Uniaxial versus Biaxial Character of Nematic Equilibria in Three Dimensions

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Abstract

We study defect structures in global minimizers of the Landau-de Gennes energy on arbitrary three-dimensional (3D), simply connected geometries with physically realistic Dirichlet boundary conditions. We prove that global Landau-de Gennes minimizers must be biaxial for sufficiently low temperatures. This follows from (i) a rigorous local characterization of defect profiles in uniaxial critical points that satisfy an energy bound, in terms of the well-known radial-hedgehog (RH) solution and (ii) the local instability of the RH solution with respect to biaxial perturbations for low temperatures.

1 Introduction

Nematic liquid crystals (LCs) are anisotropic liquids wherein the constituent rod-shaped molecules exhibit a degree of long-range orientational order [7, 28]. Nematic LC textures often exhibit intricate defect patterns, the commonest examples being Schlieren textures with striking optical properties [12], [4, 9]. These defect patterns are generic in condensed matter systems and are a source of fascinating new problems for analysts, physicists and engineers. Equally importantly, defects play a crucial role in non-equilibrium dynamic processes such as switching mechanisms in LC devices, examples of which can be found in [23].

The mathematics of LC defects offers plenty of open non-trivial questions, particularly related to the structure of a defect core, the energy concentration within defects, stability of defect structures and pattern formation etc. [1], [18], [22], [6]. In a previous paper, we study defect structures within three-dimensional spherical nematic droplets with homeotropic or radial boundary conditions, for low temperatures well below the nematic-isotropic transition temperature [11]. This model problem has been widely studied in the literature, particularly within the powerful continuum Landau-de Gennes (LdG) theory for LCs [10], [24], [26], [27], [13]. It is generally believed that there are two competing static equilibria for this model problem, (i) the radial-hedgehog solution (RH) and (ii) the biaxial torus (BT) solution. The RH solution is analogous to a degree $+1$-vortex in superconductivity [22]. It is a perfectly uniaxial, spherically symmetric solution with a single distinguished direction of molecular alignment, referred to as the director. The RH director is identically aligned along the radial unit-vector with an isolated, isotropic point at the droplet centre. The LC state loses all orientational order at the isotropic point and consequently, the isotropic point is interpreted to be a defect point. The BT solution has lesser symmetry than the RH solution i.e. it is not radially symmetric about the droplet centre but has a biaxial band, with two distinguished directions of molecular alignment, around the droplet centre. It is analytically and numerically known that the RH solution is unstable with respect to higher-dimensional biaxial perturbations for low temperatures and the asymmetric BT solution is energetically preferable to the RH solution for low temperatures [10, 13, 27, 26]. However, this does not exclude the existence of other competing uniaxial equilibria which may have lower energy than both the RH and BT solutions.

It has long been believed that the RH solution is the unique uniaxial candidate for a LdG energy minimizer on a 3D spherical droplet with radial boundary conditions for sufficiently low temperatures and we give rigorous results in support of this conjecture in [11]. In [11], we adapt the division trick in [19] and the radial symmetry results for the Ginzburg-Landau theory for superconductivity [2, 18], to the LdG theory for nematic LCs. We prove that if a global LdG minimizer is indeed uniaxial, for a 3D spherical droplet with radial boundary conditions, then the uniaxial minimizer must have a point isotropic defect near the droplet centre and the local structural profile is indeed described by the RH solution (modulo a rotation), in the low-temperature limit. This combined with the known instability of the RH solution with respect to biaxial perturbations [15, 20] suffices to prove that global LdG minimizers cannot be purely uniaxial i.e. must be biaxial, for sufficiently low temperatures.

In this paper, we generalize the results in [11] to an arbitrary 3D simply-connected geometry with topologically non-trivial, physically realistic Dirichlet conditions. We follow the same strategy as in [11]. We assume the existence of a sequence of uniaxial global LdG minimizers for low temperatures and exploit the assumed uniaxial structure to prove that the uniaxial sequence converges strongly (in the Sobolev space $W^{1,2}$) to a minimizing, limiting harmonic map. The topologically non-trivial Dirichlet boundary condition necessarily implies that every uniaxial minimizer must have an isotropic or zero set and the strong convergence result gives us precise information about the localization of the zero/isotropic set near the singular set of the limiting harmonic map, for low temperatures. We then adapt the methods in [11] to *locally* resolve the defect profile and recover the RH profile *locally* near the isotropic points of the assumed uniaxial minimizer. This local characterization of defect profiles in uniaxial minimizers, when combined with the known instability of the RH solution with respect to biaxial perturbations, suffices to prove our main result: global LdG minimizers cannot be purely uniaxial for low temperatures. In other words, biaxiality is not an artefact of a special geometry and choice of boundary conditions as in [11] but is generic for low temperatures and 3D simply-connected geometries, for physically realistic topologically non-trivial Dirichlet conditions.

There are two main new mathematical ingredients in this paper: (i) a Bochner-type inequality (analogous to inequalities derived in [17]) for uniaxial minimizers in the low-temperature limit that allows us to prove the existence of (at least) one isotropic point near each singular point of the minimizing limiting harmonic map and (ii) a local energy quantization result near each singular point of the limiting harmonic map [5] which reduces the local analysis near each isotropic point to the model problem of a 3D spherical droplet with radial boundary conditions as in [11]. In particular, our main result is a 3D result that is independent of the the details of the geometry, except for simply-connectedness. Mathematically, these tools set up analytic machinery for 'zooming into' or 'blowing up' the defect core. Indeed, these results reveal the Ginzburg-Landau-type character of uniaxial equilibria and allow us to identify the mathematical differences in the analysis of uniaxial and biaxial equilibria. From a practical point of view, the uniaxial versus biaxial character of LC equilibria is a question of great interest in the physical sciences community [7, 10, 21, 28]. In particular, biaxiality may offer new possibilities for LC-based applications and rigorous analysis on these lines, such as ours, may aid future experimental work. For example, we believe that our methods can be generalized to polymer dispersed LC systems and systems with enlarged defect cores e.g. LC systems in external fields, macro-molecular systems etc.

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 [17]

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

and we use the Einstein summation convention throughout the paper.

