Uniaxial versus Biaxial Character of Nematic Equilibria in Three Dimensions

July 31, 2015

Apala Majumdar
Department of Mathematical Sciences, University of Bath, Bath, BA2 7AY, United Kingdom

Adriano Pisante
Dipartimento di Matematica "G. Castelnuovo", Sapienza, Università di Roma, 00185 Rome, Italy

Duvan Henao
Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Casilla 306, Correo 22, Santiago, Chile

Abstract

We study global minimizers of the Landau-de Gennes (LdG) energy functional for nematic liquid crystals, on arbitrary three-dimensional simply connected geometries with topologically non-trivial and physically relevant Dirichlet boundary conditions. Our results are specific to the low-temperature limit. We prove (i) that (re-scaled) global LdG minimizers converge uniformly to a (minimizing) limiting harmonic map, away from the singular set of the limiting map; (ii) there exist both a point of maximal biaxiality and a nonempty Lebesgue-null set of uniaxial points near each singular point of the limiting harmonic map (this improves the recent results of [9]); (iii) estimates for the size of "strongly biaxial" regions in terms of the reduced temperature t. We further show that global LdG minimizers in the restricted class of uniaxial $\mathbf{Q}$-tensors cannot be stable critical points of the LdG energy for low temperatures.

1 Introduction

Nematic liquid crystals (LCs) are anisotropic liquids with long-range orientational order i.e. the constituent rod-like molecules have full translational freedom but align along certain locally preferred directions [10, 35]. The existence of distinguished directions renders nematics sensitive to light and external fields leading to unique electromagnetic, optical and rheological properties [10, 15, 29]. The analysis of nematic spatio-temporal patterns is a fascinating source of problems for mathematicians, physicists and engineers alike, especially in the context of defects or material singularities [15, 12].

In recent years, mathematicians have turned to the analysis of the celebrated Landau-de Gennes (LdG) theory for nematic liquid crystals, particularly in two asymptotic limits: the vanishing elastic constant and the low-temperature limit; see for example [22, 14, 7, 9] which is not an exhaustive list but are directly relevant to our paper. The LdG theory is a variational theory with an associated energy functional, defined in terms of a macroscopic order parameter, known as the $\mathbf{Q}$-tensor order parameter [10, 35, 19]. The LdG energy typically comprises an elastic energy, convex in $\nabla \mathbf{Q}$ with several elastic constants, and a non-convex bulk potential, f_B defined in terms of the temperature and the eigenvalues of $\mathbf{Q}$-tensor [26]. With the one-constant approximation for the elastic energy density, the LdG energy functional has a similar structure to the Ginzburg-Landau (GL) functional for superconductivity [4, 27, 8] and in certain asymptotic limits (limit of vanishing elastic constant and low-temperature limit), we can borrow several ideas from GL theory to make qualitative predictions about global energy minimizers, at least away from singularities. However, there is an important distinction between the GL theory and LdG theory. In the GL-framework, researchers study maps, $\mathbf{u} : \mathbb{R}^d \to \mathbb{R}^d$, $d = 2, 3$ (see e.g. [4, 2, 23]), whereas the LdG variable is a five-dimensional map, $\mathbf{Q} : \mathbb{R}^3 \to \mathbb{R}^5$. A uniaxial $\mathbf{Q}$-tensor has three degrees of freedom (with an order parameter and a single distinguished direction) and in the uniaxial case, there is broader scope for methodology transfer from GL-based techniques (see for example, [14]). A biaxial $\mathbf{Q}$-tensor has five degrees of freedom and there are a plethora of open questions about how the two extra degrees of freedom manifest in the mathematics and physics of biaxial systems.

We re-visit questions related to the uniaxial versus biaxial structure of global LdG minimizers in the low-temperature limit. We work with “nice” three-dimensional (3D) domains as described in the abstract and with fixed topologically non-trivial Dirichlet boundary conditions. In particular, the Dirichlet condition is a minimizer of the potential, f_B, in the LdG energy. Our first result concerns the uniform convergence of global energy minimizers to a (minimizing) limiting harmonic map, away from the singular set of the limiting harmonic map, in the low-temperature limit. The uniform convergence follows from a Bochner-type inequality for the LdG energy density, first derived in [22] in the vanishing elastic constant limit. There are subtle mathematical differences between the low-temperature and vanishing elastic constant limits; in particular, the bulk potential f_B comprises two terms that diverge at different rates in the low temperature limit. This is explained in more detail after the proof of Lemma 3.3 and requires us to consider mathematical cases or scenarios which do not arise in the vanishing elastic constant case. The uniform convergence gives a fairly good description of global energy minimizers away from the singular set, Σ, of the limiting harmonic map. The singular set, Σ, consists of a discrete set of point defects. In [9], the authors prove the existence of a point of maximal biaxiality for global minimizers, in the low-temperature limit but do not comment on the number of such points. We appeal to a topological result in [7] to deduce the existence of a point of maximal biaxiality and a point of uniaxiality near each singular point in Σ, in the low-temperature limit. Maximal biaxiality is understood in terms of the biaxiality parameter which varies between 0 and unity (see [35, 25] and subsequent sections for a definition of the biaxiality parameter). We make the notion of "strongly biaxial" regions in global energy minimizers more precise by computing estimates for the size of such regions in terms of the reduced temperature, t. The proof depends on scaling and blow-up arguments and well-established results in GL-theory and the theory of harmonic maps (e.g. [5, 31]). We consider all admissible scenarios and exclude all but one scenario, based on the arguments above and find that the size of "strongly biaxial" regions scales as $t^{-1/4}$ as $t \to \infty$.

In [14], we study global LdG energy minimizers on a 3D droplet with radial boundary conditions, in the low temperature limit. We appeal to GL-based techniques (see [2, 24]) to show that global minimizers, if uniaxial, must have the radial-hedgehog (RH) structure for low temperatures. The RH solution is a radially-symmetric critical point of the LdG energy on a 3D droplet, with a single isotropic point (with $\mathbf{Q} = 0$) at the droplet centre and perfect uniaxial symmetry away from the centre i.e. the molecules point radially outwards everywhere away from the centre [25, 14]. Further, it is known that the RH-solution is unstable with respect to symmetry-breaking biaxial higher-dimensional perturbations for low temperatures [25, 21]. In [14], it is shown that global minimizers, in the restricted class of uniaxial tensors, cannot be stable critical points of the LdG energy on a 3D droplet, for low temperatures, since they converge to the RH solution in the low-temperature limit. In [18], the author uses symmetry-based arguments and the structure of the LdG Euler-Lagrange equations to prove that the radial-hedgehog solution (modulo a rotation) is the unique uniaxial critical point on a 3D droplet with radial boundary conditions, for all temperatures.

Our second theorem in this paper generalizes the results in [14] to arbitrary three-dimensional geometries with arbitrary physically relevant topologically non-trivial Dirichlet conditions. There exists a global LdG energy minimizer in the restricted class of uniaxial **Q**-tensors, for all temperatures. These restricted uniaxial minimizers necessarily have non-negative scalar order parameter and satisfy a physically relevant energy bound. We show that these restricted minimizers cannot be stable critical points of the LdG energy for low temperatures. The argument proceeds by contradiction. Appealing to topological arguments, we show that any uniaxial critical point of the LdG energy has an isotropic point near each singular point of the limiting harmonic map, for sufficiently low-temperatures. We then proceed with a local version of the global analysis in [14], equipped with certain energy quantization results for harmonic maps [5] and blow-up techniques, to deduce the local RH-structure near each isotropic point. In other words, we reduce the local analysis near an isotropic or a defect point (in the uniaxial case) to the model problem of uniaxial equilibria on a 3D droplet with radial boundary conditions and the local instability of the RH-profile suffices for our purposes. In fact, we believe that the universal RH-defect profile for uniaxial critical points is not specific to the low-temperature limit but also extends to the vanishing elastic constant limit (for all $t > 0$) and indeed any limit for which we are guaranteed uniform convergence to a (minimizing) limiting harmonic map, away from the singularities of the limiting harmonic map. It is known from [5] that point defects for minimizing harmonic maps have a local radial profile (modulo a rotation) and we believe that the uniaxial defect profiles have the same radial profile, weighted by an appropriate scalar order parameter, which is precisely the RH solution. The analysis of defect profiles near points of maximal biaxiality remains an open problem for analysts, although some key steps are given in [34, 30, 16].

The paper is organized as follows. In Section 2, we review the theoretical background and state our main results. In Section 3, we give the proofs and in Section 4, we conclude with future perspectives.

2 Statement of results

Let $\Omega \subset \mathbb{R}^3$ be an arbitrary simply-connected 3D domain with smooth boundary. Let $\mathbb{S}^2$ be the set of unit vectors in $\mathbb{R}^3$ and let S_0 denote the set of symmetric, traceless 3×3 matrices i.e.

$$S_0 = \left\{ \mathbf{Q} \in M^{3\times 3}; \mathbf{Q}_{ij} = \mathbf{Q}_{ji}; \mathbf{Q}_{ii} = 0 \right\}, \tag{1}$$

where $M^{3\times 3}$ is the set of 3×3 matrices. The corresponding matrix norm is defined to be [22]

$$|\mathbf{Q}|^2 = \mathbf{Q}_{ij}\mathbf{Q}_{ij} \quad i,j = 1\dots 3 \tag{2}$$

and we use the Einstein summation convention throughout the paper.

We work with the Landau-de Gennes (LdG) theory for nematic liquid crystals [10] whereby a LC state is described by a macroscopic order parameter: the $\mathbf{Q}$-tensor order parameter. The $\mathbf{Q}$-tensor is a macroscopic measure of the LC anisotropy. Mathematically, the LdG $\mathbf{Q}$-tensor order parameter is a symmetric, traceless 3×3 matrix in the space S_0 in (1). A LC state is said to be (i) isotropic (disordered with no orientational ordering) when $\mathbf{Q} = 0$, (ii) uniaxial when $\mathbf{Q}$ has two degenerate non-zero eigenvalues and (iii) biaxial when $\mathbf{Q}$ has three distinct eigenvalues. A uniaxial $\mathbf{Q}$-tensor can be written as

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

for some $s(\mathbf{x}) \in \mathbb{R}$ and some unit-vector $\mathbf{n}(\mathbf{x}) \in \mathbb{S}^2$, for a.e. $\mathbf{x} \in \Omega$. We include $s = 0$ in our definition although $s = 0$ corresponds to the isotropic phase. The unit-vector, $\mathbf{n}$, is the director or equivalently, the single distinguished direction of molecular alignment in the sense that all directions orthogonal to $\mathbf{n}$ are physically equivalent for an uniaxial nematic. We recall the definition of the biaxiality parameter [25], [35],

$$\beta^2 = 1 - \frac{6(\mathrm{tr}\mathbf{Q}^3)^2}{|\mathbf{Q}|^6} \in [0,1]\,. \tag{4}$$

In particular, $\beta^2 = 0$ if and only if $\mathbf{Q}$ is uniaxial i.e. if and only if $|\mathbf{Q}|^6 = 6\left(\mathrm{tr}\mathbf{Q}^3\right)^2$.

