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SYMMETRY OF UNIAXIAL GLOBAL LANDAU–DE GENNES MINIMIZERS IN THE THEORY OF NEMATIC LIQUID CRYSTALS*

DUVAN HENAO† AND APALA MAJUMDAR‡

Abstract. We extend the recent radial symmetry results by Pisante [*J. Funct. Anal.*, 260 (2011), pp. 892–905] and Millot and Pisante [*J. Eur. Math. Soc.* (*JEMS*), 12 (2010), pp. 1069–1096] (who show that the equivariant solutions are the only entire solutions of the three-dimensional Ginzburg–Landau equations in superconductivity theory) to the Landau–de Gennes framework in the theory of nematic liquid crystals. In the low temperature limit, we obtain a characterization of global Landau–de Gennes minimizers, in the restricted class of uniaxial tensors, in terms of the well-known radial-hedgehog solution. We use this characterization to prove that global Landau–de Gennes minimizers cannot be purely uniaxial for sufficiently low temperatures.

Key words. liquid crystals, Landau–de Gennes, Ginzburg–Landau, low-temperature limit, radial symmetry, radial hedgehog, uniaxiality, biaxiality, instability, asymptotic analysis

AMS subject classifications. 35B06, 35B35, 35B40, 35B44, 35J50, 49K20, 49K30, 76A15

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1. Introduction.

Nematic liquid crystals are anisotropic liquids with long-range orientational ordering [8, 22]. Continuum theories for nematics, e.g., Oseen–Frank, Ericksen, and Landau–de Gennes theories, have received considerable attention in the mathematical literature, of which the Landau–de Gennes theory is the most general [4, 5, 7, 11, 14]. The Landau–de Gennes theory is popular in the context of studying intricate defect patterns in nematic textures. However, it is remarkable that the Landau–de Gennes theory predicts no analytic singularities for the corresponding equilibria, and a rigorous mathematical description of defects in the Landau–de Gennes framework is missing to date.

We study the model problem of nematics confined to a spherical droplet subject to radial anchoring conditions. This problem has been widely studied in the literature and there are (at least) two competing equilibria: (i) the radial-hedgehog solution and (ii) the biaxial torus solution [9, 25]. The radial-hedgehog solution is purely uniaxial everywhere, except for an isolated defect at the droplet center, in the sense that the constituent molecules have perfect radial alignment everywhere away from the center. The biaxial torus solution does not have perfect radial symmetry, the constituent molecules have two distinguished directions of alignment around the droplet center, and, hence, we have a high degree of biaxiality around the center. The instability of the radial-hedgehog solution has been demonstrated for sufficiently low temperatures [9, 18] and it is known that the biaxial torus solution has lower free-energy than the radial-hedgehog solution in the low temperature limit. However, this does not exclude

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the existence of other competing uniaxial solutions, in the low temperature regime, which may potentially have lower energy than the biaxial torus solution.

There are two principal aims of this paper: (i) to obtain a complete characterization of all uniaxial equilibria, within the Landau–de Gennes framework, in the low temperature limit and (ii) to prove the nonexistence of globally stable purely uniaxial equilibria for sufficiently low temperatures, in the Landau–de Gennes framework. To accomplish (i), we adapt results on the equivariant Ginzburg–Landau vortex in arbitrary dimensions [23] to the Landau–de Gennes framework. More precisely in [23] the author studies entire solutions $\mathbf{u} : \mathbb{R}^N \to \mathbb{R}^N$ of the Ginzburg–Landau equations

$$\Delta \mathbf{u} + \mathbf{u}\left(1 - |\mathbf{u}|^2\right) = 0$$

for $N \geq 3$. One of the central results in [23] is the following.

THEOREM (see [23]). *Let $N \geq 3$ and let $\mathbf{u} \in W^{1,2}_{loc}\left(\mathbb{R}^N;\mathbb{R}^N\right) \cap L^4_{loc}\left(\mathbb{R}^N;\mathbb{R}^N\right)$ be an entire solution of the Ginzburg–Landau equations. The following statements are equivalent:* (a) $\mathbf{u}$ *satisfies $|\mathbf{u}(\mathbf{x})| \to 1$ as $|\mathbf{x}| \to \infty$, $deg_\infty \mathbf{u} = \pm 1$ and*