We work with the Landau-de Gennes (LdG) theory for nematic liquid crystals [7] whereby a LC state is described by a macroscopic order parameter: the **Q**-tensor order parameter. The **Q**-tensor is a macroscopic measure of the LC anisotropy. Mathematically, the LdG **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 **Q** has two degenerate non-zero eigenvalues and (iii) biaxial when **Q** has three distinct eigenvalues. The LdG theory is a variational theory and has an associated LdG free energy. The LdG energy density is a nonlinear function of **Q** and its spatial derivatives [7, 21]. 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 [17, 21] :

$$\mathbf{I_{LG}}\left[\mathbf{Q}\right] = \int_\Omega \frac{L}{2}|\nabla \mathbf{Q}|^2 + f_B\left(\mathbf{Q}\right)\ dV. \tag{3}$$

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 phase of the nematic configuration : isotropic/uniaxial/biaxial. For our purposes, we take f_B to be a quartic polynomial in the $\mathbf{Q}$-tensor invariants:

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

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 [21, 15]. 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 [15, 16]

$$\mathbf{Q}_{\min} = \left\{\mathbf{Q} \in S_0; \mathbf{Q} = s_+\left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}}{3}\right),\ \mathbf{n} \in \mathbb{S}^2\right\}, \tag{5}$$

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

$$s_+ = \frac{B + \sqrt{B^2 + 24|A|C}}{4C}. \tag{6}$$

Our aim is to study the uniaxial versus biaxial character of defect cores in global minimizers and critical points of the LdG energy in (3), subject to topologically non-trivial Dirichlet boundary conditions. In what follows, we take the Dirichlet boundary condition to be

$$\mathbf{Q}_{b,A}(\mathbf{x}) = s_+\left(\mathbf{n}_b \otimes \mathbf{n}_b - \frac{\mathbf{I}}{3}\right) \tag{7}$$

for some arbitrary smooth unit-vector field, $\mathbf{n}_b$, with topological degree $d \neq 0$ (see, e.g., [1] for the definition and the main properties of the topological degree).We take our admissible space to be

$$\mathcal{A}_A = \left\{\mathbf{Q} \in W^{1,2}\left(\Omega; S_0\right); \mathbf{Q} = \mathbf{Q}_{b,A} \text{ on } \partial\Omega\right\}, \tag{8}$$

where $W^{1,2}(\Omega; S_0)$ is the Soboblev space of square-integrable $\mathbf{Q}$-tensors with square-integrable first derivatives [8], with norm

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

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 [8]; 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,

$$L\Delta\mathbf{Q} = A\mathbf{Q} - B\left(\mathbf{Q}^2 - \left(\mathrm{tr}\mathbf{Q}^2\right)\frac{\mathbf{I}}{3}\right) + C\left(\mathrm{tr}\mathbf{Q}^2\right)\mathbf{Q}, \tag{9}$$

where $\frac{B}{3}\left(\mathrm{tr}\mathbf{Q}^2\right)\frac{\mathbf{I}}{3}$ is a Lagrange multiplier accounting for the tracelessness constraint [17].

We recall a few definitions from [10, 11, 17] to motivate and state our main results.

Definition 1. *Let Ω be a measurable subset of $\mathbb{R}^3$. We say that a tensor-valued map, $\mathbf{Q} : \Omega \to S_0$, is purely uniaxial if $\mathbf{Q}(\mathbf{x})$ can be written as*

$$\mathbf{Q}(\mathbf{x}) = s(\mathbf{x})\left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{\mathbf{I}}{3}\right), \tag{10}$$

for some $s(\mathbf{x}) \in \mathbb{R}$ and some unit-vector $\mathbf{n}(\mathbf{x}) \in \mathbb{S}^2$, for a.e. $\mathbf{x} \in \Omega$. 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.

The set (5) is the set of uniaxial $\mathbf{Q}$-tensors with constant order parameter, s_+. Next, we recall the definitions of the *reduced temperature* t, the *uniaxial nematic correlation length* ξ_b and a *limiting harmonic map* as shown below

$$t = \frac{27|A|C}{B^2}, \qquad \xi_b = \sqrt{\frac{L}{|A|}} = \sqrt{\frac{27CL}{B^2 t}}. \tag{11}$$

Definition 2. *A (minimizing) limiting harmonic map with respect to the Dirichlet condition* (7) *is a uniaxial map of the form*

$$\mathbf{Q}^0 = \sqrt{\frac{3}{2}}\left(\mathbf{n}^0 \otimes \mathbf{n}^0 - \frac{\mathbf{I}}{3}\right), \tag{12}$$

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

$$I[\mathbf{n}] = \int_\Omega |\nabla\mathbf{n}|^2 \, dV \tag{13}$$

in the admissible space $\mathcal{A}_{\mathbf{n}_b} = \left\{\mathbf{n} \in W^{1,2}\left(\Omega; \mathbb{S}^2\right); \mathbf{n} = \mathbf{n}_b \text{ on } \partial\Omega\right\}$ [25].

Our two main theorems are:

Theorem 1. *Let $\Omega \subset \mathbb{R}^3$ be simply-connected, open, bounded, and with a smooth boundary. Let $\{A_j\}_{j\in\mathbb{N}}$ and $\{\mathbf{Q}_j\}_{j\in\mathbb{N}}$ be such that*

- $A_j \overset{j\to\infty}{\longrightarrow} -\infty$,
- *for each $j \in \mathbb{N}$, $\mathbf{Q}_j \in \mathcal{A}_{A_j}$ is a critical point of the LdG energy i.e. is an analytic solution of the Euler-Lagrange equations (9),*
- *for each $j \in \mathbb{N}$, $\mathbf{Q}_j$ is uniaxial with non-negative scalar order parameter as shown below:*

$$\mathbf{Q}_j(\mathbf{x}) = s_j(\mathbf{x}) \left(\mathbf{n}_j(\mathbf{x}) \otimes \mathbf{n}_j(\mathbf{x}) - \frac{\mathbf{I}}{3} \right), \tag{14}$$

for some $s_j(\mathbf{x}) \geq 0$ and a unit-vector field $\mathbf{n}_j(\mathbf{x}) \in \mathbb{S}^2$, for a.e. $\mathbf{x} \in \Omega$,

- *for each $j \in \mathbb{N}$, $\mathbf{Q}_j$ satisfies the following energy bound*

$$\limsup_{j\to\infty} \frac{1}{s_+^2} \mathbf{I_{LG}}[\mathbf{Q}_j] \leq L \left(\inf_{\mathbf{n}\in\mathcal{A}_{\mathbf{n}_b}} I[\mathbf{n}] \right), \tag{15}$$

with $I[\mathbf{n}]$ and $\mathcal{A}_{\mathbf{n}_b}$ as in (13).