The LdG theory is a variational theory and has an associated LdG free energy. The LdG energy density is a nonlinear function of $\mathbf{Q}$ and its spatial derivatives [10, 26]. We work with the simplest form of the LdG energy functional that allows for a first-order nematic-isotropic phase transition and spatial inhomogeneities as shown below [22, 26]:

$$\mathbf{I_{LG}}\left[\mathbf{Q}\right] = \int_\Omega \frac{L}{2}|\nabla\mathbf{Q}|^2 + f_B\left(\mathbf{Q}\right)\, dV. \tag{5}$$

Here, $L > 0$ is a small material-dependent elastic constant, $|\nabla\mathbf{Q}|^2 = \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}$ (note that $\mathbf{Q}_{ij,k} = \frac{\partial\mathbf{Q}_{ij}}{\partial\mathbf{x}_k}$) with $i,j,k = 1,2,3$ is an *elastic energy density* and $f_B : S_0 \to \mathbb{R}$ is the *bulk energy density* that dictates the preferred nematic phase: isotropic/uniaxial/biaxial. For our purposes, we take f_B to be a quartic polynomial in the $\mathbf{Q}$-tensor invariants:

$$f_B(\mathbf{Q}) = \frac{A(T)}{2}\mathrm{tr}\mathbf{Q}^2 - \frac{B}{3}\mathrm{tr}\mathbf{Q}^3 + \frac{C}{4}\left(\mathrm{tr}\mathbf{Q}^2\right)^2 \tag{6}$$

where $\mathrm{tr}\mathbf{Q}^3 = \mathbf{Q}_{ij}\mathbf{Q}_{jp}\mathbf{Q}_{pi}$ with $i, j, p = 1, 2, 3$; $A(T) = \alpha(T - T^*)$; $\alpha, B, C > 0$ are material-dependent constants, T is the absolute temperature and T^* is a characteristic temperature below which the isotropic phase, $\mathbf{Q} = 0$, loses its stability [26, 20]. We work in the low temperature regime with $T << T^*$ (or $A < 0$) and subsequently investigate the $A \to -\infty$ limit, known as the *low temperature* limit. One can readily verify that f_B is bounded from below and attains its minimum on the set of $\mathbf{Q}$-tensors given by [20, 21]

$$\mathbf{Q}_{\mathrm{min}} = \left\{\mathbf{Q} \in S_0; \mathbf{Q} = s_+\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right),\ \mathbf{n} \in \mathbb{S}^2\right\}, \tag{7}$$

$\mathbf{I}$ is the 3×3 identity matrix and

$$s_+ = \frac{B + \sqrt{B^2 + 24|A|C}}{4C}. \tag{8}$$

The set, (7), is the set of uniaxial $\mathbf{Q}$-tensors with constant order parameter, s_+.

In what follows, we take the Dirichlet boundary condition to be

$$\mathbf{Q}_{b,A}(\mathbf{x}) = s_+\left(\mathbf{n}_b\otimes\mathbf{n}_b - \frac{\mathbf{I}}{3}\right) \tag{9}$$

for some arbitrary smooth unit-vector field, $\mathbf{n}_b$, with topological degree $d \neq 0$ (see, e.g., [6] and [5] for the definition and the main properties of the topological degree). The corresponding admissible space is

$$\mathcal{A}_A = \left\{\mathbf{Q} \in W^{1,2}\left(\Omega; S_0\right); \mathbf{Q} = \mathbf{Q}_{b,A} \text{ on } \partial\Omega\right\}, \tag{10}$$

where $W^{1,2}\left(\Omega; S_0\right)$ is the Soboblev space of square-integrable $\mathbf{Q}$-tensors with square-integrable first derivatives [11], with norm

$$||\mathbf{Q}||_{W^{1,2}} = \left(\int_\Omega |\mathbf{Q}|^2 + |\nabla\mathbf{Q}|^2\ dV\right)^{1/2}.$$

In what follows, we identify the degree of a uniaxial $\mathbf{Q}$-tensor in $\mathcal{A}_A$ on the boundary, with the degree of the director field, $\mathbf{n} \in W^{1,2}\left(\Omega; S^2\right)$ on the boundary, $\deg\left(\mathbf{n}, \partial\Omega\right)$, which is well defined because $\mathbf{n}_b$ is smooth. The existence of a global minimizer of $\mathbf{I_{LG}}$ in the admissible space, $\mathcal{A}_A$, is immediate from the direct method in the calculus of variations [11]; the details are omitted for brevity. It follows from standard arguments in elliptic regularity that all global minimizers are smooth and real analytic solutions of the Euler-Lagrange equations associated with $\mathbf{I_{LG}}$ on Ω,

$$L\Delta\mathbf{Q} = A\mathbf{Q} - B\left(\mathbf{Q}^2 - \left(\mathrm{tr}\mathbf{Q}^2\right)\frac{\mathbf{I}}{3}\right) + C\left(\mathrm{tr}\mathbf{Q}^2\right)\mathbf{Q}, \tag{11}$$

where $B\left(\mathrm{tr}\mathbf{Q}^2\right)\frac{\mathbf{I}}{3}$ is a Lagrange multiplier accounting for the tracelessness constraint [22].

Define the re-scaled maps, $\bar{\mathbf{Q}} := \frac{1}{s_+}\sqrt{\frac{3}{2}}\mathbf{Q}$. Let

$$t := \frac{27|A|C}{B^2},\ h_+ = \frac{3+\sqrt{9+8t}}{4},\ \xi_b = \sqrt{\frac{27LC}{B^2 t}} \quad \text{and} \quad \bar{L} := \frac{27C}{2B^2}L. \tag{12}$$

Then $s_+ = \frac{B}{3C}h_+$ and the minimum of the bulk energy density, f_B in (6), is

$$\min_{\mathbf{Q}\in S_0} f_B\left(\mathbf{Q}\right) = -\frac{1}{8}\left(t + h_+\right). \tag{13}$$

The low-temperature limit corresponds to $t \to \infty$.

The re-scaled LdG energy is then given by

$$\frac{3\bar{L}}{2Ls_+^2}\mathbf{I}_{LG}[\bar{\mathbf{Q}}] = \int_\Omega \frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}|^2 + \frac{t}{8}\left(1-|\bar{\mathbf{Q}}|^2\right)^2 + \frac{h_+}{8}(1+3|\bar{\mathbf{Q}}|^4 - 4\sqrt{6}\mathrm{tr}\bar{\mathbf{Q}}^3)\, dV \tag{14}$$

Note that the bulk potential has two contributions in (14), both of which are both nonnegative in view of (4). The first term vanishes for $\bar{\mathbf{Q}} \in \mathbb{S}^4$ and the second term vanishes if and only if $\bar{\mathbf{Q}}$ is uniaxial with unit norm (from (4) again). The re-scaled boundary condition is $\bar{\mathbf{Q}}_b = \sqrt{\frac{3}{2}}\left(\mathbf{n}_b\otimes\mathbf{n}_b - \frac{\mathbf{I}}{3}\right)$. **In what follows, all statements are to be understood in terms of the re-scaled variables and we drop the bars from the variables for brevity. We recall the definition of a minimizing limiting harmonic map.**

Definition 1. *A (minimizing) limiting harmonic map with respect to the re-scaled Dirichlet condition in* (9)*, is a uniaxial map of the form*

$$\mathbf{Q}^0 = \sqrt{\frac{3}{2}}\left(\mathbf{n}^0\otimes\mathbf{n}^0 - \frac{\mathbf{I}}{3}\right), \tag{15}$$

where $\mathbf{n}^0$ *is a minimizer of the Dirichlet energy*

$$I[\mathbf{n}] = \int_\Omega |\nabla \mathbf{n}|^2 \, dV \tag{16}$$

in the admissible space $\mathcal{A}_{\mathbf{n}_b} = \left\{ \mathbf{n} \in W^{1,2}\left(\Omega; \mathbb{S}^2\right); \mathbf{n} = \mathbf{n}_b \text{ on } \partial\Omega \right\}$ *[31].*

In particular, $\mathbf{n}_0$ is a harmonic map into $\mathbb{S}^2$, i.e., a solution of the harmonic map equations $\Delta\mathbf{n} + |\nabla\mathbf{n}|^2\mathbf{n} = 0$. The singular set of $\mathbf{n}_0$, denoted by $\Sigma = \{\mathbf{x}_1 \dots \mathbf{x}_N\} \subset \Omega$, is a finite set of points [31, 32].

We have two main theorems.

Theorem 1. *Let* $\Omega \subset \mathbb{R}^3$ *be as above. Let* $\{t_j\}_{j\in\mathbb{N}}$ *with* $t_j \overset{j\to\infty}{\longrightarrow} +\infty$ *and let* $\{\mathbf{Q}_j\}_{j\in\mathbb{N}}$ *be a corresponding global minimizer of the LdG energy in (14), in the admissible space* $\bar{\mathcal{A}}_A = \left\{ \mathbf{Q} \in W^{1,2}\left(\Omega; S_0\right); \mathbf{Q} = \sqrt{\frac{3}{2}}\left(\mathbf{n}_b \otimes \mathbf{n}_b - \frac{\mathbf{I}}{3}\right) \text{ on } \partial\Omega \right\}$. *Then (up to a subsequence), we have the following results.*

(i) $\{\mathbf{Q}_j\}$ *converges to a limiting harmonic map,* $\mathbf{Q}^0$ *defined in (15), strongly in* $W^{1,2}(\Omega; S_0)$ *and uniformly away from* Σ*, as* $j \to \infty$.

(ii) Let $\Sigma_\epsilon = \{\mathbf{x} \in \Omega : dist\,(\mathbf{x}, \Sigma) < \epsilon\} = \bigcup_{\mathbf{x}_i\in\Sigma} B_\epsilon(\mathbf{x}_i)$ *where* $B_\epsilon(\mathbf{x}_i)$ *denotes a ball of radius* ϵ *centered at* $\mathbf{x}_i$*, and* $B^j_\delta = \left\{\mathbf{x} \in \Omega : \beta^2\left(\mathbf{Q}_j(\mathbf{x})\right) > \delta\right\}$*, for a fixed* $\epsilon > 0$ *and* $\delta \in (0,1)$*. Then* $B^j_\delta \subseteq \Sigma_\epsilon$ *for* j *large enough.*

(iii) $|\mathbf{Q}_j| \to 1$ *uniformly on* Ω *as* $j \to \infty$.

(iv) For each $\mathbf{x}_i \in \Sigma$*, we have for* j *large enough,*

$$\min_{\mathbf{x}\in\overline{B_\epsilon(\mathbf{x}_i)}} \beta^2\left(\mathbf{Q}_j(\mathbf{x})\right) = 0, \qquad \max_{\mathbf{x}\in\overline{B_\epsilon(\mathbf{x}_i)}} \beta^2\left(\mathbf{Q}_j(\mathbf{x})\right) = 1, \tag{17}$$

and $\mathcal{L}^n(\{\mathbf{x} \in \overline{B_\epsilon(\mathbf{x}_i)} : \beta^2\left(\mathbf{Q}_j(\mathbf{x})\right) = 0\}) = 0$.

(v) For each $\mathbf{x}_i \in \Sigma$ *and* $\delta \in (0,1)$*, we have*

$$diam\left(B_\epsilon(\mathbf{x}_i) \cap B^j_\delta\right) \sim t_j^{-1/4} \tag{18}$$

for j *sufficiently large.*

An immediate consequence is that global energy minimizers cannot be purely uniaxial, as also stated in [9] where the authors prove the existence of at least a single point of maximal biaxiality for global LdG minimizers.

Theorem 2. *Let $\Omega \subset \mathbb{R}^3$ be as above. Let $\{t_j\}_{j\in\mathbb{N}}$ be such that $t_j \to \infty$ as $j \to \infty$. For each $j \in \mathbb{N}$, let $\{\mathbf{Q}_j\}_{j\in\mathbb{N}}$ be a global minimizer of the LdG energy (14) in the restricted class of uniaxial $\mathbf{Q}$-tensors of the form (3). Then $\mathbf{Q}_j$ has non-negative scalar order parameter and $\mathbf{Q}_j$ satisfies the following energy bound*

$$\frac{3\bar{L}}{2Ls_+^2}\mathbf{I}_{LG}[\mathbf{Q}_j] \leq \frac{3\bar{L}}{2} \cdot \inf_{\mathbf{n}\in\mathcal{A}_{\mathbf{n}_b}} I[\mathbf{n}], \tag{19}$$

with $I[\mathbf{n}]$ and $\mathcal{A}_{\mathbf{n}_b}$ as in (16), for each $j \in \mathbb{N}$. For j sufficiently large, $\mathbf{Q}_j$ cannot be a stable critical point of the LdG energy in (14) in the admissible space, $\bar{\mathcal{A}}_A = \left\{\mathbf{Q} \in W^{1,2}(\Omega; S_0); \mathbf{Q} = \sqrt{\frac{3}{2}}\left(\mathbf{n}_b \otimes \mathbf{n}_b - \frac{\mathbf{I}}{3}\right) \text{ on } \partial\Omega\right\}$.