$$E\left(\mathbf{u}, B_R\right) = \int_{B(0,R)} \frac{1}{2}|\nabla \mathbf{u}|^2 + \frac{1}{4}\left(1 - |\mathbf{u}|^2\right)^2 \, dV = \frac{1}{2}\frac{N-1}{N-2}\left|S^{N-1}\right| R^{N-2} + o(R^{N-2})$$

as $R \to \infty$, where $B(0,R) \subset \mathbb{R}^N$ is the N-dimensional ball of radius R centered at the origin and $|S^{N-1}|$ is the surface area of the N-dimensional unit sphere; (b) *up to a translation on the domain and an orthogonal transformation on the image,* $\mathbf{u}$ *is $O(N)$-equivariant, i.e., $\mathbf{u}(\mathbf{x}) = \frac{\mathbf{x}}{|\mathbf{x}|} f(|\mathbf{x}|)$, where $f : [0,\infty) \to [0,1)$ is the unique solution of an explicit boundary-value problem.*

We work in the low temperature limit and after a suitable rescaling, the study of global Landau–de Gennes minimizers in the restricted class of uniaxial states reduces to the study of entire solutions of the tensor-valued Ginzburg–Landau equations (see equation (28) below). This is a well-posed problem and the radial anchoring conditions are an example of a topologically nontrivial boundary condition with nonzero topological degree. The correct energy bound (as in (a) above) is ensured by the energy minimality in the restricted class of uniaxial states in the Landau–de Gennes framework. Of key importance in our analysis is the concept of a limiting harmonic map. We demonstrate that any sequence of purely uniaxial global Landau–de Gennes minimizers converges strongly, in $W^{1,2}$, to a limiting harmonic map [16]. This strong convergence result contains information about the location of defects in uniaxial minimizers, and as a consequence, all defects are concentrated near the droplet center for sufficiently low temperatures. We are then able to prove that for all sufficiently low temperatures, global Landau–de Gennes minimizers, in the restricted class of uniaxial states, can be approximated arbitrarily closely (up to an orthogonal transformation) by the well-studied radial-hedgehog solution.

To accomplish (ii), we study the second variation of the Landau–de Gennes energy as in [9] and use the characterization of global uniaxial Landau–de Gennes minimizers in terms of the radial-hedgehog solution above. This is sufficient to demonstrate that global Landau–de Gennes minimizers in the restricted class of uniaxial states lose stability with respect to biaxial perturbations, when we move to sufficiently low temperatures. The paper is organized as follows. In section 2, we recall the main mathematical constituents of the Landau–de Gennes theory and state our principal results. In section 3, we obtain results and estimates for global Landau–de Gennes minimizers under the restriction of uniaxiality, in the low temperature limit. In section 4, we use the division trick, as introduced in [20] and used in [23], to obtain

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a characterization of global Landau–de Gennes minimizers, under the constraint of uniaxiality, in terms of the well-known radial-hedgehog solution. Finally, in section 5, we relax the constraint of uniaxiality and use a second variation argument to demonstrate the nonexistence of purely uniaxial global Landau–de Gennes minimizers for this model problem for sufficiently low temperatures.

2. Statement of results. Let $B(0, R_0) \subset \mathbb{R}^3$ denote a three-dimensional spherical droplet of radius $R_0 > 0$, centered at the origin. 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 [16]

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

and we will use the Einstein summation convention throughout the paper.

We work with the Landau–de Gennes theory for nematic liquid crystals [8], whereby a liquid crystal configuration is described by a macroscopic order parameter, known as the $\mathbf{Q}$-tensor order parameter. Mathematically, the Landau–de Gennes $\mathbf{Q}$-tensor order parameter is a symmetric, traceless 3×3 matrix belonging to the space S_0 in (1). A nematic configuration is said to be (i) isotropic (disordered with no orientational ordering) when $\mathbf{Q} = 0$, (ii) uniaxial when $\mathbf{Q}$ has two degenerate nonzero eigenvalues, and (iii) biaxial when $\mathbf{Q}$ has three distinct eigenvalues. The liquid crystal energy is given by the Landau–de Gennes energy functional and the associated energy density is a nonlinear function of $\mathbf{Q}$ and its spatial derivatives [8, 22]. We work with the simplest form of the Landau–de Gennes energy functional that allows for a first-order nematic-isotropic phase transition and spatial inhomogeneities as shown below [16, 22]:

$$\mathbf{I_{LG}}[\mathbf{Q}] = \int_{B(0,R_0)} \frac{L}{2}|\nabla \mathbf{Q}|^2 + f_B(\mathbf{Q}) \; dV. \tag{3}$$