Then, passing to a subsequence (still indexed by j),

(i) as $j \to \infty$, the rescaled maps, $\left\{ \frac{1}{s_+}\sqrt{\frac{3}{2}}\mathbf{Q}_j \right\}$, converge strongly in $W^{1,2}(\Omega; S_0)$, to a (minimizing) limiting harmonic map $\bar{\mathbf{Q}}^0 = \sqrt{\frac{3}{2}}\left(\mathbf{n}^0 \otimes \mathbf{n}^0 - \frac{\mathbf{I}}{3}\right)$, such that $\bar{\mathbf{Q}}^0$ has a finite number of isolated, interior point defects, $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, with $N \geq d$ (where d is the topological degree of the field $\mathbf{n}_b$ defined in (7)), in Ω,

(ii) $\frac{1}{s_+}\sqrt{\frac{3}{2}}|\mathbf{Q}_j(\mathbf{x})| \overset{j\to\infty}{\longrightarrow} 1$ for every $\mathbf{x} \in \Omega \setminus \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, the convergence being uniform in every compact set $K \subset \overline{\Omega} \setminus \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$,

(iii) given any compact set $K \subset \Omega \setminus \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, there exists a constant C, depending only on K, such that $\frac{1}{s_+}\sqrt{\frac{3}{2}}\|\nabla\mathbf{Q}_j\|_{L^\infty(K)} \leq C$, for all $j \in \mathbb{N}$,

(iv) 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* $\mathbf{x}_i^{(j)} \xrightarrow{j\to\infty} \mathbf{x}_i$*,*

(v) 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* $\left\{\tilde{\mathbf{x}} \mapsto \frac{1}{s_+}\sqrt{\frac{3}{2}}\mathbf{Q}_{j_k}\left(\mathbf{x}^{(j_k)} + \xi_b\tilde{\mathbf{x}}\right)\right\}_{k\in\mathbb{N}}$ *converge to*

$$\mathbf{H}_{\mathbf{T}}(\tilde{\mathbf{x}}) := \sqrt{\frac{3}{2}}h(|\tilde{\mathbf{x}}|)\left(\frac{\mathbf{T}\tilde{\mathbf{x}} \otimes \mathbf{T}\tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^2} - \frac{\mathbf{I}}{3}\right), \quad \tilde{\mathbf{x}} \in \mathbb{R}^3, \tag{16}$$

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*

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h^3 - h, \qquad h(0) = 0, \qquad \lim_{r\to\infty} h(r) = 1. \tag{17}$$

Theorem 1 gives us 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 simply given by

$$\mathbf{H}(\tilde{\mathbf{x}}) := \sqrt{\frac{3}{2}}h(|\tilde{\mathbf{x}}|)\left(\frac{\tilde{\mathbf{x}} \otimes \tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^2} - \frac{\mathbf{I}}{3}\right), \quad \tilde{\mathbf{x}} \in \mathbb{R}^3 \tag{18}$$

where h is defined as in (17). The boundary-value problem (17) has been studied in detail in [14, 16], in connection to existence and qualitative properties of solutions. The RH solution is locally unstable with respect to biaxial perturbations, as has been demonstrated in [15, 20]. Hence, we conclude that

Theorem 2. *Let* $\Omega \subset \mathbb{R}^3$ *be simply-connected, open, bounded, and with a smooth boundary. There exists* $A_0 < 0$ *such that for every* $A < A_0$*, the minimizer of* $\mathbf{I_{LG}}[\mathbf{Q}]$ *in the space* $\mathcal{A}_A$ *(defined in* (8)*), is not purely uniaxial.*

The proofs of Theorems 1 and 2 frequently require us to recall Propositions 4, 8 and Theorem 3 from [11]. In fact, Theorem 1 is a local version of the global results for a 3D spherical droplet with radial boundary conditions, contained in Propositions 4 and 8 of [11]. For completeness, we recall Propositions 4, 8 and Theorem 3 from [11].

Proposition 2.1. *[Proposition 4, [11]] For each $t > 0$, let $\tilde{\mathbf{Q}}^t \in W^{1,2}(B(0,\tilde{R}_t); S_0)$ be a uniaxial minimizer of the dimensionless LdG energy, $\tilde{\mathcal{I}}_{LG}$, on a re-scaled spherical droplet, $B(0,\tilde{R}_t) = \left\{ \tilde{\mathbf{x}} = \frac{\mathbf{x}}{\xi_b} \in \mathbb{R}^3; |\tilde{\mathbf{x}}| \leq \frac{R_0}{\xi_b} \right\}$, where R_0 is independent of t, ξ_b is the nematic correlation length defined above and*

$$\tilde{\mathcal{I}}_{LG}[\tilde{\mathbf{Q}}] = \int_{B(0,\tilde{R}_t)} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}|^2 - \frac{\operatorname{tr}\tilde{\mathbf{Q}}^2}{2} - \frac{\sqrt{6}h_+}{t}\operatorname{tr}\tilde{\mathbf{Q}}^3 + \frac{h_+^2}{2t}\left(\operatorname{tr}\tilde{\mathbf{Q}}^2\right)^2 + C(t)\ dV. \quad (19)$$

Here $h_+ = \frac{3+\sqrt{9+8t}}{4}$ and $C(t)$ is an additive constant. We add the constant $C(t)$ to ensure that the bulk potential is non-negative. Then, for every sequence $\{t_j\}_{j\in\mathbb{N}}$ with $t_j \to \infty$ as $j \to \infty$, there exists a sequence $\{\tilde{\mathbf{x}}_j^*\}_{j\in\mathbb{N}} \subset \mathbb{R}^3$ such that

(i) $\tilde{\mathbf{x}}_j^* \in B(0,\tilde{R}_{t_j})$ *for each* $j \in \mathbb{N}$ *and* $\lim_{j\to\infty} \frac{\tilde{\mathbf{x}}_j^*}{\tilde{R}_{t_j}} = 0$,

(ii) $\tilde{\mathbf{Q}}^{t_j}(\tilde{\mathbf{x}}_j^*) = 0$ *for every* $j \in \mathbb{N}$,

(iii) $\tilde{\mathbf{Q}}^{t_j}$ *has non-negative scalar order parameter*

(iv) the sequence of maps, $\{\tilde{\mathbf{x}} \mapsto \tilde{\mathbf{Q}}^{t_j}(\tilde{\mathbf{x}} + \tilde{\mathbf{x}}_j^*)\}_{j\in\mathbb{N}}$, has a subsequence that converges to a uniaxial solution, $\tilde{\mathbf{Q}}^\infty \in C^\infty(\mathbb{R}^3; S_0)$, of the Ginzburg-Landau equations (20)

$$\Delta\tilde{\mathbf{Q}} = (|\tilde{\mathbf{Q}}|^2 - 1)\tilde{\mathbf{Q}}, \qquad \tilde{\mathbf{x}} \in \mathbb{R}^3, \quad (20)$$

in $C^k_{\mathrm{loc}}(\mathbb{R}^3; S_0)$ for every $k \in \mathbb{N}$, with $\tilde{\mathbf{Q}}^\infty(0) = 0$ and

$$\frac{1}{R}\int_{B(0,R)} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}^\infty|^2 + \frac{(1-|\tilde{\mathbf{Q}}^\infty|^2)^2}{4}\ dV \leq 12\pi \quad (21)$$

for all $R > 0$.