Theorem 2 is a consequence of Proposition 2.1 below and Propositions 3 and 8 of [14].

Proposition 2.1. *Let $\Omega \subset \mathbb{R}^3$ be as above. Let $\{t_j\}_{j\in\mathbb{N}}$ be such that $t_j \to \infty$ as $j \to \infty$. Let $\mathbf{Q}_j$ be a sequence of uniaxial critical points of the re-scaled LdG energy in (14) with non-negative scalar order parameter and satisfying the energy bound (19) for all $j > 0$. Then, passing to a subsequence (still indexed by j), the sequence $\{\mathbf{Q}_j\}$ converges uniformly to a (minimizing) limiting harmonic map, $\mathbf{Q}^0$ as $j \to \infty$, everywhere away from the singular set $\Sigma = \{\mathbf{x}_1 \ldots \mathbf{x}_N\}$ of $\mathbf{Q}^0$. We have that*

(i) for each $i = 1, \ldots, N$, there exists $\{\mathbf{x}_i^{(j)}\}_{j\in\mathbb{N}}$ such that $\mathbf{Q}_j(\mathbf{x}_i^{(j)}) = \mathbf{0}$ for all $j \in \mathbb{N}$ and $\mathbf{x}_i^{(j)} \stackrel{j\to\infty}{\longrightarrow} \mathbf{x}_i$ and

(ii) given any sequence, $\{\mathbf{x}^{(j)}\}_{j\in\mathbb{N}} \subset \Omega$, such that $\mathbf{Q}_j(\mathbf{x}^{(j)}) = \mathbf{0}\ \forall j \in \mathbb{N}$, there exists a subsequence $\{j_k\}_{k\in\mathbb{N}}$ and an orthogonal transformation $\mathbf{T} \in \mathcal{O}(3)$ (which may depend on the subsequence) such that the shifted maps $\left\{\tilde{\mathbf{x}} \mapsto \mathbf{Q}_{j_k}\left(\mathbf{x}^{(j_k)} + \xi_b\tilde{\mathbf{x}}\right)\right\}_{k\in\mathbb{N}}$ converge to

$$\mathbf{H}_{\mathbf{T}}(\tilde{\mathbf{x}}) := \sqrt{\frac{3}{2}}h(|\tilde{\mathbf{x}}|)\left(\frac{\mathbf{T}\tilde{\mathbf{x}} \otimes \mathbf{T}\tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^2} - \frac{\mathbf{I}}{3}\right), \quad \tilde{\mathbf{x}} \in \mathbb{R}^3, \tag{20}$$

in $C^r_{\mathrm{loc}}(\mathbb{R}^3; S_0)$ for all $r \in \mathbb{N}$, where $h : [0, \infty) \to \mathbb{R}^+$ is the unique, monotonically increasing solution, with $r = |\tilde{\mathbf{x}}|$, of the boundary-value problem

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h^3 - h, \qquad h(0) = 0, \qquad \lim_{r\to\infty} h(r) = 1. \tag{21}$$

Proposition 2.1 provides a local description of the structural profile near a set of isotropic points in the uniaxial critical points, $\mathbf{Q}_j$, in terms of the well-known RH solution. The RH solution is a rare example of an explicit critical point of the LdG energy simply given by

$$\mathbf{H}(\tilde{\mathbf{x}}) := \sqrt{\frac{3}{2}} h(|\tilde{\mathbf{x}}|) \left(\frac{\tilde{\mathbf{x}} \otimes \tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^2} - \frac{\mathbf{I}}{3} \right), \quad \tilde{\mathbf{x}} \in \mathbb{R}^3, \tag{22}$$

where h is defined as in (21). The boundary-value problem (21) has been studied in detail, see for example in [17, 21]. The RH solution is locally unstable with respect to biaxial perturbations, as has been demonstrated in [20, 25].

3 Proof of the theorems

Recall that the re-scaled LdG energy is given by

$$\frac{3\bar{L}}{2Ls_+^2} \mathbf{I}_{LG}^j[\mathbf{Q}] = \int_\Omega \frac{\bar{L}}{2} |\nabla \mathbf{Q}|^2 + \bar{L} f(\mathbf{Q}, t_j) \; dV, \tag{23}$$

with

$$\bar{L} f(\mathbf{Q}, t) = \frac{t}{8} \left(1 - |\mathbf{Q}|^2\right)^2 + \frac{h_+}{8} \left(1 + 3|\mathbf{Q}|^4 - 4\sqrt{6} \mathrm{tr} \mathbf{Q}^3\right), \tag{24}$$

and that for all $t > 0$ the potential $f(\mathbf{Q}, t)$ is minimized on the set

$$\mathbf{Q}_{\min} = \left\{ \sqrt{\frac{3}{2}} \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}}{3} \right) : \mathbf{n} \in \mathbb{S}^2 \right\}. \tag{25}$$

Denote the LdG energy density by

$$e(\mathbf{Q}, t) = \frac{1}{2} |\nabla \mathbf{Q}|^2 + f(\mathbf{Q}, t). \tag{26}$$

In Theorem 1 we consider global minimizers $\mathbf{Q}_j$ of $\mathbf{I}_{LG}^j$ in the admissible space $\bar{\mathcal{A}}_A = \left\{ \mathbf{Q} \in W^{1,2}(\Omega; S_0) ; \mathbf{Q} = \sqrt{\frac{3}{2}} \left(\mathbf{n}_b \otimes \mathbf{n}_b - \frac{\mathbf{I}}{3} \right) \text{ on } \partial\Omega \right\}$ for each $t_j > 0$, the existence of which is guaranteed by the direct method of the calculus of variations. Standard elliptic regularity arguments (presented in [22, Prop. 13]) show that each minimizer $\mathbf{Q}_j$ is a real analytic solution of the Euler-Lagrange equations

$$\triangle \mathbf{Q}_{ij} = \Gamma_{ij}, \tag{27}$$

where

$$\bar{L}\Gamma_{ij} = \frac{t}{2}\mathbf{Q}_{ij}\left(|\mathbf{Q}|^2 - 1\right) + \frac{3h_+}{2}\left[|\mathbf{Q}|^2\mathbf{Q}_{ij} - \sqrt{6}\mathbf{Q}_{ip}\mathbf{Q}_{pj} + \sqrt{6}|\mathbf{Q}|^2\delta_{ij}/3\right].$$

Theorem 2 is proved by assuming that a sequence $\{\mathbf{Q}_j\}_{j\in\mathbb{N}}$ of minimizers in the restricted class of uniaxial $\mathbf{Q}$-tensors is composed of stable critical points of the LdG energy and then reaching a contradiction. In both cases, we consider classical solutions of (27) that satisfy the energy bound (19) (this follows from the fact that any minimizing limiting harmonic map $\mathbf{Q}^0$ belongs to $\bar{\mathcal{A}}_A$, so it can be used as a trial function). As done in [14, 9], the arguments in [22, Lemmas 2 and 3; Props. 3, 4, and 6] can be adapted to prove the following preliminary results.

Proposition 3.1. *Let $t_j \to +\infty$ and, for each $j \in \mathbb{N}$, let $\mathbf{Q}_j \in \bar{\mathcal{A}}_A$ be a classical solution of the corresponding equations* (27)*, satisfying the energy bound* (19)*. Then, passing to a subsequence,*

(i) $\{\mathbf{Q}_j\}_{j\in\mathbb{N}}$ *converges strongly to a (minimizing) limiting harmonic map $\mathbf{Q}^0$ in $W^{1,2}(\Omega; S_0)$,*

(ii) $\|\mathbf{Q}_j\|_{L^\infty} \leq 1$ *and* $\|\nabla\mathbf{Q}_j\|_{L^\infty} \leq C\sqrt{\frac{t_j}{L}}$ *for some C independent of j,*

(iii) $\displaystyle\frac{1}{r}\int_{B(\mathbf{x},r)} e(\mathbf{Q}_j, t_j)\; dV \leq \frac{1}{R}\int_{B(\mathbf{x},R)} e(\mathbf{Q}_j, t_j)\; dV$ *for all $\mathbf{x} \in \Omega$ and $r \leq R$ so that $B(\mathbf{x}, R) \subset \Omega$,*

(iv) for any compact $K \subset \overline{\Omega} \setminus \Sigma$, where Σ denotes the singular set of $\mathbf{Q}^0$,

$$\frac{1}{8}\left(1 - |\mathbf{Q}_j|^2\right)^2 + \frac{h_+}{8t}(1 + 3|\mathbf{Q}_j|^4 - 4\sqrt{6}\,\mathrm{tr}\,\mathbf{Q}_j^3) \to 0 \qquad (28)$$

uniformly in K.

However, this only ensures that $|\mathbf{Q}_j| \to 1$ uniformly as $j \to \infty$, away from Σ. We want to prove the following stronger result.

Proposition 3.2. *Under the hypotheses of Proposition 3.1, $\{\mathbf{Q}_j\}_{j\in\mathbb{N}}$ converges uniformly to $\mathbf{Q}^0$ away from Σ, as $t_j \to \infty$.*

The key step is to prove a Bochner inequality of the form

Lemma 3.3. *There exist $\epsilon_1 > 0$ and a constant $C > 0$ independent of t such that if $\mathbf{Q} \in C^3(\Omega; S_0)$ is a solution of* (27) *then*

$$-\triangle e\left(\mathbf{Q}, t\right)(\mathbf{x}) \leq Ce^2\left(\mathbf{Q}, t\right)(\mathbf{x}) \qquad (29)$$

for all $\mathbf{x} \in \Omega$ *satisfying*

$$1 - \epsilon_1 \leq |\mathbf{Q}(\mathbf{x})| \leq 1. \tag{30}$$

This inequality was proven in [22, Lemmas 5–7] in the case when $\mathbf{Q}_j$ is close to the manifold $\mathbf{Q}_{\min}$, defined in (25), which does not necessarily hold in our case as explained in detail after the proof of Lemma 3.3.

Proof of Lemma 3.3. The same proof of [22, Lemma 5] shows that there exists a positive constant $\epsilon_0 > 0$ such that:

$$\frac{t}{C} f(\mathbf{Q}, t) \leq |\Gamma|^2(\mathbf{Q}, t) \leq C t f(\mathbf{Q}, t) \tag{31}$$

for all $\mathbf{Q} \in S_0$ such that $\left|\mathbf{Q} - \sqrt{\frac{3}{2}}\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right)\right| \leq \epsilon_0$ for some $\mathbf{n} \in \mathbb{S}^2$, the positive constant C being independent of t. Let ϵ_1 be a positive constant (depending only on C and ϵ_0 above) such that

$$0 \leq |\mathbf{Q}|^3 - \sqrt{6}\,\mathrm{tr}\,\mathbf{Q}^3 \leq \epsilon_1 \tag{32}$$

and (30) collectively ensure that $\left|\mathbf{Q} - \sqrt{\frac{3}{2}}\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right)\right| \leq \epsilon_0$ for some $\mathbf{n} \in \mathbb{S}^2$.