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 $i, j, k = 1 \ldots 3$ 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 as shown below:

$$f_B(\mathbf{Q}) = \frac{\alpha(T - T^*)}{2}\mathrm{tr}\mathbf{Q}^2 - \frac{b^2}{3}\mathrm{tr}\mathbf{Q}^3 + \frac{c^2}{4}\left(\mathrm{tr}\mathbf{Q}^2\right)^2, \tag{4}$$

where $\mathrm{tr}\mathbf{Q}^3 = \mathbf{Q}_{ij}\mathbf{Q}_{jp}\mathbf{Q}_{pi}$ with $i, j, p = 1 \ldots 3$, $\alpha, b^2, c^2 > 0$ 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. We work in the low temperature regime with $T \ll T^*$ and hence we can rewrite (4) as

$$f_B(\mathbf{Q}) = -\frac{a^2}{2}\mathrm{tr}\mathbf{Q}^2 - \frac{b^2}{3}\mathrm{tr}\mathbf{Q}^3 + \frac{c^2}{4}\left(\mathrm{tr}\mathbf{Q}^2\right)^2, \tag{5}$$

where $a^2 > 0$ is a temperature-dependent parameter and we will subsequently investigate the $a^2 \to \infty$ limit, known as the *low temperature* limit. One can readily verify

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that f_B is bounded from below and attains its minimum on the set of $\mathbf{Q}$-tensors given by [15, 18]

$$\mathbf{Q}_{\min} = \left\{ \mathbf{Q} \in S_0; \mathbf{Q} = s_+ \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}}{3} \right), \ \mathbf{n} \in \mathbb{S}^2 \right\}, \tag{6}$$

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

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \tag{7}$$

We are interested in characterizing global minimizers of the Landau–de Gennes energy functional in (3) on spherical droplets with *homeotropic* or *radial anchoring conditions* [18]. The global Landau–de Gennes minimizers correspond to physically observable liquid crystal configurations and hence are of both mathematical and practical importance. We take our admissible $\mathbf{Q}$-tensors to belong to the space

$$\mathcal{A} = \left\{ \mathbf{Q} \in W^{1,2}\left(B(0,R_0); S_0\right); \mathbf{Q} = \mathbf{Q}_b \ on \ \partial B(0,R_0) \right\}, \tag{8}$$

where $W^{1,2}\left(B(0,R_0); S_0\right)$ is the Soboblev space of square-integrable $\mathbf{Q}$-tensors with square-integrable first derivatives [6], with norm

$$||\mathbf{Q}||_{W^{1,2}} = \left(\int_{B(0,R_0)} |\mathbf{Q}|^2 + |\nabla \mathbf{Q}|^2 \, dV \right)^{1/2}.$$

The Dirichlet boundary condition $\mathbf{Q}_b$ is given by

$$\mathbf{Q}_b(\mathbf{x}) = s_+ \left(\frac{\mathbf{x} \otimes \mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3} \right) \in \mathbf{Q}_{\min}, \tag{9}$$

where $\mathbf{x} \in \mathbb{R}^3$ is the position vector and $\frac{\mathbf{x}}{|\mathbf{x}|}$ is the unit vector in the radial direction. The existence of a global minimizer of $\mathbf{I_{LG}}$ in the admissible space $\mathcal{A}$ is immediate from the direct method in the calculus of variations [6]; 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 $B(0,R_0)$,

$$L\Delta \mathbf{Q}_{ij} = -a^2 \mathbf{Q}_{ij} - b^2 \left(\mathbf{Q}_{ip}\mathbf{Q}_{pj} - \frac{1}{3}\mathbf{Q}_{pq}\mathbf{Q}_{pq}\delta_{ij} \right) + c^2 \left(\mathrm{tr}\mathbf{Q}^2 \right) \mathbf{Q}_{ij} \quad i,j,p,q = 1 \ldots 3, \tag{10}$$

where $\frac{b^2}{3}\mathbf{Q}_{pq}\mathbf{Q}_{pq}\delta_{ij}$ is a Lagrange multiplier for the constraint that $\mathbf{Q}$ should be traceless [16].