Proposition 2.2 (Proposition 8, [11])**.** *Let $\mathbf{Q} \in C^2(\mathbb{R}^3; S_0)$ be a uniaxial solution of* (20) *with $\mathbf{Q}(0) = 0$ and non-negative scalar order parameter, satisfying the energy bound* (21)*. Let h denote the unique solution for the boundary-value problem* (17)*. Then there exists an orthogonal matrix $\mathbf{T} \in \mathcal{O}(3)$ such that*

$$\mathbf{Q}(\mathbf{x}) = \sqrt{\frac{3}{2}}h(|\mathbf{x}|)\left(\frac{\mathbf{T}\mathbf{x} \otimes \mathbf{T}\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3}\right), \quad \mathbf{x} \in \mathbb{R}^3. \quad (22)$$

Proposition 2.3 (Radial-hedgehog solution; Theorem 3 [11])**.** *For every t sufficiently large, there exists a unique solution, $h_t : [0, \tilde{R}_t] \to \mathbb{R}$, for the ordinary differential equation*

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h^3 - h + \frac{3h_+}{t}\left(h^3 - h^2\right) \tag{23}$$

subject to the boundary conditions

$$h(0) = 0, \qquad h(\tilde{R}_t) = 1 \tag{24}$$

(recall the definition of h_+ and $\tilde{R}_t = \frac{R_0}{\xi_b}$; for $t = \infty$, the boundary-value problem is to be understood as in (17)). Define the radial-hedgehog solution to be

$$\mathbf{H}^t(\mathbf{x}) = \sqrt{\frac{3}{2}}h_t(r)\left(\frac{\mathbf{x}\otimes\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3}\right). \tag{25}$$

Then $\mathbf{H}^t$ is a solution of the Euler-Lagrange equations associated with the dimensionless LdG energy in (19) and there exists a $t^* > 0$, such that $\mathbf{H}^t$ is an unstable equilibrium of $\tilde{\mathcal{I}}_{LG}$ for all $t > t^*$.

3 Proof of the theorems

Proof of Theorem 1. Part (i) is proved as [11, Prop. 2]; we sketch the proof for completeness. Define the re-scaled maps, $\bar{\mathbf{Q}}_j := \frac{1}{s_+}\sqrt{\frac{3}{2}}\mathbf{Q}_j$. Let

$$t_j := \frac{27|A_j|C}{B^2}, \quad h_+ = \frac{3+\sqrt{9+8t_j}}{4}, \xi_b = \sqrt{\frac{27LC}{B^2t}} \quad \text{and} \quad \bar{L} := \frac{27C}{2B^2}L. \tag{26}$$

Then

$$s_+ = \frac{B}{3C}h_+ \tag{27}$$

and the minimum of the bulk energy density, f_B in (4), is

$$\min_{\mathbf{Q}\in S_0} f_B\left(\mathbf{Q}\right) = -\frac{1}{8}\left(t + h_+\right). \tag{28}$$

The sequence $\left\{\bar{\mathbf{Q}}_j\right\}$ is uniaxial by assumption. By [3, 11] (see for example Lemma 1 in [11]), $\bar{\mathbf{Q}}$ is uniaxial if and only if $\left(\operatorname{tr}\bar{\mathbf{Q}}^2\right)^3 = 6\left(\operatorname{tr}\bar{\mathbf{Q}}^3\right)^2$. Since

$\bar{\mathbf{Q}}_j$ has non-negative scalar order parameter by assumption (for each j), we necessarily have that

$$\operatorname{tr}\bar{\mathbf{Q}}^3 = \frac{|\bar{\mathbf{Q}}|^3}{\sqrt{6}}.$$

The re-scaled LdG energy functional for the uniaxial sequence, $\{\bar{\mathbf{Q}}_j\}$, is then given by

$$\frac{3\bar{L}}{2Ls_+^2}\mathbf{I}_{LG}^j[\bar{\mathbf{Q}}_j] = \int_\Omega \frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}_j|^2 + t_j\bar{g}_j(\bar{\mathbf{Q}}_j)\ dV, \tag{29}$$

where

$$\bar{g}_j(\bar{\mathbf{Q}}_j) := \frac{1}{8}\left(1-|\bar{\mathbf{Q}}_j|^2\right)^2 + \frac{h_+}{8t_j}(1+3|\bar{\mathbf{Q}}_j|^4 - 4|\bar{\mathbf{Q}}_j|^3). \tag{30}$$

The re-scaled energy follows from (3), from which we have subtracted (28), to ensure that the integrand is strictly non-negative.

The associated Euler-Lagrange equations for $\{\bar{\mathbf{Q}}_j\}$ are

$$\bar{L}\Delta\bar{\mathbf{Q}}_j = \frac{t_j}{2}(|\bar{\mathbf{Q}}_j|^2-1)\bar{\mathbf{Q}}_j + \frac{3h_+}{2}(|\bar{\mathbf{Q}}_j|^2 - |\bar{\mathbf{Q}}_j|)\bar{\mathbf{Q}}_j. \tag{31}$$

and by a standard maximum principle argument (taking the product with $\bar{\mathbf{Q}}_j$), we obtain the global bound

$$|\bar{\mathbf{Q}}_j(\mathbf{x})| \leq 1 \quad \text{for all } \mathbf{x}\in\Omega. \tag{32}$$

This global bound, in particular, implies that

$$(1+3|\bar{\mathbf{Q}}_j|^4 - 4|\bar{\mathbf{Q}}_j|^3) \geq 0$$

for all $\mathbf{Q}_j$ in the sequence. The right-hand side vanishes if and only if $\bar{\mathbf{Q}}$ is of the form (12).

The scaled maps satisfy the boundary condition, $\bar{\mathbf{Q}}_j = \sqrt{\frac{3}{2}}\left(\mathbf{n}_b\otimes\mathbf{n}_b - \frac{\mathbf{I}}{3}\right)$, on $\partial\Omega$. The corresponding admissible space is non-empty and from the energy bound (15) in Theorem 1, the re-scaled energy (29) can be bounded independently of t_j as $t_j\to+\infty$. Therefore, the sequence $\{\nabla\bar{\mathbf{Q}}_j\}_{j\in\mathbb{N}}$ is bounded in $W^{1,2}(\Omega;S_0)$ and after passing to a subsequence, $\bar{\mathbf{Q}}_j \overset{W^{1,2}}{\rightharpoonup} \bar{\mathbf{Q}}_0$ for some $\bar{\mathbf{Q}}^0\in W^{1,2}(\Omega;S_0)$.