Such an ϵ_1 exists because the biaxiality parameter (see (4))

$$\beta^2(\mathbf{Q}) = \frac{|\mathbf{Q}|^3 - \sqrt{6}\,\mathrm{tr}\,\mathbf{Q}^3}{|\mathbf{Q}|^3}\frac{|\mathbf{Q}|^3 + \sqrt{6}\,\mathrm{tr}\,\mathbf{Q}^3}{|\mathbf{Q}|^3} \tag{33}$$

$$\leq \frac{|\mathbf{Q}|^3 - \sqrt{6}\,\mathrm{tr}\,\mathbf{Q}^3}{(1-\epsilon_1)^3} \cdot \frac{|\mathbf{Q}|^3 + |\mathbf{Q}|^3}{|\mathbf{Q}|^3} \leq \frac{\epsilon_1}{(1-\epsilon_1)^3} \cdot 2 \overset{\epsilon_1 \to 0}{\longrightarrow} 0. \tag{34}$$

The quantity $|\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3$ plays an important role in the following proof and we note the following elementary inequality

$$0 \leq \left(|\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3\right) \leq \frac{\left(3 - \mathrm{sgn}\,\mathrm{tr}\mathbf{Q}^3\right)}{2}|\mathbf{Q}|^3. \tag{35}$$

As in [22], we use the Euler-Lagrange equations (27) to derive the following inequality:

$$-\triangle e\left(\mathbf{Q}, t\right) + |\Gamma|^2 \leq -2\frac{\partial^2 f}{\partial \mathbf{Q}_{ij}\partial \mathbf{Q}_{pq}}\mathbf{Q}_{ij,k}\mathbf{Q}_{pq,k}. \tag{36}$$

Moreover, we have

$$\bar{L}^2|\Gamma|^2 = \frac{t^2}{4}|\mathbf{Q}|^2\left(1-|\mathbf{Q}|^2\right)^2 + \frac{9h_+^2}{4}(1-|\mathbf{Q}|)^2|\mathbf{Q}|^4 + $$
$$+\frac{3h_+t}{2}(1-|\mathbf{Q}|^2)(|\mathbf{Q}|^3-|\mathbf{Q}|^4) + \frac{3h_+t}{2}(|\mathbf{Q}|^2-1)(|\mathbf{Q}|^3-\sqrt{6}\mathrm{tr}\mathbf{Q}^3) + $$
$$+\frac{9h_+^2}{2}(|\mathbf{Q}|^3-\sqrt{6}\mathrm{tr}\mathbf{Q}^3)|\mathbf{Q}|^2 \tag{37}$$

and

$$-\bar{L}\frac{\partial^2 f}{\partial \mathbf{Q}_{ij}\partial \mathbf{Q}_{pq}}\mathbf{Q}_{ij,k}\mathbf{Q}_{pq,k} = \frac{t}{2}|\nabla\mathbf{Q}|^2(1-|\mathbf{Q}|^2) - t(\mathbf{Q}\cdot\nabla\mathbf{Q})^2 - $$
$$-3h_+\left(\mathbf{Q}\cdot\nabla\mathbf{Q}\right)^2 - \frac{3h_+}{2}\left|\mathbf{Q}\right|^2\left|\nabla\mathbf{Q}\right|^2 + 3\sqrt{6}h_+\mathbf{Q}_{\beta j}\mathbf{Q}_{\alpha j,k}\mathbf{Q}_{\alpha\beta,k}. \tag{38}$$

We consider three separate cases according to the sign of $\mathrm{tr}\mathbf{Q}^3$ and the magnitude of $|\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3$.

Case I: $0 \leq |\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3 \leq \epsilon_1$. This, when combined with (30), implies that $\mathrm{tr}\mathbf{Q}^3 > 0$ and that $\left|\mathbf{Q} - \sqrt{\frac{3}{2}}\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right)\right| \leq \epsilon_0$ for some $\mathbf{n} \in S^2$ (by definition of ϵ_1). In this case, we can repeat all the arguments in [22, Lemmas 5-7]; we state the key steps for completeness.

We start with inequality (31) above. We denote the eigenvectors of $\mathbf{Q}$ by $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ respectively and let $\lambda_3 > 0$ and λ_1, λ_2 denote the corresponding eigenvalues. Define

$$\mathbf{Q}^* = \sqrt{\frac{2}{3}}\mathbf{n}_3\otimes\mathbf{n}_3 - \sqrt{\frac{1}{6}}\left(\mathbf{n}_1\otimes\mathbf{n}_1 + \mathbf{n}_2\otimes\mathbf{n}_2\right).$$

From the inequality $\left|\mathbf{Q} - \sqrt{\frac{3}{2}}\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right)\right| \leq \epsilon_0$ with $\mathbf{n} = \mathbf{n}_3$, we necessarily have that

$$\left(\lambda_1 + \sqrt{\frac{1}{6}}\right)^2 + \left(\lambda_2 + \sqrt{\frac{1}{6}}\right)^2 + \left(\lambda_3 - \sqrt{\frac{2}{3}}\right)^2 \leq \epsilon_0^2.$$

The proof of the Bochner inequality now follows from the chain of inequalities below:

$$
\begin{aligned}
-\triangle e(\mathbf{Q},t) + |\Gamma|^2 &\leq -2\frac{\partial^2 f}{\partial \mathbf{Q}_{ij}\partial \mathbf{Q}_{pq}} \mathbf{Q}_{ij,k}\mathbf{Q}_{pq,k} \leq \\
&\leq \delta \sum_{i,j,m=1}^{3} \left(\frac{\partial^3 f}{\partial \mathbf{Q}_{ij} \mathbf{Q}_{pq} \partial \mathbf{Q}_{mn}} \left(\mathbf{Q}^*\right) \right)^2 \left(\mathbf{Q}-\mathbf{Q}^*\right)^2 \qquad (39) \\
&\qquad + \delta \sum_{i,j,m=1}^{3} \left(\mathcal{R}^{ijmn}\right)^2 \left(\mathbf{Q},\mathbf{Q}^*\right) + \frac{1}{\delta}|\nabla \mathbf{Q}|^4 \leq \\
&\leq C_1 \delta t^2 \left|\mathbf{Q}-\mathbf{Q}^*\right|^2 + \frac{1}{\delta}|\nabla \mathbf{Q}|^4 \leq \\
&\leq C_2 \delta t f(\mathbf{Q},t) + \frac{1}{\delta}|\nabla \mathbf{Q}|^4. \qquad (40)
\end{aligned}
$$

In Equation (39) above, we have carried out a Taylor series expansion of the right-hand side of (36) about $\mathbf{Q}^*$, $\left(\mathcal{R}^{ijmn}\right)$ is the remainder term in the Taylor series expansion which is well-controlled and the constants C_1 and C_2 are independent of t but dependent on $\bar{L}$ (which does not matter since $\bar{L}$ is fixed). For δ sufficiently small, we can absorb the $C_2\delta t f(\mathbf{Q},t)$-term on the right by the $|\Gamma|^2(\mathbf{Q})$-contribution on the left so that

$$
|\Gamma|^2\left(\mathbf{Q}_j\right) - C_2 \delta t f(\mathbf{Q},t) \geq 0
$$

for δ sufficiently small (from (31)), yielding the Bochner inequality

$$
-\triangle e(\mathbf{Q},t) \leq \frac{1}{\delta}|\nabla \mathbf{Q}|^4
$$

for $\delta > 0$ independent of t, as required.

Case II: $\mathrm{tr}\mathbf{Q}^3 > 0$ and $\epsilon_1 < |\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3 \leq 1$.

We refer to the relations (36)-(38) and use the Cauchy-Schwarz inequality in (37) to see that

$$
\frac{3h_+ t}{2}(|\mathbf{Q}|^2-1)(|\mathbf{Q}|^3-\sqrt{6}\mathrm{tr}\mathbf{Q}^3) \geq -\delta t^2(|\mathbf{Q}|^2-1)^2 - \frac{9h_+^2}{16}\frac{1}{\delta}(|\mathbf{Q}|^3-\sqrt{6}\mathrm{tr}\mathbf{Q}^3)^2.
$$

For $\frac{3}{16} < \delta < \frac{1-2\epsilon_1}{4}$ and ϵ_1 chosen as above, we have

$$
\begin{aligned}
&\bar{L}^2|\Gamma|^2 \geq \alpha t^2 |\mathbf{Q}|^2(1-|\mathbf{Q}|)^2 + \frac{9h_+^2}{4}(1-|\mathbf{Q}|)^2|\mathbf{Q}|^4 + \\
&+\frac{3h_+ t}{2}|\mathbf{Q}|^3(1-|\mathbf{Q}|)^2(1+|\mathbf{Q}|) + \eta h_+^2(|\mathbf{Q}|^3-\sqrt{6}\mathrm{tr}\mathbf{Q}^3) \qquad (41)
\end{aligned}
$$

for positive constants α, η independent of t and $\bar{L}$ is fixed for our purposes. Finally, we appeal to (38) to obtain

$$-\bar{L}\frac{\partial^2 f}{\partial \mathbf{Q}_{ij}\partial \mathbf{Q}_{pq}}\mathbf{Q}_{ij,k}\mathbf{Q}_{pq,k} \leq \delta_1\frac{t^2}{4}(1-|\mathbf{Q}|^2)^2 + \\ +\delta_2 h_+^2|\mathbf{Q}|^2 + \frac{1}{\delta_5(\delta_1,\delta_2)}|\nabla\mathbf{Q}|^4. \tag{42}$$

For δ_2 sufficiently small, we can absorb the $h_+^2|\mathbf{Q}|^2$ term in (42) by the $\eta h_+^2(|\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3)$ term in (41). Choosing δ_1, δ_2 small enough (and independent of t), recalling (36), the lower bound (41) and the upper bound (42), we have

$$-\triangle e\left(\mathbf{Q}, t\right) \leq \frac{1}{\delta_5}|\nabla\mathbf{Q}|^4 \tag{43}$$

which is precisely the Bochner inequality.

Case III: $\mathrm{tr}\mathbf{Q}^3 \leq 0$ so that $(1-\epsilon_1)^3 \leq |\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3 \leq 2|\mathbf{Q}|^3$.

A large part of the computations for Case II carry over to Case III. In particular, (42) is unchanged and it remains to note that for $\mathrm{tr}\mathbf{Q}^3 < 0$, the bulk potential $\bar{L}f(\mathbf{Q},t) \geq \frac{t}{8}\left(1-|\mathbf{Q}|^2\right)^2 + \frac{h_+}{8}$. In particular,

$$\frac{h_+^2}{64\bar{L}^2} \leq e^2(\mathbf{Q},t). \tag{44}$$

Define σ and γ to be

$$1-|\mathbf{Q}|^2 = \sigma\frac{h_+}{t} \\ \gamma = |\mathbf{Q}|^3 - \sqrt{6}\mathrm{tr}\mathbf{Q}^3 \tag{45}$$

where $\mathrm{tr}\mathbf{Q}^3 \leq 0$ by assumption. The second, third and fifth terms in (37) are positive, hence

$$\bar{L}^2|\Gamma|^2 \geq \frac{|\mathbf{Q}|^2}{4}\sigma^2 h_+^2 - \frac{3h_+^2}{2}\sigma\gamma \geq \\ \geq \frac{h_+^2}{8}(\sigma^2 - 12\sigma\gamma) \geq \frac{h_+^2}{8}((\sigma-6\gamma)^2 - 36\gamma^2) \geq -\frac{9h_+^2}{2}\gamma^2. \tag{46}$$

Since $\gamma = |\mathbf{Q}|^3 - \sqrt{6}\,\mathrm{tr}\,\mathbf{Q}^3 \leq 2$, we get $\bar{L}^2|\Gamma|^2 \geq -18h_+^2$ and therefore, the Bochner inequality (29) then follows from (36), (46), (44).

□

Comment: The Bochner-inequality for the Landau-de Gennes energy density was derived in [22], for global LdG minimizers, away from the singular set, Σ, of a limiting harmonic map, in the vanishing elastic constant limit i.e. in the $L \to 0$ limit. There is an important mathematical difference between the $L \to 0$ limit and the low-temperature limit ($A \to -\infty$) considered in our manuscript. As $L \to 0$, we can use the monotonicity formula [22, Lemma 2 and Proposition 4] to deduce that a global LdG minimizer, denoted by $\mathbf{Q}_L$, is "almost" uniaxial with unit norm away from Σ as $L \to 0$ i.e. they are close to the uniaxial manifold $\left\{\sqrt{\frac{3}{2}}\left(\mathbf{m}\otimes\mathbf{m} - \frac{\mathbf{I}}{3}\right)\right\}$ for some arbitrary $\mathbf{m} \in \mathbb{S}^2$. In [22], the authors use this proximity to the uniaxial manifold, away from Σ, to derive the Bochner-inequality which, in turn, yields uniform convergence to a (minimizing) limiting harmonic map, away from Σ.