Our goal is to prove that in the low temperature limit, global Landau–de Gennes minimizers in the admissible space $\mathcal{A}$ cannot be *purely uniaxial*.

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*

$$\mathbf{Q}(\mathbf{x}) = s(\mathbf{x}) \left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{\mathbf{I}}{3} \right) \tag{11}$$

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

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THEOREM 1. *Let $B(0,R_0) \subset \mathbb{R}^3$ denote a spherical droplet of radius R_0, centered at the origin. For each $a^2 > 0$, let $\mathbf{Q}^a$ denote a global minimizer of $\mathbf{I_{LG}}$ (defined in* (3)*) in the space $\mathcal{A}$ defined in* (8)*. There exists a_0 (which depends on L, b, c and R_0) such that for $a^2 > a_0^2$, the minimizer $\mathbf{Q}^a$ is not purely uniaxial.*

In order to prove the above result, we study the auxiliary problem of minimizing the Landau–de Gennes energy functional in the restricted class $\mathcal{A}_u \subset \mathcal{A}$ of purely uniaxial $\mathbf{Q}$-tensors:

$$\mathcal{A}_u = \{\mathbf{Q} \in \mathcal{A} : \mathbf{Q} \text{ is purely uniaxial}\}. \tag{12}$$

Proposition 1 shows that the auxiliary problem is well posed. Moreover, proceeding as in [16, Lem. 3], it can be seen that after a suitable rescaling in $\mathbf{Q}$ (note that $s_+ \to \infty$ as $a^2 \to \infty$; see (35) in Proposition 2), any sequence of minimizers, $\{\mathbf{Q}^a\} \in \mathcal{A}_u$, converges strongly in $W^{1,2}(B(0,R_0); S_0)$, as $a^2 \to \infty$, to a *limiting harmonic map* $\mathbf{Q}^0$. A limiting harmonic map, as defined in [16], is a uniaxial map of the form

$$\mathbf{Q}^0 = s_+ \left(\mathbf{n}^0 \otimes \mathbf{n}^0 - \frac{\mathbf{I}}{3}\right), \tag{13}$$

where s_+ is defined in (7) and $\mathbf{n}^0$ is a minimizer of the Dirichlet energy [21, 24]

$$I[\mathbf{n}] = \int_{B(0,R_0)} |\nabla \mathbf{n}|^2 \, dV \tag{14}$$

in the admissible space $\mathcal{A}_{\mathbf{n}} = \{\mathbf{n} \in W^{1,2}(B(0,R_0); \mathbb{S}^2); \mathbf{n} = \frac{\mathbf{x}}{|\mathbf{x}|} \text{ on } \partial B(0,R_0)\}$; in the case of a spherical droplet with homeotropic boundary conditions, $\mathbf{n}^0$ is unique and $\mathbf{n}^0 = \frac{\mathbf{x}}{|\mathbf{x}|}$ [13, 14]. Hence $\mathbf{Q}^0 = \mathbf{Q}_b$, where $\mathbf{Q}_b$ is the boundary condition defined in (9).

This strong convergence result, in the $a^2 \to \infty$ limit, shows that for a uniaxial sequence of minimizers $\{\mathbf{Q}^a\} \in \mathcal{A}_u$, $|\mathbf{Q}^a| \to |\mathbf{Q}_b| = \sqrt{\frac{2}{3}} s_+$ uniformly away from the singular set of the limiting harmonic map $\mathbf{Q}^0$, i.e., away from the origin (Proposition 2(iv)). $\mathbf{Q}^a$ must necessarily have isotropic regions because of the topologically nontrivial boundary condition $\mathbf{Q}_b$ and for a^2 sufficiently large (i.e., if the temperature is sufficiently low), these isotropic points are concentrated or localized near the origin (Proposition 2(v)). However, for the purpose of proving that global minimizers of the Landau–de Gennes energy are not uniaxial, it is not enough to know that $\mathbf{Q}^a$ converges to $\mathbf{Q}^0$ as $a^2 \to \infty$. It is also necessary to understand the nature of this convergence. More precisely, it is necessary to blow up at the point $\mathbf{x} = 0$ and to compute the optimal decay profile for $|\mathbf{Q}^a|$ around the origin. Keeping this in mind, we keep L, b^2, and c^2 fixed in (3) and (5) and introduce the following dimensionless variables as in [18]:

$$\xi_b = \sqrt{\frac{27c^2L}{tb^4}}, \ \tilde{\mathbf{x}} = \frac{\mathbf{x}}{\xi_b}, \ \tilde{\mathbf{Q}}(\tilde{\mathbf{x}}) = \frac{1}{h_+}\sqrt{\frac{27c^4}{2b^4}}\mathbf{Q}(\mathbf{x}), \ \tilde{\mathcal{I}}_{LG} = \frac{1}{h_+^2}\sqrt{\frac{27c^6t}{4b^4L^3}}\hat{\mathbf{I}}_{\mathbf{LG}}, \tag{15}$$

where

$$t = \frac{27a^2c^2}{b^4} > 0 \tag{16}$$

is the *reduced temperature* [9] (so that the $a^2 \to \infty$ limit corresponds to the $t \to \infty$ limit),

$$h_+ = \frac{3c^2}{b^2}s_+ = \frac{3+\sqrt{9+8t}}{4} \sim \sqrt{\frac{t}{2}} \quad \text{as } t \to \infty \tag{17}$$

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and

$$\hat{\mathbf{I}}_{\mathbf{LG}}[\mathbf{Q}] = \int_{B(0,R_0)} \frac{L}{2}|\nabla \mathbf{Q}|^2 + f_B(\mathbf{Q}) - \min_{\mathbf{Q}\in S_0} f_B(\mathbf{Q})\ dV. \tag{18}$$

(It is clear that $\mathbf{Q}^* \in \mathcal{A}$ is a minimizer of $\hat{\mathbf{I}}_{\mathbf{LG}}$ if and only if $\mathbf{Q}^*$ is a minimizer of $\mathbf{I}_{\mathbf{LG}}$ in (3) and, hence, it suffices to study minimizers of the modified functional in (18).) The position vector $\mathbf{x}$ has been rescaled in (15), so that the droplet $B(0,R_0)$ is rescaled to $B(0,\tilde{R}_t)$ with

$$\tilde{R}_t = \sqrt{\frac{b^4 t}{27c^2 L}} R_0 \to \infty \quad \text{as } t \to \infty. \tag{19}$$

The corresponding dimensionless Landau–de Gennes energy functional is given by

$$\tilde{\mathcal{I}}_{LG}[\tilde{\mathbf{Q}}] = \int_{B(0,\tilde{R}_t)} \frac{1}{2}|\nabla \tilde{\mathbf{Q}}|^2 - \frac{\operatorname{tr}\tilde{\mathbf{Q}}^2}{2} - \frac{\sqrt{6}h_+}{t}\operatorname{tr}\tilde{\mathbf{Q}}^3 + \frac{h_+^2}{2t}\left(\operatorname{tr}\tilde{\mathbf{Q}}^2\right)^2 + C(t)\ dV, \tag{20}$$

where

$$C(t) = -\frac{1}{h_+^2}\sqrt{\frac{27c^6 t}{4b^4L^3}}\xi_b^3 \min_{\mathbf{Q}\in S_0} f_B(\mathbf{Q}) = -\frac{1}{h_+^2}\sqrt{\frac{27c^6 t}{4b^4L^3}}\xi_b^3 f_B(\mathbf{Q}_b) = \frac{1}{2} + \frac{h_+}{t} - \frac{h_+^2}{2t}$$

is the additive constant that ensures that

$$-\frac{1}{2}\operatorname{tr}\tilde{\mathbf{Q}}^2 - \frac{\sqrt{6}h_+}{t}\operatorname{tr}\tilde{\mathbf{Q}}^3 + \frac{h_+^2}{2t}\left(\operatorname{tr}\tilde{\mathbf{Q}}^2\right)^2 + C(t) \geq 0 \quad \forall \tilde{\mathbf{Q}} \in S_0. \tag{21}$$

From (9) and (17), after rescaling the limiting harmonic map becomes

$$\tilde{\mathbf{Q}}^0(\tilde{\mathbf{x}}) = \sqrt{\frac{3}{2}}\left(\frac{\tilde{\mathbf{x}}\otimes\tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^2} - \frac{\mathbf{I}}{3}\right), \quad \tilde{\mathbf{x}} \in B(0,\tilde{R}_t), \tag{22}$$

and from (8), the admissible $\mathbf{Q}$-tensors for the auxiliary problem (12) belong to the space

$$\mathcal{A}_{\mathbf{Q}} = \left\{\tilde{\mathbf{Q}} \in W^{1,2}\left(B(0,\tilde{R}_t); S_0\right);\ \tilde{\mathbf{Q}} \text{ is uniaxial and } \tilde{\mathbf{Q}} = \tilde{\mathbf{Q}}_b \text{ on } \partial B(0,\tilde{R}_t)\right\}. \tag{23}$$