Passing to a subsequence converging pointwise a.e. and noting that the constraint of uniaxiality, $6\left(\operatorname{tr}\mathbf{Q}^3\right)^2 = |\mathbf{Q}|^6$, is weakly closed (with non-negative scalar order parameter), we deduce that $\bar{\mathbf{Q}}^0$ is uniaxial. From (32), (29), (30) and the energy bound it follows that

$$\int_\Omega (1-|\bar{\mathbf{Q}}^0|^2)^2\,\mathrm{d}V \leq \limsup_{j\to\infty}\left(\frac{8}{t_j}\cdot\frac{27^2C^3}{4h_+^2B^2}\mathbf{I}_{LG}^j[\mathbf{Q}_j]+\frac{\gamma}{\sqrt{t_j}}\right)=0 \tag{33}$$

for some constant $\gamma>0$. Therefore, $|\bar{\mathbf{Q}}^0|=1$ a.e. and from the orientability result in [3, Th. 2], $\bar{\mathbf{Q}}^0$ can be written as, $\bar{\mathbf{Q}}^0=\sqrt{\frac{3}{2}}(\mathbf{n}^0\otimes\mathbf{n}^0-\frac{\mathbf{I}}{3})$ for some $\mathbf{n}^0\in W^{1,2}(\Omega;\mathbb{S}^2)$. From (29) and the energy upper bound, we obtain

$$\begin{aligned}\frac{3\bar{L}}{2}\int_\Omega|\nabla\mathbf{n}^0|^2\,\mathrm{d}V &= \int_\Omega\frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}^0|^2\,\mathrm{d}V\\ &\leq \limsup_{j\to\infty}\int_\Omega\frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}_j|^2\,\mathrm{d}V \leq \frac{3\bar{L}}{2}\left(\inf_{\mathbf{n}\in\mathcal{A}_{\mathbf{n}_b}}\int_\Omega|\nabla\mathbf{n}|^2\,\mathrm{d}V\right),\end{aligned} \tag{34}$$

i.e. $\bar{\mathbf{Q}}^0$ is a (minimizing) limiting harmonic map and the above inequalities are in fact equalities. This convergence of the L^2-norms of the gradients implies that the weak convergence to $\bar{\mathbf{Q}}^0$ in $W^{1,2}$ is, in fact, a strong convergence. From the theory of harmonic maps, it is known that $\mathbf{n}^0$ has a finite number, $N\geq d$, of isolated interior point defects, $\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$, and each of these defects has degree ±1 [1, 5].

Proof of (ii): we refer the reader to [17, Props. 4 and 6]. From the energy bound (v) in Theorem 1 and the strong convergence to a minimizing limiting harmonic map (as defined in (12)), we have that

$$\lim_{j\to+\infty}\int_\Omega t_j\left\{\frac{1}{8}\left(1-|\bar{\mathbf{Q}}_j|^2\right)^2+\frac{h_+}{8t_j}(1+3|\bar{\mathbf{Q}}_j|^4-4|\bar{\mathbf{Q}}_j|^3)\right\}\,dV=0.$$

We combine the above with the monotonicity inequality for solutions of the Euler-Lagrange equations (31) (as derived in [17]):

$$\frac{1}{R_1}\int_{B(\mathbf{x},R_1)}\frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}_j|^2+t_j\bar{g}_j(\bar{\mathbf{Q}}_j)\,dV\leq\frac{1}{R_2}\int_{B(\mathbf{x},R_2)}\frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}_j|^2+t_j\bar{g}_j(\bar{\mathbf{Q}}_j)\,dV$$

for all $\mathbf{x}\in\Omega$, $R_1<R_2$ such that $B(\mathbf{x},R_2)\subset\Omega$, to obtain the following pointwise convergence result

$$\lim_{j\to\infty}\left[\frac{1}{8}\left(1-|\bar{\mathbf{Q}}_j|^2\right)^2+\frac{h_+}{8t_j}(1+3|\bar{\mathbf{Q}}_j|^4-4|\bar{\mathbf{Q}}_j|^3)\right]=0,$$

everywhere away from the singular set of $\bar{\mathbf{Q}}^0$. We can then argue as in Proposition 4 in [17] to deduce the uniform convergence in the interior. We can deduce the uniform convergence up to the boundary, away from the singular set of the minimizing limiting harmonic map, by using the boundary monotonicity lemma derived in [17, Lemma 9] and arguing as above.

Proof of (iii): The proof closely follows Lemma 6, Lemma 7 and Proposition 5 in [17]. The key step is to prove a Bochner-type inequality of the form

$$-\Delta\left(\frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}_j|^2 + t_j\bar{g}_j(\bar{\mathbf{Q}}_j)\right) \leq C(K)|\nabla\bar{\mathbf{Q}}_j|^4 \tag{35}$$

on any compact subset, $K \subset \Omega \setminus \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, that does not contain any singularities of the limiting harmonic map, $\bar{\mathbf{Q}}^0$. A direct computation shows that

$$-\Delta\left(\frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}_j|^2 + t_j\bar{g}_j(\bar{\mathbf{Q}}_j)\right) = -\bar{L}\bar{\mathbf{Q}}_{j,\alpha\beta}\cdot\bar{\mathbf{Q}}_{j,\alpha\beta} - \bar{L}\Delta\bar{\mathbf{Q}}_{j,\alpha}\cdot\bar{\mathbf{Q}}_{j,\alpha} \tag{36}$$

$$- t_j(D\bar{g}_j)_{,\alpha}\cdot\bar{\mathbf{Q}}_{j,\alpha} - t_jD\bar{g}_j\cdot\Delta\bar{\mathbf{Q}}_j. \tag{37}$$

We define

$$D\bar{g}_j(\bar{\mathbf{Q}}) = \frac{\partial\bar{g}_j(\bar{\mathbf{Q}})}{\partial\bar{\mathbf{Q}}} = -\left(\frac{1}{2}(1-|\bar{\mathbf{Q}}|^2)\bar{\mathbf{Q}} + \frac{3h_+}{2t_j}(|\bar{\mathbf{Q}}| - |\bar{\mathbf{Q}}|^2)\bar{\mathbf{Q}}\right), \tag{38}$$

and this is directly related to the Euler-Lagrange equations, (31), by

$$\bar{L}\Delta\bar{\mathbf{Q}}_j = t_jD\bar{g}_j(\bar{\mathbf{Q}}_j(\mathbf{x})). \tag{39}$$

Therefore,

$$-\Delta\left(\frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}_j|^2 + t_j\bar{g}_j(\bar{\mathbf{Q}}_j)\right) \leq -2t_j(D\bar{g}_j)_{,\alpha}\cdot\bar{\mathbf{Q}}_{j,\alpha} - \frac{t_j^2}{\bar{L}}|D\bar{g}_j|^2. \tag{40}$$

In order to prove (35), note that

$$\begin{aligned} -t_j\Big(D\bar{g}_j(\bar{\mathbf{Q}}_j(\mathbf{x}))\Big)_{,\alpha}\cdot\bar{\mathbf{Q}}_{j,\alpha} &= -\bar{L}\Delta\bar{\mathbf{Q}}_{j,\alpha}\cdot\bar{\mathbf{Q}}_{j,\alpha} \\ &= -\left(t_j + \frac{3h_+}{2}\left(2 - \frac{1}{|\bar{\mathbf{Q}}_j|}\right)\right)\sum_{\alpha=1}^{3}|\bar{\mathbf{Q}}_j\cdot\bar{\mathbf{Q}}_{j,\alpha}|^2 \qquad (41) \\ &\quad + \left(t_j\frac{1+|\bar{\mathbf{Q}}_j|}{2} + \frac{3h_+}{2}|\bar{\mathbf{Q}}_j|\right)(1-|\bar{\mathbf{Q}}_j|)|\nabla\bar{\mathbf{Q}}_j|^2 \end{aligned}$$

and

$$\frac{t_j^2}{\bar{L}}|D\bar{g}_j|^2 = \frac{t_j^2}{\bar{L}} \times \left\{ \frac{1}{4}\left(1-|\bar{\mathbf{Q}}_j|^2\right)^2 |\bar{\mathbf{Q}}_j|^2 + \left(\frac{3h_+}{2t_j}\right)^2 |\bar{\mathbf{Q}}_j|^4 \left(1-|\bar{\mathbf{Q}}_j|\right)^2 + \right. \\ \left. + \frac{3h_+}{2t_j}|\bar{\mathbf{Q}}_j|^3(1+|\bar{\mathbf{Q}}_j|)(1-|\bar{\mathbf{Q}}_j|)^2 \right\}. \tag{42}$$