In the low-temperature limit ($A \to -\infty$), we can only prove that a global LdG minimizer, denoted by $\mathbf{Q}_A$, satisfies $|\mathbf{Q}_A| \to 1$ uniformly away from Σ, without any information about uniaxiality or biaxiality (since the prefactor $\frac{h_+}{t}$ of the second term in (28) vanishes as $t \to \infty$). This is weaker information than what is available as $L \to 0$. We use the information about $|\mathbf{Q}_A|$ as $A \to -\infty$ to derive the Bochner inequality and this requires us to consider three separate cases, depending on $\mathrm{tr}\mathbf{Q}_A^3$ and the degree of biaxiality. Once we derive the Bochner inequality for the energy density, we can prove uniform convergence of a sequence of global energy minimizers to a limiting minimizing harmonic map, away from Σ.

From the maximum principle (see [20]) and the uniform convergence $|\mathbf{Q}_j| \to 1$ away from the singularities of $\mathbf{Q}^0$ (see Proposition 3.1), we see that (30) is satisfied for all t sufficiently large, so we obtain Bochner's inequality away from Σ for large t. This enables us to deduce the following ϵ-regularity property, exactly as in [22, Lemma 7]:

Lemma 3.4. *Let $K \subset \Omega$ be a compact subset that does not contain any singularity of $\mathbf{Q}^0$. Then there exist j_0 and constants $C_1, C_2 > 0$ (independent of j) so that if for $\mathbf{a} \in K$ and $0 < r < \mathrm{dist}\,(\mathbf{a}, \partial K)$, we have*

$$\frac{1}{r}\int_{B(\mathbf{a},r)} e\left(\mathbf{Q}_j, t_j\right)\, dV \le C_1, \tag{47}$$

then

$$r^2 \sup_{B(\mathbf{a},r/2)} e\left(\mathbf{Q}_j, t_j\right) \le C_2 \tag{48}$$

for all $j \ge j_0$.

Proof of Proposition 3.2. The normalized energy, $\frac{1}{r}\int_{B(a,r)} e\left(\mathbf{Q}_j, t_j\right)\, dV$, can be controlled away from Σ, by simply (i) using the strong convergence of the sequence, $\{\mathbf{Q}_j\}$ to $\mathbf{Q}^0$ as $j \to \infty$ in $W^{1,2}$ and (ii) the fact that $|\nabla \mathbf{Q}^0|$ is bounded away from Σ, independently of t_j. Thus, the uniform convergence, $\mathbf{Q}_j \to \mathbf{Q}^0$, away from Σ as $j \to \infty$, follows immediately from Lemma 3.4, combining (47) and (48) and Ascoli-Arzelá Theorem. □

We are almost ready to prove the main theorems. It only remains to state an elementary result from homotopy theory and to recall that the Landau-de Gennes energy functional has a Ginzburg-Landau like structure by blowing-up at scale $t^{-1/2}$ and working in the $t \to \infty$ limit.

Lemma 3.5. *Let* $\mathbf{Q}^*(\mathbf{x}) := \sqrt{\frac{3}{2}}\left(\mathbf{n}^*(\mathbf{x}) \otimes \mathbf{n}^*(\mathbf{x}) - \frac{\mathbf{I}}{3}\right)$ *for some* $\mathbf{n}^* \in C(\partial B; \mathbb{S}^2)$, *where* B *is a ball* $B(\mathbf{a}, \epsilon) \subset \mathbb{R}^3$. *Suppose that* $\mathbf{Q}^*$ *is homotopic in* $C(\partial B; \mathbf{Q}_{\min})$ *(see* (25)*) to* $\mathbf{Q}|_{\partial B}$ *for some* $\mathbf{Q} \in C(\overline{B}; \mathbf{Q}_{\min})$. *Then* $\deg \mathbf{n}^* = 0$.

Proof. Since $\mathbf{Q}|_{\partial B}$ has a continuous $\mathbf{Q}_{\min}$-valued extension inside $\overline{B}$, it is homotopic in $C(\partial B; \mathbf{Q}_{\min})$ to the constant tensor $\mathbf{Q}(\mathbf{a})$. Hence, combining the two homotopies, we deduce that $\mathbf{Q}^*$ is homotopic to a constant in $C(\partial B; \mathbf{Q}_{\min})$.

Since ∂B is simply-connected and $\mathbb{S}^2$ is a universal cover of $\mathbf{Q}_{\min} \cong \mathbb{R}P^2$, the latter homotopy lifts to $\mathbb{S}^2$, implying that $\mathbf{n}^*$ is homotopic to a constant in $C(\partial B; \mathbb{S}^2)$ and hence, $\deg \mathbf{n}^* = 0$, as needed. □

Lemma 3.6. *Let* $t_j \to +\infty$ *and, for each* $j \in \mathbb{N}$, *let* $\mathbf{Q}_j \in \bar{\mathcal{A}}_A$ *be a classical solution of* (27). *Suppose that* $\mathbf{Q}_j$ *converges strongly in* $W^{1,2}$ *to a minimizing limiting harmonic map* $\mathbf{Q}^0$. *Let* $\mathbf{x}_j^*$ *be a sequence of points converging to some* $\mathbf{x}^*$ *in the singular set* Σ *of* $\mathbf{Q}^0$. *Then (up to a subsequence) the rescaled maps*

$$\xi_j := \sqrt{\frac{\bar{L}}{t_j}}, \qquad \tilde{\mathbf{x}} := \frac{\mathbf{x} - \mathbf{x}_j^*}{\xi_j}, \qquad \tilde{\mathbf{Q}}_j(\tilde{\mathbf{x}}) := \mathbf{Q}_j(\mathbf{x}_j^* + \xi_j \tilde{\mathbf{x}}) \tag{49}$$

converge in $C^k_{\mathrm{loc}}(\mathbb{R}^3; S_0)$ *for all* $k \in \mathbb{N}$ *to a smooth solution of the Ginzburg-Landau equations* $\Delta \tilde{\mathbf{Q}} = (|\tilde{\mathbf{Q}}|^2 - 1)\tilde{\mathbf{Q}}$, *in* $\mathbb{R}^3$, *which satisfies the energy bound*

$$\frac{1}{R}\int_{|\tilde{\mathbf{x}}|<R} \frac{1}{2}|\nabla \tilde{\mathbf{Q}}^\infty(\tilde{\mathbf{x}})|^2 + \frac{(1 - |\tilde{\mathbf{Q}}^\infty|^2)^2}{8}\ \mathrm{d}V \le 12\pi \quad \forall R > 0. \tag{50}$$

Proof. The proof follows from the celebrated energy quantization result for minimizing harmonic maps at singular points, established in [5]:

$$\lim_{r\to 0}\frac{1}{r}\int_{B(\mathbf{x}^*,r)}\frac{1}{2}|\nabla\mathbf{n}^0|^2\,\mathrm{d}V = 4\pi,\quad i=1,\ldots,N. \tag{51}$$

We begin by noting that $|\nabla\mathbf{Q}^0|^2 = 3|\nabla\mathbf{n}^0|^2$, therefore

$$\frac{1}{r}\int_{B(\mathbf{x}^*,r)}\frac{1}{2}|\nabla\mathbf{Q}_j|^2 + f(\mathbf{Q}_j,t_j)\ \mathrm{d}V \overset{j\to\infty}{\longrightarrow} \frac{3}{r}\int_{B(\mathbf{x}^*,r)}\frac{1}{2}|\nabla\mathbf{n}^0|^2\ \mathrm{d}V \tag{52}$$

for every small $r>0$.

By the monotonicity formula, Proposition 3.1 (iii), for every fixed $R>0$, every small $r>|\mathbf{x}_j^*-\mathbf{x}^*|+\xi_jR$, and every j sufficiently large, we have that

$$\frac{1}{R}\int_{|\tilde{\mathbf{x}}|<R}\frac{1}{2}|\nabla\tilde{\mathbf{Q}}_j(\tilde{\mathbf{x}})|^2 + \frac{(1-|\tilde{\mathbf{Q}}_j|^2)^2}{8}\,\mathrm{d}V \tag{53}$$

$$\leq \frac{1}{\xi_jR}\int_{|\mathbf{x}-\mathbf{x}_j^*|<\xi_jR}\frac{1}{2}|\nabla\mathbf{Q}_j(\mathbf{x})|^2 + f(\mathbf{Q}_j(\mathbf{x}),t_j)\ \mathrm{d}V \tag{54}$$

$$\leq \frac{1}{r-|\mathbf{x}_j^*-\mathbf{x}^*|}\int_{B(\mathbf{x}_j^*,r-|\mathbf{x}_j^*-\mathbf{x}^*|)}\frac{1}{2}|\nabla\mathbf{Q}_j(\mathbf{x})|^2 + f(\mathbf{Q}_j(\mathbf{x}),t_j)\ \mathrm{d}V \tag{55}$$

$$\leq \frac{r}{r-|\mathbf{x}_j^*-\mathbf{x}^*|}\cdot\frac{1}{r}\int_{B(\mathbf{x}^*,r)}\frac{1}{2}|\nabla\mathbf{Q}_j(\mathbf{x})|^2 + f(\mathbf{Q}_j(\mathbf{x}),t_j)\ \mathrm{d}V \tag{56}$$

(we have used the inequality $\frac{t}{8L}(1-|\tilde{\mathbf{Q}}_j|^2)^2 \leq f(\tilde{\mathbf{Q}}_j,t_j)$ above). This combined with (52) and (51) yields the following inequality

$$\begin{aligned}\limsup_{j\to\infty}\frac{1}{R}\int_{|\tilde{\mathbf{x}}|<R}\frac{1}{2}|\nabla\tilde{\mathbf{Q}}_j(\tilde{\mathbf{x}})|^2 + \frac{(1-|\tilde{\mathbf{Q}}_j|^2)^2}{8}\ \mathrm{d}V\\ \leq 3\left(\limsup_{r\to 0^+}\frac{1}{r}\int_{B(\mathbf{x}^*,r)}\frac{1}{2}|\nabla\mathbf{n}^0|^2\ \mathrm{d}V\right)\leq 12\pi\end{aligned} \tag{57}$$

for every $R>0$.

Using the energy bound above, we can extract a diagonal subsequence, converging weakly in $W^{1,2}_{\mathrm{loc}}\cap L^4_{\mathrm{loc}}(\mathbb{R}^3;S_0)$, to a limit map $\tilde{\mathbf{Q}}^\infty$ satisfying the energy bound (50). One can check that $\tilde{\mathbf{Q}}^\infty$ solves the weak form of the Ginzburg-Landau equations in $\mathbb{R}^3$ (write the weak form of the partial differential equations for $\tilde{\mathbf{Q}}_{j_k}$ and pass to the limit when $k\to\infty$). Standard arguments in elliptic regularity then show that $\tilde{\mathbf{Q}}^\infty$ is a classical solution of the Ginzburg-Landau equations and that the diagonal subsequence converges in $\bigcap_{k\in\mathbb{N}}C^k_{\mathrm{loc}}$ to $\tilde{\mathbf{Q}}^\infty$. □

Proof of Theorem 1. (i) It follows from Propositions 3.1 and 3.2.

(ii) This is an immediate consequence of the uniform convergence, $\mathbf{Q}_j \to \mathbf{Q}^0$ as $j \to \infty$, away from the singular set, $\Sigma = \{\mathbf{x}_1 \ldots \mathbf{x}_N\}$ of $\mathbf{Q}^0$. $\mathbf{Q}^0$ is purely uniaxial by definition i.e. $\beta^2\left(\mathbf{Q}^0\right) = 0$ (see (4) for the definition of the biaxiality parameter, $\beta^2(\mathbf{Q})$). The map $\mathbf{Q} \mapsto \beta^2(\mathbf{Q})$ is continuous for $\mathbf{Q} \neq 0$ and the conclusion, $B^j_\delta \subseteq \Sigma_\epsilon$, follows for any fixed ϵ, provided j is large enough.

