (n \cdot \nabla p)^2 \right] = \frac{1}{3L} \left( 2c^2S_L^3 - b^2S_L^2 - 3a^2S_L^2R_L^2 + 3b^2R_L^2 \right)
\]

\[
\Delta R_L - R_L \left( |\nabla m|^2 + |\nabla p|^2 \right) + \left[ S_L(m \cdot \nabla n)^2 - S_L(p \cdot \nabla n)^2 - 2R_L(m \cdot \nabla p)^2 \right] = \frac{1}{L} \left( 2c^2R_L^3 + \frac{2c^2S_L^2R_L}{3} + \frac{2b^2S_LR_L}{3} - a^2R_L \right).
\]

**Proof.** The equations (167) and (168) follow from tedious but straightforward manipulations of the Euler-Lagrange equations (27). The details are omitted for brevity.

7. **Generalizations.** This paper focuses on qualitative properties of small energy sequences of solutions associated with the Landau-de Gennes energy functional on 2D and 3D domains. This is a general framework that includes local and global energy minimizers. In the 2D case, we focus on energy minimizers, show that the Landau-de Gennes theory is equivalent to the 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 far away from the defect set.

In the 3D case, we focus on the vanishing core limit, expressed in terms of a dimensionless parameter $L \to 0$, which is relevant for macroscopic domains that are much larger than the uniaxial correlation length. We demonstrate that the results for global Landau-de Gennes minimizers in [17] carry over to small energy sequences of solutions in the $L \to 0$ limit. Of key importance here is the energy bound (5). We derive a lower bound for the Landau-de Gennes energy using the concept of a null lagrangian. It is likely that these estimates can be further refined to get exact expressions for the minimum energy, as a function of the geometry and material parameters, in certain prototype examples. We define the singular set to be the set of points where we observe energy concentration within balls of radius on the order of the nematic correlation length. We plan to use this definition to obtain strong results on the dimension of the singular set i.e. does the singular set consist of isolated points etc.

The second half of the paper deals with uniaxial small energy sequences because this is the first step in a rigorous study of arbitrary minimizers. We derive the governing equations for the scalar order parameter and the leading eigenvector; these equations reflect the coupling between the two quantities. We establish the $C^{1,\alpha}$-convergence of uniaxial small energy sequences to a limiting harmonic map, everywhere away from the singular set of the limiting harmonic map, in the vanishing core limit. We use this convergence result to obtain an expansion for the scalar order parameter in terms of $L$, 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. Topological defects have a straightforward interpretation within the uniaxial framework; they are contained inside the corresponding isotropic set. We establish the equivalence between our new definition of the singular set and the isotropic set in the vanishing core limit. We also obtain an upper bound for the size of the singular set in the vanishing core limit.

There has been very interesting recent work on three-dimensional Ginzburg-Landau theory [20]. In [20], the authors obtain a characterization of local Ginzburg-Landau energy minimizers on $\mathbb{R}^3$. We plan to adapt their methods to the uniaxial case, since the uniaxial case can be viewed as a generalized Ginzburg-Landau theory from $\mathbb{R}^3$ to $\mathbb{R}^3$ in spite of important technical differences. A complete characterization of uniaxial local minimizers (if they exist) will be very useful for understanding the interplay between uniaxiality and biaxiality and the nature of the accompanying defects in each case.

A complete analysis of Landau-de Gennes global energy minimizers can be accomplished only if we have a better understanding of the full Euler-Lagrange equations (27). One strategy is to decompose the system (27) as follows -

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

where we can think of the first term as being a Ginzburg-Landau component (because of its similarity to Ginzburg-Landau equations for superconductors [20]) and the second term as being a remainder component. We need to understand the coupling between the Ginzburg-Landau and the remainder components and to establish quantitative estimates on the magnitude of the remainder 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 (13).

Other future directions are to study qualitative properties of minimizers for different choices of the boundary conditions i.e. when $Q_b \notin Q_{\text{min}}$ where $Q_{\text{min}}$ has been defined in (8), to study minimizers in different temperature regimes where the bulk energy density $f_B$ in (4) has two competing minima and to study the multiplicity of solutions of (169) in different parameter regimes. We plan to report on these problems in future work.

Acknowledgments. A. Majumdar is supported by Award No. KUK-C1-013-04, made by King Abdullah University of Science and Technology (KAUST), to the Oxford Centre for Collaborative Applied Mathematics and an EPSRC Career Acceleration Fellowship EP/J001686/1. The author thanks John Ball, Cameron Hall and Luc Nguyen for helpful conversations. The author thanks Arghir Zarnescu for suggesting improvements on an earlier version of the paper.

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Received November 2010; revised November 2011.

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