Finally, we use the global bound $|\bar{\mathbf{Q}}_j| \leq 1$ a.e. and the uniform convergence, $|\bar{\mathbf{Q}}_j| \to 1$ uniformly in K as $j \to +\infty$, to obtain

$$-2t_j(D\bar{g}_j)_{,\alpha} \cdot \bar{\mathbf{Q}}_{j,\alpha} \leq 2t_j\left(1+\frac{3h_+}{2t_j}\right)(1-|\bar{\mathbf{Q}}_j|)|\nabla\bar{\mathbf{Q}}_j|^2 \tag{43}$$

$$\leq C\delta(1-|\bar{\mathbf{Q}}_j|)^2 t_j^2 + \frac{1}{\delta}|\nabla\bar{\mathbf{Q}}_j|^4; \tag{44}$$

$$-\frac{t_j^2}{\bar{L}}|D\bar{g}_j|^2 \leq -\frac{t_j^2}{\bar{L}}\left(1+\frac{3h_+}{2t_j}\right)(1-|\bar{\mathbf{Q}}_j|)^2. \tag{45}$$

The last step is to choose δ sufficiently small and j sufficiently large so that inequality (35) follows. The rest of the proof is identical to Lemma 7 and Proposition 5 of [17].

Proof of (iv): we prove that for each $i = 1, \ldots, N$ 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 $\bar{\mathbf{Q}}_j$ 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 $\min_{B(\mathbf{x}_i,r_0)} |\bar{\mathbf{Q}}_{j_k}| > 0$ for all $k \in \mathbb{N}$. Then, we can apply the orientability result in [3, Th. 2] to $\frac{\bar{\mathbf{Q}}_{j_k}}{|\bar{\mathbf{Q}}_{j_k}|} = \sqrt{\frac{3}{2}}\left(\mathbf{n}_{j_k} \otimes \mathbf{n}_{j_k} - \frac{\mathbf{I}}{3}\right)$ in $B(\mathbf{x}_i, r_0)$ to conclude, without loss of generality, that the corresponding director, $\mathbf{n}_{j_k} \in W^{1,2}(B(\mathbf{x}_i, r_0); \mathbb{S}^2)$ (in (14)). The gradient, $\nabla\mathbf{n}_{j_k}$, can be estimated as shown below

$$\sqrt{\frac{3}{2}}\mathbf{n}_{j_k,\alpha} = \mathbf{n}\left(\frac{\bar{\mathbf{Q}}_{j_k}}{|\bar{\mathbf{Q}}_{j_k}|}\right)_{,\alpha} = \frac{1}{|\bar{\mathbf{Q}}_{j_k}|}\Big(\bar{\mathbf{Q}}_{j_k,\alpha} - \frac{\bar{\mathbf{Q}}_{j_k}}{|\bar{\mathbf{Q}}_{j_k}|^2}(\bar{\mathbf{Q}}_{j_k} \cdot \bar{\mathbf{Q}}_{j_k,\alpha})\Big). \tag{46}$$

We have that $|\nabla\bar{\mathbf{Q}}_{j_k}|$ is uniformly bounded (independently of t_{j_k}) and that $|\bar{\mathbf{Q}}_{j_k}| \to 1$ uniformly away from the singularities of the limiting harmonic map, for j_k sufficiently large. Therefore, $\mathbf{n}_{j_k}$ and $\bar{\mathbf{Q}}_{j_k}$ are Lipschitz-continuous in $B(\mathbf{x}_i, r_0) \setminus B(\mathbf{x}_i, r_0/2)$, uniformly with respect to k. For a.e. $r_0/2 < r < r_0$, we can use Fubini's theorem to extract a subsequence, which may possibly depend on r and is still labelled by j_k, such that

$$\begin{aligned}&\mathbf{n}_{j_k} \to \mathbf{n} \text{ uniformly on } \partial B(\mathbf{x}_i, r) \text{ for some } \mathbf{n} : \partial B(\mathbf{x}_i, r) \to \mathbb{S}^2, \text{ and} \\ &\bar{\mathbf{Q}}_{j_k}(\mathbf{x}) \to \sqrt{\frac{3}{2}}\left(\mathbf{n}^0(\mathbf{x}) \otimes \mathbf{n}^0(\mathbf{x}) - \frac{\mathbf{I}}{3}\right) \text{ for } \mathcal{H}^{n-1}\text{-a.e. } \mathbf{x} \in \partial B(\mathbf{x}_i, r),\end{aligned} \tag{47}$$

where $\mathbf{n}^0 \in W^{1,2}(\Omega; \mathbb{S}^2)$ is related to the (minimizing) limiting harmonic map, $\bar{\mathbf{Q}}^0$, as in part (i) of Theorem 1. We combine the two ingredients above to obtain that $\mathbf{n} \otimes \mathbf{n} = \mathbf{n}^0 \otimes \mathbf{n}^0$ so that $\mathbf{n}(\mathbf{x}) = \pm \mathbf{n}^0(\mathbf{x})$ for a.e. $\mathbf{x} \in \partial B(\mathbf{x}_i, r)$. Since $\mathbf{n} \cdot \mathbf{n}^0 \in W^{1,2}(\partial B(\mathbf{x}_i, r))$ (because $\mathbf{n} : \partial B(\mathbf{x}_i, r) \to \mathbb{S}^2$ is also Lipschitz) and hence is absolutely continuous on almost every curve on $\partial B(\mathbf{x}_i, r)$, then either $\mathbf{n}(\mathbf{x}) = \mathbf{n}_0(\mathbf{x})$ for a.e. $\mathbf{x}$ or $\mathbf{n}(\mathbf{x}) = -\mathbf{n}_0(\mathbf{x})$ for a.e. $\mathbf{x}$. In particular, $|\deg(\mathbf{n}, \partial B(\mathbf{x}_i, r))| = |\pm \deg(\mathbf{n}_0, \partial B(\mathbf{x}_i, r))| = 1$ (recall that each singular point of $\bar{\mathbf{Q}}^0$ has degree, $d = \pm 1$, from standard results in the theory of minimizing harmonic maps, see [5]). By the continuity of the degree with respect to the uniform convergence, this implies that $\deg(\mathbf{n}_{j_k}, \partial B(\mathbf{x}_i, r)) = \pm 1$ for all k sufficiently large. However, $\bar{\mathbf{Q}}_{j_k}$ is uniaxial and $\inf_{\overline{B}(\mathbf{x}_i, r_0)} \bar{\mathbf{Q}}_{j_k} > 0$ by assumption and therefore, $\bar{\mathbf{Q}}_{j_k}$ has two degenerate non-zero eigenvalues on $\overline{B}(\mathbf{x}_i, r_0)$. The leading eigenvector, $\mathbf{n}_{j_k}$, has the same degree of regularity as $\bar{\mathbf{Q}}_{j_k}$ as long as the number of distinct eigenvalues does not change [17]. The map $\bar{\mathbf{Q}}_{j_k}$ is analytic and consequently, $\mathbf{n}_{j_k}$ is analytic on $\overline{B}(\mathbf{x}_i, r_0)$, since $\bar{\mathbf{Q}}_{j_k}$ is free of any isotropic points in $\overline{B}(\mathbf{x}_i, r_0)$. This leads to a contradiction since $\deg(\mathbf{n}_{j_k}, \partial B(\mathbf{x}_i, r)) = \pm 1$ for all k sufficiently large and the proof is now complete.