(iii) This can be proven as in [9], where the authors prove that $|\mathbf{Q}_j(\mathbf{x})| > 0$ on Ω, for j large enough. We argue by contradiction and we assume that there exist points $\mathbf{x}^*_j \in \Omega$ such that $\left|\mathbf{Q}_j\left(\mathbf{x}^*_j\right)\right| \leq 1 - \eta$ (for some $\eta > 0$ independent of j), for all j in the sequence.

In view of part (i), we may assume $\mathbf{x}^*_j \to \mathbf{x}^*$ for some $\mathbf{x}^* \in \Sigma$ and repeat the arguments in Lemma 3.1 and 4.1 of [9] i.e. perform a blow-up analysis of the re-scaled maps, $\mathbf{Q}^*_j(\mathbf{x}) = \mathbf{Q}_j\left(\mathbf{x}^*_j + \frac{\mathbf{x}}{\sqrt{t_j}}\right)$. By Lemma 3.6 and [9, Lemma 3.1], the rescaled minimizers converge locally smoothly to a minimizer, $\mathbf{Q}_\infty \in C^2(\mathbb{R}^3; S_0)$, of the Ginzburg-Landau energy,

$$GL(\mathbf{Q}; A) = \int_A |\nabla \mathbf{Q}|^2 + \frac{1}{4}(1 - |\mathbf{Q}|^2)^2 dV \tag{58}$$

(on open sets with compact closure $\subset \mathbb{R}^3$ with respect to its own boundary conditions) with the energy growth $GL(\mathbf{Q}; B_R(0)) = \mathcal{O}(R)$ as $R \to \infty$. In addition we have $|\mathbf{Q}_\infty(0)| \leq 1 - \eta$ because of the normalization. We can then use the same blow-down analysis as in [9] to show that $\mathbf{Q}_R(\mathbf{x}) = \mathbf{Q}_\infty(R\mathbf{x})$ as $R \to \infty$ converges strongly in $W^{1,2}_{loc}$ to a $\mathbb{S}^4$-valued minimizing harmonic map, labelled by $\hat{\mathbf{Q}}_\infty$. Indeed, one can use the well-known Luckhaus interpolation Lemma as in [28], Proposition 4.4, still for a sequence of functionals converging to the Dirichlet integral for maps into a manifold, showing that minimality persist in the limit and the convergence is actually strong in $W^{1,2}_{loc}$.

From the monotonicity formula for the Ginzburg-Landau energy, $\hat{\mathbf{Q}}_\infty$ is a degree-zero homogeneous harmonic map, hence it is smooth away from the origin by partial regularity theory [31]. Since the latter is constant by [33], the GL minimizer $\mathbf{Q}_\infty$ is also a constant matrix of norm one from the monotonicity formula for the GL energy. Thus, $|\mathbf{Q}^*_j(0)| \to |\mathbf{Q}_\infty(0)| = 1$ which yields the desired contradiction.

(iv) Let $\delta \in (0, 1)$ be fixed. From part (i), (ii) and since $\epsilon > 0$ is fixed and arbitrary, we necessarily have

$$\beta^2\left(\mathbf{Q}_j\right)|_{\partial B_\epsilon(\mathbf{x}_i)} \leq \delta \tag{59}$$

for j sufficiently large, $\mathbf{x}_i \in \Sigma$ (depending only on ϵ). From (iii) above, we have that $|\mathbf{Q}_j| \to 1$ uniformly on $\overline{B_\epsilon(\mathbf{x}_i)}$ as $j \to \infty$.

Thus, if we define the set

$$\mathcal{N}_\sigma = \{\mathbf{Q} \in S_0 \ s.t.\ \beta^2(\mathbf{Q}) \leq \sigma \text{ and } 1-\sigma \leq |\mathbf{Q}| \leq 1\} \tag{60}$$

for each $0 \leq \sigma < 1$ and let $\delta < \sigma$, we have the following:

- The restriction of $\mathbf{Q}_j$ to the boundary, $\mathbf{Q}_j \in C(\partial B_\epsilon(\mathbf{x}_i); \mathcal{N}_\delta)$ for j large enough (depending only on ϵ (by (59)) and $\mathbf{Q}^0 \in C(\partial B_\epsilon(\mathbf{x}_i); \mathcal{N}_\delta)$ (in view of the inclusion $\mathbf{Q}_{min} = \mathcal{N}_0 \subset \mathcal{N}_\delta$).
- For $\delta < \sigma < 1$, the maps $\mathbf{Q}_j$ and $\mathbf{Q}^0$ are homotopic in $C(\partial B_\epsilon(\mathbf{x}_i); \mathcal{N}_\sigma)$ (thanks to the uniform convergence; composing pointwise with the affine homotopy in S_0 keeps the images inside $\mathcal{N}_\sigma$ for j large enough).
- $\mathcal{N}_\sigma \supset \mathcal{N}_0$ retracts homotopically onto $\mathcal{N}_0 = \mathbf{Q}_{min} \sim \mathbb{R}P^2$ for every $\sigma < 1$, see [7, Lemma 3.10]; see also [9], Corollary 1.2 and Section 5 therein.

Suppose, for a contradiction, that $\max_{\overline{B_\epsilon(\mathbf{x}_i)}} \beta^2(\mathbf{Q}_j) < 1$ and let $\sigma \in (\max\{\delta, \max_{\overline{B_\epsilon(\mathbf{x}_i)}} \beta^2(\mathbf{Q}_j)\}, 1)$. Then the composition of the aforementioned retraction with $\mathbf{Q}_j$ yields a map $\mathbf{Q}_j^* \in C(\overline{B}_\epsilon; \mathbf{Q}_{\min})$ whose trace $\mathbf{Q}_j^*|_{\partial B_\epsilon}$ is homotopic in $C(\partial B_\epsilon; \mathbf{Q}_{\min})$ to $\mathbf{Q}^0|_{\partial B_\epsilon}$. By Lemma 3.5 we would conclude that $\deg \mathbf{n}^0|_{\partial B_\epsilon} = 0$, a contradiction with the fact that $\deg\ \mathbf{n}^0|_{\partial B_\epsilon} = \pm 1$ near each singular point, for ϵ small enough fixed at the beginning.

Similarly, assume that $\min_{\overline{B_\epsilon(\mathbf{x}_i)}} \beta^2(\mathbf{Q}_j) > 0$ for infinitely many j in the sequence. Then $\mathbf{Q}_j(\mathbf{x})$ is purely biaxial for all $\mathbf{x} \in B_\epsilon(\mathbf{x}_i)$ (recall that there are no isotropic points from part (iii)). Let $\mathbf{n}_j(\mathbf{x}) \in \mathbb{S}^2$ be the eigenvector corresponding to the maximum eigenvalue (which is uniquely defined up to a sign). Recall that $\mathbf{Q}_j$ is continuous in $\overline{B_\epsilon(\mathbf{x}_i)}$, hence $\mathbf{x} \in \Omega \mapsto \mathbf{n}_j \otimes \mathbf{n}_j \in \mathbb{R}P^2$ is continuous (if $\mathbf{x}_k \to \mathbf{x}$ and $\mathbf{n}_j(\mathbf{x}_k) \overset{k\to\infty}{\longrightarrow} \mathbf{n}'$ then clearly $\mathbf{n}'$ maximizes $\mathbf{n} \cdot \mathbf{Q}_j(\mathbf{x})\mathbf{n}$ in $\mathbb{S}^2$ and the maximal eigenvalue is simple). As a consequence, we choose $\mathbf{n}_j$ to be a continuous lifting so that $\mathbf{n}_j \in C(\overline{B_\epsilon(\mathbf{x}_i)}; \mathbb{S}^2)$.

Now, $\mathbf{Q}_j$ converges uniformly to $\mathbf{Q}^0$ on ∂B_ϵ. Therefore, $|\mathbf{Q}_j| \to 1$ and $\beta(\mathbf{Q}_j) \to 0$ uniformly on ∂B_ϵ. This implies that $\mathbf{n}_j \otimes \mathbf{n}_j \to \mathbf{n}^0 \otimes \mathbf{n}^0$ uniformly on ∂B_ϵ since

$$\left| \sqrt{\frac{3}{2}} \left(\mathbf{n}_j \otimes \mathbf{n}_j - \frac{\mathbf{I}}{3} \right) - \frac{\mathbf{Q}_j}{|\mathbf{Q}_j|} \right| + \left| \frac{\mathbf{Q}_j}{|\mathbf{Q}_j|} - \mathbf{Q}^0 \right| \overset{j\to\infty}{\longrightarrow} 0.$$

We conclude that $\mathbf{Q}^0|_{\partial B_\epsilon}$ is homotopic to $\sqrt{\frac{3}{2}}(\mathbf{n}_j\otimes\mathbf{n}_j-\frac{\mathbf{I}}{3})$, first in $C(\partial B_\epsilon,\mathcal{N}_\sigma)$ for some small σ (composing pointwise with the affine homotopy in S_0) and then in $C(\partial B_\epsilon,\mathbf{Q}_{\min})$ (composing with the retraction from $\mathcal{N}_\sigma$ to $\mathbf{Q}_{\min}$). Since $\sqrt{\frac{3}{2}}(\mathbf{n}_j\otimes\mathbf{n}_j-\frac{\mathbf{I}}{3})$ has a continuous extension inside $\overline{B_\epsilon}$, we recall Lemma 3.5 and obtain a contradiction with the fact that $\deg \mathbf{n}^0|_{\partial B_\epsilon}=\pm 1$ for every $\epsilon>0$ small enough.

The uniaxial set has zero Lebesgue-measure, as has already been established in [22, Prop. 14].

(v) For each $\mathbf{x}_i\in\Sigma$ and $\delta\in(0,1)$ fixed, consider the biaxiality set, $B_\epsilon(\mathbf{x}_i)\cap B^j_\delta$, around $\mathbf{x}_i$ and its diameter, $d_j:=\operatorname{diam}\left(B_\epsilon(\mathbf{x}_i)\cap B^j_\delta\right)$. We have $d_j=o(1)$ as $j\to\infty$ from (i) and (ii) above.

We claim that $d_j\sim t_j^{-1/4}$ as $j\to\infty$, which follows by blowing up $\mathbf{Q}_j$, at scale d_j, and excluding remaining decay rates. Firstly, let $\mathbf{p}_j,\mathbf{q}_j\in B_\epsilon(\mathbf{x}_i)\cap B^j_\delta$ such that $d_j=|\mathbf{p}_j-\mathbf{q}_j|$ and let $\hat{\mathbf{x}}_j:=(\mathbf{p}_j+\mathbf{q}_j)/2$. Clearly $\left(B_\epsilon(\mathbf{x}_i)\cap B^j_\delta\right)\subseteq B(\hat{\mathbf{x}}_j,\frac{3d_j}{2})$ and $\hat{\mathbf{x}}_j\to\mathbf{x}_i$ as $j\to\infty$. Then by defining $B^j:=B^j(\hat{\mathbf{x}}_j,d_j/2)$ and by (ii), we immediately have $\beta^2(\mathbf{Q}_j)\le\delta$ on $\partial B(\hat{\mathbf{x}}_j,\frac{3d_j}{2})$, $\beta^2(\mathbf{Q}_j)=\delta$ at two antipodal points on ∂B^j, and $\max_{\overline{B}(\hat{\mathbf{x}}_j,\frac{3d_j}{2})}\beta^2(\mathbf{Q}_j)=1$, for j large enough.

Define $\hat{\mathbf{Q}}_j(\mathbf{x})=\mathbf{Q}_j(\hat{\mathbf{x}}_j+d_j\mathbf{x}/2)$ and we get, up to a sequence of rotations which we do not specify explicitly,

$$\beta^2\left(\hat{\mathbf{Q}}_j\right)|_{\partial(\frac{3}{2}B)}\le\delta\,,\quad \beta^2\left(\hat{\mathbf{Q}}_j(0,0,\pm1)\right)=\delta\,,\quad \max_{(\frac{3}{2}B)}\beta^2\left(\hat{\mathbf{Q}}_j\right)=1 \qquad (61)$$

on the unit ball $B=B(0,1)$. The the rescaled maps $\hat{\mathbf{Q}}_j$ are defined on the family of expanding domains, $2(\Omega-\hat{\mathbf{x}}_j)/d_j\to\mathbb{R}^3$ and are local minimizers on compact subdomains of the functionals

$$I_j\left[\hat{\mathbf{Q}}_j\right]:=\int\frac{\bar{L}}{2}|\nabla\hat{\mathbf{Q}}_j|^2+\frac{d_j^2}{4}\left[\frac{t_j}{8}\left(1-|\hat{\mathbf{Q}}_j|^2\right)^2+\frac{h_+}{8}\left(1+3|\hat{\mathbf{Q}}_j|^2-4\sqrt{6}\operatorname{tr}\hat{\mathbf{Q}}_j^3\right)\right]dV \qquad (62)$$

with $h_+\sim\sqrt{t_j}$ as $j\to\infty$. Taking into account the Euler-Lagrange equations (corresponding to (62)), we can exclude the following regimes: (a) $d_j<<t_j^{-1/2}$ since we easily deduce that (up to subsequences) $\hat{\mathbf{Q}}_j\to\mathbf{Q}_*$ in $C^k_{loc}\left(\mathbb{R}^3\right)$ for $k\in\mathbb{N}$ by the uniform L^∞-bound and elliptic regularity. Indeed, for $d_j<<t_j^{-1/2}$, the nonlinear terms in the Euler-Lagrange equations vanish as $j\to\infty$. Thus $\mathbf{Q}_*\in C^2\left(\mathbb{R}^3\right)$ is bounded and harmonic, hence constant (of

norm one from (iii) above) by Liouville's Theorem and this fact contradicts (61) which holds for the limiting map $\mathbf{Q}_*$ by uniform convergence. (b) $d_j \sim t_j^{-1/2}$; this regime has already been discussed in item (iii) above and hence, up to a subsequence, $\hat{\mathbf{Q}}_j \to \mathbf{Q}_{**}$ in $C^k_{loc}\left(\mathbb{R}^3\right)$ for $k \in \mathbb{N}$. Here $\mathbf{Q}_{**}$ is a bounded Ginzburg-Landau local minimizer on the whole of $\mathbb{R}^3$ such that $\int_{B_R} \frac{1}{2}|\nabla \mathbf{Q}_{**}|^2 + \left(1 - |\mathbf{Q}_{**}|^2\right)^2 = \mathcal{O}(R)$ as $R \to \infty$. Arguing as in Lemma 3.6 and item (iii) above, we infer that $\mathbf{Q}_{**}$ is a constant matrix of norm one, contradicting (61) which still passes to the limit under smooth convergence and clearly cannot hold for constant maps.

(c) $t_j^{-1/2} << d_j << t_j^{-1/4}$. Here (up to a subsequence), the limiting map is a local minimizer of $\int |\nabla \mathbf{Q}|^2$ among $\mathbb{S}^4$-valued maps. Indeed the sequence is locally bounded in $H^1_{\mathrm{loc}}(\mathbb{R}^3)$ by the monotonicity formula and hence converges weakly in H^1_{loc} (up to a subsequence). The limiting map is clearly $\mathbb{S}^4$-valued, as can be seen by applying Fatou's Lemma to (62). Additionally, we can prove strong convergence to the limiting map and the minimality of the limiting map, arguing as in item (iii) above, i.e. using the well-known Luckhaus interpolation Lemma as in [28], Proposition 4.4, for a sequence of functionals converging to the Dirichlet integral for maps into a manifold.

Therefore, $\hat{\mathbf{Q}}_j \to \mathbf{Q}_h$ in $H^1_{loc}\left(\mathbb{R}^3\right)$ and $\mathbf{Q}_h \in W^{1,2}_{loc}\left(\mathbb{R}^3, \mathbb{S}^4\right)$ is a minimizing harmonic map. By the regularity theory of minimizing harmonic maps [31], the map $\mathbf{Q}_h$ is smooth away from a locally finite set and indeed $\mathbf{Q}_h \in C^\infty(\mathbb{R}^3; \mathbb{S}^4)$ by the constancy of stable tangent maps into spheres proven in [33]. Further, we have the energy bound, $\int_{B_R} |\nabla \mathbf{Q}_h|^2 \leq CR$ for a positive constant C, by the monotonicity formula which allows us to blow-down $\mathbf{Q}_h$ from infinity. Thus, $\mathbf{Q}_h$ has minimizing tangent maps at infinity and the rescaled harmonic maps converge strongly to the tangent maps (up to a subsequence) by Luckhaus compactness theorem for harmonic maps. We use the constancy of stable tangent maps into spheres from [33] and the monotonicity formula, arguing by analogy with case (b), to infer that $\mathbf{Q}_h$ is a constant matrix of norm one. In view of this constancy property, we can improve the convergence $\hat{\mathbf{Q}}_j \to \mathbf{Q}_h$ in $H^1_{loc}\left(\mathbb{R}^3\right)$ to a smooth convergence (we just need to use the argument based on the Bochner inequality from (i) above). Since biaxiality is constant for constant maps, we contradict (61).

Finally, we consider the regime (d) $t_j^{-1/4} << d_j << 1$. Here, the limiting energy is again the Dirichlet energy, $\int |\nabla \mathbf{Q}|^2 \, dV$, for $\mathbf{Q}_{min}$-valued maps in $H^1_{\mathrm{loc}}(\mathbb{R}^3)$, as can be seen by applying Fatou's Lemma to (62). We again have $\hat{\mathbf{Q}}_j \to \mathbf{Q}_h$ in $H^1_{loc}\left(\mathbb{R}^3\right)$, arguing similarly to part (c) above. However, from the uniaxiality of the limiting tensor and the lifting results in [3], we lift

$\mathbf{Q}_h$ to an $\mathbb{S}^2$-valued minimizing harmonic map $\bar{\mathbf{n}} \in H^1_{loc}(\mathbb{R}^3;\mathbb{S}^2)$. From the classification result for harmonic unit-vector fields, such as $\bar{\mathbf{n}}$, in [1, Thm. 2.2], we either have $\mathbf{Q}_h = constant$ or $\mathbf{Q}_h = \sqrt{\frac{3}{2}}\left(\frac{\mathbf{x}\otimes\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3}\right)$, again as in step (c) with locally smooth convergence except at most at one point (combining the smoothness of the limiting map with small energy regularity to infer smooth convergence). This contradicts (61) since $\beta^2(\mathbf{Q}_h) = 0$ everywhere except possibly for the origin, since $\mathbf{Q}_h$ is uniaxial for $\mathbf{x} \neq \mathbf{0}$.

□

Proof of Theorem 2. We can prove the existence of a global LdG minimizer $\mathbf{Q}_j$, of the re-scaled energy (14), in the restricted class of uniaxial $\mathbf{Q}$-tensors, for each t_j, from the direct methods in the calculus of variations. It suffices to note that the uniaxiality constraint, $6\left(\mathrm{tr}\mathbf{Q}^3\right)^2 = |\mathbf{Q}|^6$ is weakly closed and the existence result follows immediately.

The limiting harmonic map $\mathbf{Q}^0$ is uniaxial and hence, the energy bound (19) follows immediately since the upper bound is simply the re-scaled LdG energy of $\mathbf{Q}^0$. The uniaxial map, $\mathbf{Q}_j = s_j\left(\mathbf{n}_j \otimes \mathbf{n}_j - \frac{\mathbf{I}}{3}\right)$, necessarily has non-negative scalar order parameter. Indeed, note that by uniaxiality, $\det \mathbf{Q}(x) > 0$ (resp. $\det \mathbf{Q}(x) < 0$) iff $\mathbf{Q}(x)$ has positive (resp. negative) scalar order parameter and also that $\det \mathbf{Q}(x) = 0$ iff $\mathbf{Q}(x) = 0$ at any $x \in \Omega$. We set $\Omega_j := \{\det \mathbf{Q}_j(x) < 0\} \subset \Omega$, which is an open subset (possibly empty), since $\mathbf{Q}_j$ is globally Lipschitz in Ω. If $\Omega_j \neq \emptyset$, then we define the uniaxial admissible perturbation

$$\mathbf{Q}^*_j(\mathbf{r}) = \begin{cases} \mathbf{Q}_j & \mathbf{r} \in \Omega \setminus \Omega_j \\ -\mathbf{Q}_j & \mathbf{r} \in \Omega_j \end{cases} \tag{63}$$

and one can easily check that $\mathbf{Q}^*_j$ is globally Lipschitz in Ω and $\frac{3\bar{L}}{2Ls_+^2}\mathbf{I}^j_{LG}[\mathbf{Q}^*_j] < \frac{3\bar{L}}{2Ls_+^2}\mathbf{I}^j_{LG}[\mathbf{Q}_j]$, contradicting the assumed global minimality of $\mathbf{Q}_j$ in the restricted class of uniaxial $\mathbf{Q}$-tensors. We can then appeal to Proposition 2.1 and proceed by contradiction. We assume that the global LdG-minimizers, $\mathbf{Q}_j$, in the restricted class of uniaxial $\mathbf{Q}$-tensors, are stable critical points of the LdG energy, for j large enough. The sequence, $\{\mathbf{Q}_j\}$, then satisfies the hypothesis of Proposition 2.1, for large j. We thus, conclude that each $\mathbf{Q}_j$, has a set of isotropic points $\mathbf{x}^{(j)}_i$ (at least one near each singular point $\mathbf{x}_i$ of $\mathbf{Q}^0$) and $\mathbf{Q}_j$ is asymptotically described by the RH-profile near each isotropic point $\mathbf{x}^{(j)}_i$ as $j \to \infty$ in the sense of Proposition 2.1. Recall that the RH-solution, (20) is known to be unstable with respect to biaxial perturbations localized around the origin [20], [25]. This suffices to prove that global minimizers in the restricted class of uniaxial $\mathbf{Q}$-tensors cannot be stable critical points of the LdG energy in the low-temperature limit, since stability of $\mathbf{Q}_j$ would pass to the limit under smooth convergence. □

Proof of Proposition 2.1. Proof of (i): By Propositions 3.1 and 3.2, after extracting a subsequence, we have that $\{\mathbf{Q}_j\}$ converges strongly in $W^{1,2}$ and uniformly away from the singular set $\Sigma = \{\mathbf{x}_1 \dots \mathbf{x}_N\}$, to a (minimizing) limiting harmonic map, $\mathbf{Q}^0$. We prove that for each $i = 1, \dots, N$ and every fixed $r_0 > 0$ sufficiently small, there exists $j_0 \in \mathbb{N}$ such that for every $j \geq j_0$, the map $\mathbf{Q}_j$ has an isotropic point, $\mathbf{x}_i^{(j)}$, in $\overline{B}(\mathbf{x}_i, r_0)$. The stated conclusion then follows by a diagonal argument on r_0. Suppose, for a contradiction, that we can find a subsequence, $\{j_k\}_{k\in\mathbb{N}}$, such that $\min_{B(\mathbf{x}_i, r_0)} |\mathbf{Q}_{j_k}| > 0$ for all $k \in \mathbb{N}$. Since $\mathbf{Q}_j$ is purely uniaxial for all j by assumption, we have that $\frac{\mathbf{Q}_{j_k}}{|\mathbf{Q}_{j_k}|}$ is continuous on $\overline{B(\mathbf{x}_i, r_0)}$ and the uniform convergence to $\mathbf{Q}^0$ implies that $\frac{\mathbf{Q}_{j_k}}{|\mathbf{Q}_{j_k}|}$ converges uniformly to $\mathbf{Q}^0$ on ∂B_ϵ. Arguing as in the proof of Theorem 1 (iv) we obtain a contradiction.