Proof of (v): The aim is to prove that $\bar{\mathbf{Q}}_j$ has a radial-hedgehog type of profile, (16), near each singular point of the limiting harmonic map, for j sufficiently large. The proof follows from the strong $W^{1,2}$-convergence of the rescaled $\mathbf{Q}$-tensors, $\bar{\mathbf{Q}}_j$, to a limiting harmonic map; the celebrated energy quantization result for the energy of minimizing harmonic maps at singular points, established in [5]:

$$\lim_{r \to 0} \frac{1}{r} \int_{B(\mathbf{x}_i, r)} \frac{1}{2} |\nabla \mathbf{n}^0|^2 \, \mathrm{d}V = 4\pi, \quad i = 1, \ldots, N \tag{48}$$

and Propositions 4 and 8 in [11], quoted in Section 2.

We begin by noting that for each $i = 1 \ldots N$ in $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, we can extract a sequence, $\left\{\mathbf{x}^{(j)}\right\}$, such that $\bar{\mathbf{Q}}_j\left(\mathbf{x}^{(j)}\right) = 0$ and $\mathbf{x}^{(j)} \to \mathbf{x}_i$ as $j \to \infty$, from (iv) above. The inequalities in (34), together with the strong $W^{1,2}$-convergence, imply that

$$\frac{1}{r}\int_{B(\mathbf{x}_i,r)} \frac{1}{2}|\nabla\bar{\mathbf{Q}}_j|^2 + \frac{t_j}{\bar{L}}\bar{g}_j(\bar{\mathbf{Q}}_j)\ \mathrm{d}V \overset{j\to\infty}{\longrightarrow} \frac{3}{r}\int_{B(\mathbf{x}_i,r)} \frac{1}{2}|\nabla\mathbf{n}^0|^2\ \mathrm{d}V \tag{49}$$

for every small $r > 0$. Let

$$\xi_j := \sqrt{\frac{2\bar{L}}{t_j}}, \qquad \tilde{\mathbf{x}} := \frac{\mathbf{x}-\mathbf{x}^{(j)}}{\xi_j}, \qquad \tilde{\mathbf{Q}}_j(\tilde{\mathbf{x}}) := \bar{\mathbf{Q}}_j(\mathbf{x}^{(j)} + \xi_j\tilde{\mathbf{x}}). \tag{50}$$

The goal is to prove that a subsequence of $\{\tilde{\mathbf{Q}}_j\}_{j\in\mathbb{N}}$ converges to the radial-hedgehog solution in (16), in $C^r_{\mathrm{loc}}(\mathbb{R}^3; S_0)$ for all $r \in \mathbb{N}$. By the monotonicity formula in [17, Lemma 2], for every fixed $R > 0$, every small $r > |\mathbf{x}^{(j)} - \mathbf{x}_i| + \xi_j R$, and every j sufficiently large, we have that

$$\begin{aligned}
&\frac{1}{R}\int_{|\tilde{\mathbf{x}}|<R} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}_j(\tilde{\mathbf{x}})|^2 + \frac{(1-|\tilde{\mathbf{Q}}_j|^2)^2}{4}\,\mathrm{d}V && (51)\\
&\quad\le \frac{1}{\xi_j R}\int_{|\mathbf{x}-\mathbf{x}^{(j)}|<\xi_j R} \frac{1}{2}|\nabla\bar{\mathbf{Q}}_j(\mathbf{x})|^2 + \frac{t_j}{\bar{L}}\bar{g}_j(\bar{\mathbf{Q}}_j(\mathbf{x}))\ \mathrm{d}V && (52)\\
&\quad\le \frac{1}{r-|\mathbf{x}^{(j)}-\mathbf{x}_i|}\int_{B(\mathbf{x}^{(j)},r-|\mathbf{x}^{(j)}-\mathbf{x}_i|)} \frac{1}{2}|\nabla\bar{\mathbf{Q}}_j(\mathbf{x})|^2 + \frac{t_j}{\bar{L}}\bar{g}_j(\bar{\mathbf{Q}}_j(\mathbf{x}))\ \mathrm{d}V && (53)\\
&\quad\le \frac{r}{r-|\mathbf{x}^{(j)}-\mathbf{x}_i|}\cdot\frac{1}{r}\int_{B(\mathbf{x}_i,r)} \frac{1}{2}|\nabla\bar{\mathbf{Q}}_j(\mathbf{x})|^2 + \frac{t_j}{\bar{L}}\bar{g}_j(\bar{\mathbf{Q}}_j(\mathbf{x}))\ \mathrm{d}V && (54)
\end{aligned}$$

(we have used the inequality $\frac{(1-|\tilde{\mathbf{Q}}_j|^2)^2}{4} \le g_j(\bar{\mathbf{Q}}_j(\mathbf{x}))$ above). This combined with (49) and (48) yields the following inequality

$$\begin{aligned}
&\limsup_{j\to\infty}\frac{1}{R}\int_{|\tilde{\mathbf{x}}|<R} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}_j(\tilde{\mathbf{x}})|^2 + \frac{(1-|\tilde{\mathbf{Q}}_j|^2)^2}{4}\ \mathrm{d}V\\
&\qquad\qquad \le 3\left(\limsup_{r\to 0^+}\frac{1}{r}\int_{B(\mathbf{x}_i,r)} \frac{1}{2}|\nabla\mathbf{n}^0|^2\ \mathrm{d}V\right) \le 12\pi
\end{aligned} \tag{55}$$

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 uniaxial limit map, $\tilde{\mathbf{Q}}^\infty$, with non-negative scalar order parameter that satisfies the following energy bound

$$\frac{1}{R}\int_{|\tilde{\mathbf{x}}|<R} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}_j(\tilde{\mathbf{x}})|^2 + \frac{(1-|\tilde{\mathbf{Q}}_j|^2)^2}{4}\ \mathrm{d}V \le 12\pi \quad \forall R > 0. \tag{56}$$