Proof of (ii): The aim is to prove that $\mathbf{Q}_j$ has a radial-hedgehog type of profile, (20), near each singular point in Σ, for j sufficiently large. The proof follows from Lemma 3.6 and Propositions 4 and 8 in [14]. We begin by noting that for each $i = 1 \dots N$ in $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, we can extract a sequence, $\left\{\mathbf{x}_j^*\right\}$, such that $\mathbf{Q}_j\left(\mathbf{x}_j^*\right) = 0$ and $\mathbf{x}_j^* \to \mathbf{x}_i$ as $j \to \infty$. By Lemma 3.6, the rescaled maps (49) converges in $\bigcap_{k\in\mathbb{N}} C^k_{\text{loc}}$ to a classical solution $\tilde{\mathbf{Q}}^\infty$ of the Ginzburg-Landau equations satisfying the energy growth (50). Moreover, it can be seen that $\tilde{\mathbf{Q}}^\infty$ is uniaxial and has a non-negative scalar order parameter. Finally $\tilde{\mathbf{Q}}^\infty(\mathbf{0}) = \mathbf{0}$ because $\tilde{\mathbf{Q}}_{j_k}(0) = \mathbf{0}$ for each k, by assumption. We conclude that the hypotheses of [14, Prop. 8] are satisfied. We reproduce the statement of [14, Prop. 8] below, for completeness.

Proposition 3.7 (Proposition 8, [14])**.** *Let $\mathbf{Q} \in C^2(\mathbb{R}^3; S_0)$ be a uniaxial solution of $\Delta\mathbf{Q} = (|\mathbf{Q}|^2 - 1)\mathbf{Q}$ with $\mathbf{Q}(0) = 0$ and non-negative scalar order parameter, satisfying the energy bound* (50)*. Let h denote the unique solution for the boundary-value problem* (21)*. Then there exists an orthogonal matrix $\mathbf{T} \in \mathcal{O}(3)$ such that*

$$\mathbf{Q}(\mathbf{x}) = \sqrt{\frac{3}{2}}h(|\mathbf{x}|)\left(\frac{\mathbf{T}\mathbf{x} \otimes \mathbf{T}\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3}\right), \quad \mathbf{x} \in \mathbb{R}^3. \tag{64}$$

This yields the conclusion of Proposition 2.1.

□

4 Conclusions

Theorem 1 focuses on global minimizers of the LdG energy on arbitrary 3D domains, with arbitrary topologically non-trivial Dirichlet conditions, for low temperatures. We prove that global minimizers are "almost" uniaxial everywhere away from the singular set of a (minimizing) limiting harmonic map, $\mathbf{Q}^0$. Further, we prove that global minimizers have at least a point of maximal biaxiality (with $\beta^2 = 1$) and a point of pure uniaxiality (with $\beta^2 = 0$) near each singular point of $\mathbf{Q}^0$ and their norm converges uniformly to unity everywhere, for low temperatures. This yields quantitative information about the expected number and location of points of maximal biaxiality and provides rigorous justification for the widely used Lyuksyutov constraint for the LdG energy in the low-temperature limit, suggesting that we may be able to analytically recover the celebrated biaxial torus solution [13, 16, 34, 30] by a blow-up analysis of the LdG energy using scalings related to the decay estimate of strongly biaxial regions derived in Theorem 1. Recall that the biaxial torus solution (numerically) exhibits a ring of maximal biaxiality and defect cores with uniaxial states that have negative order parameter and from the results in Theorem 1, we conjecture that we may find a biaxial torus solution near each singular point of a (minimizing) limiting harmonic map.

Theorem 2 focuses on global LdG minimizers within the restricted class of uniaxial $\mathbf{Q}$-tensors for low temperatures. These constrained uniaxial minimizers exist although they need not be critical points of the LdG energy. Indeed, uniaxial critical points of (11) are, in general, difficult to find. In [18], the author excludes purely uniaxial critical points of the LdG energy in 1D and 2D but the radial-hedgehog (RH) solution is a 3D uniaxial critical point of the LdG energy i.e. is a solution of the system (11) of the form (3) with $s > 0$ for $r > 0$. Indeed, one could imagine a continuous uniaxial perturbation of the RH solution that remains a solution of the system (11). An alternative scenario is that we glue together several copies of the RH solution, with a weak uniaxial perturbation of a limiting harmonic map interpolating between the distinct RH-copies, to yield an uniaxial solution of (11), at least in some approximate sense. Proposition 2.1 (of which constrained uniaxial minimizers are a special case) has a two-fold purpose: (i) firstly, it rules out the stability of such uniaxial critical points, if they can be constructed and (ii) secondly and perhaps more importantly, it establishes the universal RH-type defect profiles for uniaxial critical points (if they exist) of the LdG energy for low temperatures.

We conjecture that the universal RH-type defect profile is generic for sequences of uniaxial critical points that converge strongly to a (minimizing) limiting harmonic map, under some physically relevant hypotheses which maybe different in different asymptotic limits. For example, we can consider a sequence of physically relevant uniaxial critical points in the vanishing elastic constant limit $L \to 0$. Here, physical relevance can again be understood in terms of non-negative scalar order parameter and an appropriate energy bound. The $L \to 0$ limit has been well-studied in [22] and we can appeal to Lemmas $6-7$ of [22] or Case I of Theorem 1[(i)] to deduce that the uniaxial sequence converges uniformly to a limiting (minimizing) harmonic map, $\mathbf{Q}^0$, away from the singular set of $\mathbf{Q}^0$. We conjecture that one can repeat the arguments in Proposition 2.1 to deduce (i) the existence of an isotropic point near each singular point, $\mathbf{x}_i$, of $\mathbf{Q}^0$ and (ii) the local RH-type defect profile near each such isotropic point. We hope to make rigorous studies of uniaxial and biaxial defect profiles, in different temperature regimes, in future work.

Acknowledgements

AM is supported by an EPSRC Career Acceleration Fellowship EP/J001686/1 and EP/J001686/2, an Oxford Centre for Industrial Applied Mathematics (OCIAM) Visiting Fellowship and association with the Advanced Studies Centre, Keble College, Oxford. DH is supported by FONDECYT project n° 1150038 from the Chilean Ministry of Education. AP thanks OCCAM for supporting his collaborative visit in March 2012. DH thanks OxPDE, University of Oxford, for financial support in October 2012. DH, AM thank the Mathematics of Liquid Crystals Research Programme for supporting their stay at the Isaac Newton Institute, University of Cambridge in April 2013. We thank Giacomo Canevari and Arghir Zarnescu for helpful discussions.

References

[1] F. J. Almgren and E. Lieb. Singularities of energy minimizing maps from the ball to the sphere: examples, counterexamples, and bounds. *Ann. of Math.*, 128:483 – 530, 1988.

[2] A.Pisante. Two results on the equivariant Ginzburg-Landau vortex in arbitrary dimension. *J. Funct. Anal.*, 260:892 – 905, 2011.

[3] J.M. Ball and A. Zarnescu. Orientability and energy minimization for liquid crystals. *Arch. Rational Mech. Anal.*, 202(2):493–535, 2011.

[4] F. Bethuel, H. Brezis, and F. Hélein. Asymptotics for the minimizers of a Ginzburg-Landau functional. *Calc. Var. and Partial Differential Equations*, 1:123–148, 1993.

[5] H. Brezis, J.-M. Coron, and E. Lieb. Harmonic maps with defects. *Comm. Math. Phys.*, 107:649–705, 1986.

[6] Haim Brezis. *Degree theory: old and new. Topological nonlinear analysis, II.* Birkhuser Boston, Boston, MA, 1997.

[7] G. Canevari. Biaxiality in the asymptotic analysis of a 2D Landau-de Gennes model for liquid crystals. *ESAIM: Control, Optimisation and Calculus of Variations*, 21:101–137, 2015.

[8] S. J. Chapman, S. D. Howison, and J. R. Ockendon. Macroscopic models for superconductivity. *SIAM Rev.*, 34:529–560, 1992.

[9] Andres Contreras and Xavier Lamy. Biaxial escape in nematics at low temperature. *http://arxiv.org/abs/1405.2055*, 2014.

[10] P. G. de Gennes. *The physics of liquid crystals.* Clarendon, Oxford, 1974.

[11] L. Evans. *Partial Differential Equations.* American Mathematical Society, Providence, 1998.

[12] A. Fernandez-Nieves, V. Vitelli, A. S. Utada, D. R. Link, M. Marquez, D. R. Nelson, and D. A. Weitz. Novel defect structures in nematic liquid crystal shells. *Phys. Rev. Lett.*, 99:157801, 2007.

[13] E. C. Gartland and S.Mkaddem. On the local instability of radial hedgehog configurations in nematic liquid crystals under Landau-de Gennes free-energy models. *Phys. Rev. E.*, 59:563–567, 1999.

[14] D. Henao and A. Majumdar. Symmetry of uniaxial global Landau-de Gennes minimizers in the theory of nematic liquid crystals. *SIAM J. Math. Anal.*, 44:3217–3241, 2012.

[15] M. Kleman and O. D. Lavrentovich. *Soft Matter Physics: An Introduction.* Springer, New York, 2003.

[16] S. Kralj and E. Virga. Universal fine structure of nematic hedgehogs. *J. Phys. A*, 34:829–838, 2001.

[17] Xavier Lamy. Some properties of the nematic radial hedgehog in the Landau-de Gennes theory. *Journal of Mathematical Analysis and Applications*, 397:586–594, 2013.

[18] Xavier Lamy. Uniaxial symmetry in nematic liquid crystals. *Annales de l'Institut Henri Poincare (C) Non Linear Analysis*, In press, 2014.

[19] F. H. Lin and C. Liu. Static and dynamic theories of liquid crystals. *J. Partial Differential Equations*, 14:289–330, 2001.

[20] A. Majumdar. Equilibrium order parameters of liquid crystals in the Landau-de Gennes theory. *Eur. J. Appl. Math.*, 21:181–203, 2010.

[21] A. Majumdar. The radial-hedgehog solution in the Landau-de Gennes theory for nematic liquid crystals. *Eur. J. Appl. Math.*, 23:61–97, 2012.

[22] A. Majumdar and A. Zarnescu. The Landau-de Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond. *Arch. Ration. Mech. and Anal.*, 196:227–280, 2010.

[23] V. Millot and A. Pisante. Symmetry of local minimizers for the Ginzburg-Landau functional in 3D. *J. Eur. Math. Soc.*, 12:1069–1096, 2010.

[24] P. Mironescu. Les minimiseurs locaux pour l'équation de Ginzburg-Landau sont à symétrie radiale. *C. R. Acad. Sci. I - Math.*, 323:593–598, 1996.

[25] S. Mkaddem and E. C. Gartland. Fine structure of defects in radial nematic droplets. *Phys. Rev. E*, 62:6694–6705, 2000.

[26] N.J.Mottram and C.Newton. Introduction to **Q**-tensor theory. Research Report 10, University of Strathclyde, Department of Mathematics, 2004.

[27] F. Pacard and T. Rivière. *Linear and nonlinear aspects of vortices. The Ginzburg-Landau model.* Birkhäuser, Boston, 2000.

[28] G. Panati and A.Pisante. Bloch bundles, Marzari-Vanderbilt functional and maximally localized Wannier functions. *Comm. Math. Phys.*, 322:835–875, 2013.

[29] L. A. Parry-Jones and S. J. Elston. Flexoelectric switching in a zenithally bistable nematic device. *J. Appl. Phys.*, 97:093515, 2005.

[30] E. Penzenstadler and H.-R.Trebin. Fine structure of point defects and soliton decay in nematic liquid crystals. *J. Phys. France*, 50:1027–1040, 1989.

[31] R. Schoen and K. Uhlenbeck. A regularity theory for harmonic maps. *J. Diff. Geom.*, 17:307–335, 1982.

[32] R. Schoen and K. Uhlenbeck. Boundary regularity and the Dirichlet problem for harmonic maps. *J. Diff. Geom.*, 18:253–268, 1983.

[33] R. Schoen and K. Uhlenbeck. Regularity of minimizing harmonic maps into the sphere. *Invent. Math.*, 78:89–100, 1984.

[34] N. Schopohl and T. J. Sluckin. Defect core structure in nematic liquid crystals. *Phys. Rev. Lett.*, 59:2582–2585, 1987.

[35] E. G. Virga. *Variational theories for liquid crystals.* Chapman and Hall, London, 1994.