One can check that $\tilde{\mathbf{Q}}^\infty$ solves the weak form of the Ginzburg-Landau equations, $\Delta\tilde{\mathbf{Q}} = (|\tilde{\mathbf{Q}}|^2-1)\tilde{\mathbf{Q}}$, in $\mathbb{R}^3$ (write the weak form of the partial differential equations for $\bar{\mathbf{Q}}_{j_k}$ and pass to the limit when $k \to \infty$). Standard arguments in elliptic regularity show that $\tilde{\mathbf{Q}}^\infty$ is a classical solution of the Ginzburg-Landau equations and that the diagonal subsequence converges in $\bigcap_{r\in\mathbb{N}} C^k_{\mathrm{loc}}$ to $\tilde{\mathbf{Q}}^\infty$. Finally $\tilde{\mathbf{Q}}^\infty(\mathbf{0}) = \mathbf{0}$ because $\tilde{\mathbf{Q}}_{j_k}(\mathbf{x}^{(j_k)}) = \mathbf{0}$ for each k, by assumption. We conclude that the hypotheses of [11, Prop. 8] are satisfied, yielding the conclusion of Theorem 1. □

Proof of Theorem 2. We proceed by contradiction. Suppose that there exist sequences, $\{A_j\}_{j\in\mathbb{N}}$ with $A_j \to -\infty$, and a sequence $\{\mathbf{Q}_j\}_{j\in\mathbb{N}} \subset W^{1,2}(\Omega; S_0)$, such that for each $j \in \mathbb{N}$:

(i) $\mathbf{Q}_j(\mathbf{x})$ is uniaxial for a.e. $\mathbf{x} \in \Omega$, i.e. it can be written in the form

$$\mathbf{Q}(\mathbf{x}) = s(\mathbf{x})\left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{\mathbf{I}}{3}\right), \tag{57}$$

for some $s(\mathbf{x}) \in \mathbb{R}$ (not necessarily nonnegative) and some unit-vector field $\mathbf{n}(\mathbf{x}) \in \mathbb{S}^2$;

(ii) and $\mathbf{Q}_j$ is a global minimizer of Landau-de Gennes energy, $\mathbf{I_{LG}}[\mathbf{Q}]$, in the space $\mathcal{A}_{A_j}$.

Then, by global minimality [15, Lemma 2], $\mathbf{Q}_j$ necessarily has non-negative scalar order parameter for each $j \in \mathbb{N}$, i.e. $s(\mathbf{x})$ above is necessarily nonnegative. Also, by elliptic regularity theory, $\mathbf{Q}_j$ is a real-analytic solution of (9) (see, e.g. [17]). Finally, let $\mathbf{Q}^{(1)}$ be a minimizing limiting harmonic map with respect to the Dirichlet condition (7), as defined in (12). We are guaranteed the existence of a minimizing limiting harmonic map from direct methods in the calculus of variations [8]. Then the tensor-valued map $\sqrt{\frac{2}{3}}s_+\mathbf{Q}^{(1)} \in \mathcal{A}_{A_j}$, and since $\mathbf{Q}_j$ is a global LdG minimizer in the space $\mathcal{A}_{A_j}$, we obtain the following inequality

$$\frac{1}{s_+^2}\mathbf{I_{LG}}[\mathbf{Q}_j] \le \frac{1}{s_+^2}\mathbf{I_{LG}}[\mathbf{Q}^{(1)}] \tag{58}$$

$$= \frac{1}{s_+^2}\cdot\frac{2s_+^2}{3}\int_\Omega \frac{L}{2}|\nabla\mathbf{Q}^{(1)}|^2\,\mathrm{d}V = L\left(\inf_{\mathbf{n}\in\mathcal{A}_{\mathbf{n}_b}} I[\mathbf{n}]\right) \tag{59}$$

for every $j \in \mathbb{N}$. This is precisely the energy bound in (15) of Theorem 1. We now combine Theorem 1, part (v), with the instability result for the RH solution with respect to biaxial perturbations as in [11, Th. 3], also see [11, Sect. 5]; (the statement of [11, Th. 3] has been reproduced in Section 2 for completeness and the reader's convenience) to complete the proof. $\square$

4 Conclusions

In this paper, we generalize the results in [11] to an arbitrary three-dimensional simply-connected domain with topologically non-trivial Dirichlet conditions. In [11], we consider a specific model problem of a three-dimensional spherical droplet with radial boundary conditions. In this case, the minimizing limiting harmonic map is $\bar{\mathbf{Q}}^0 = \sqrt{\frac{3}{2}}\left(\frac{\mathbf{x}\otimes\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3}\right)$, with a single singular point at the droplet centre. For the general problem studied in this paper, the minimizing limiting harmonic map may not be unique and will have several singular points (N singular points where N is bounded from below by the topological degree of the Dirichlet boundary condition, see e.g. [1]). We derive a Bochner-type inequality for the energy density away from the singular set of the limiting harmonic map and use convergence properties of the topological degree to establish a correspondence between the isotropic set of uniaxial critical points and the singular set of a minimizing limiting harmonic map (as described in Theorem 1, part (iv)). We use energy quantization results near singular points of energy-minimizing harmonic maps (see [5]) to prove that such uniaxial critical points have a generic radial-hedgehog type of profile near sequences of isotropic points, that converge to a singular point of a minimizing limiting harmonic map in the low-temperature limit (see (16)). This characterization allows us to prove that such uniaxial critical points are unstable with respect to biaxial perturbations and hence, cannot be global energy minimizers.

There are close analogies and differences between the vanishing elastic constant limit studied in [17] and the low-temperature limit studied here and in [11]. In the vanishing elastic constant limit, any sequence of global Landau-de Gennes energy minimizers converges strongly (in $W^{1,2}$) to a minimizing limiting harmonic map. This is not the case for the low-temperature limit, i.e. arbitrary sequences do not converge strongly to minimizing limiting harmonic maps, but sequences of uniaxial critical points (as in Theorem 1) converge strongly to minimizing limiting harmonic maps. Further, we exclude the global minimality of uniaxial critical points satisfying the energy bound (15) in Theorem 1, for sufficiently low temperatures. However, these uniaxial critical points may be stable in restricted classes of uniaxial $\mathbf{Q}$-tensors or other sub-classes of $\mathbf{Q}$-tensors. It would be interesting to further investigate the existence and stability of uniaxial critical points for low temperatures.

There are several natural generalizations of the problem studied in this paper. For example, it would be physically more relevant to consider weak anchoring conditions or surface energies, as opposed to Dirichlet conditions. Our mathematical machinery heavily relies on the one-constant isotropic elastic energy density in (3). There are more general quadratic elastic energy densities in the literature [20], [28] and it is natural to ask if the conclusion of Theorem 1 holds with elastic anisotropy. This opens the door for new mathematical challenges since we do not even have a maximum principle argument for anisotropic quadratic elastic energy densities.

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