The associated Euler–Lagrange equations are [17, 16] (also see Proposition 2):

$$\Delta\tilde{\mathbf{Q}}_{ij} = -\tilde{\mathbf{Q}}_{ij} - \frac{3\sqrt{6}h_+}{t}\left(\tilde{\mathbf{Q}}_{ik}\tilde{\mathbf{Q}}_{kj} - \frac{\delta_{ij}}{3}\operatorname{tr}(\tilde{\mathbf{Q}}^2)\right) + \frac{2h_+^2}{t}\tilde{\mathbf{Q}}_{ij}\operatorname{tr}(\tilde{\mathbf{Q}}^2), \quad i,j = 1,2,3. \tag{24}$$

The following is our main result. (This is an immediate consequence of Propositions 4 and 8.)

THEOREM 2. *For every $t > 0$, let $\tilde{\mathbf{Q}}^t$ denote a minimizer of $\tilde{\mathcal{I}}_{LG}$ on $\mathcal{A}_{\mathbf{Q}}$. Then, for every sequence $\{t_j\}_{j\in\mathbb{N}}$ with $t_j \to \infty$ as $j \to \infty$, there exists a sequence $\{\tilde{\mathbf{x}}_j^*\}_{j\in\mathbb{N}} \subset \mathbb{R}^3$ and an orthogonal transformation $\mathbf{T} \in \mathcal{O}(3)$ 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* $j \in \mathbb{N}$, *and*

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(iii) *the sequence of maps* $\{\tilde{\mathbf{x}} \mapsto \tilde{\mathbf{Q}}^{t_j}(\tilde{\mathbf{x}} + \tilde{\mathbf{x}}_j^*)\}_{j\in\mathbb{N}}$ *converges in* $C^k_{\mathrm{loc}}(\mathbb{R}^3; S_0)$ *for every* $k \in \mathbb{N}$ *to the map*

$$\mathbf{H}_T(\tilde{\mathbf{x}}) = \sqrt{\frac{3}{2}} h(|\tilde{\mathbf{x}}|) \left(\frac{\mathbf{T}\tilde{\mathbf{x}} \otimes \mathbf{T}\tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^2} - \frac{1}{3}\mathbf{I} \right), \quad \tilde{\mathbf{x}} \in \mathbb{R}^3, \tag{25}$$

where $h : [0, \infty) \to \mathbb{R}^+$ *is the unique, monotonically increasing solution, with* $r = |\tilde{\mathbf{x}}|$*, of the boundary-value problem*

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h^3 - h, \qquad h(0) = 0, \qquad \lim_{r\to\infty} h(r) = 1. \tag{26}$$

Theorem 2 states that after a suitable choice of the origin $\tilde{\mathbf{x}}_j^*$ for every $j \in \mathbb{N}$, every subsequence of the original sequence of minimizing $\mathbf{Q}$-tensors has a subsequence that converges, up to a fixed orthogonal transformation, to the *radial-hedgehog* solution

$$\mathbf{H}(\tilde{\mathbf{x}}) = h(|\tilde{\mathbf{x}}|)\sqrt{\frac{3}{2}} \left(\frac{\tilde{\mathbf{x}} \otimes \tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^2} - \frac{1}{3}\mathbf{I} \right), \quad \tilde{\mathbf{x}} \in \mathbb{R}^3 \tag{27}$$

(see Proposition 5) of the tensor-valued Ginzburg–Landau equations

$$\Delta\tilde{\mathbf{Q}} = (|\tilde{\mathbf{Q}}|^2 - 1)\tilde{\mathbf{Q}}, \qquad \tilde{\mathbf{x}} \in \mathbb{R}^3. \tag{28}$$

Some questions, however, remain open. In particular, it would be interesting to show that the orthogonal transformation $\mathbf{T}$ of Theorem 2 is simply the identity matrix, which ought to be true by virtue of the imposed boundary condition $\mathbf{Q}_b$ in (9), especially in light of the strong convergence result in Proposition 2. Second, it would be interesting to establish the stronger result that $\frac{\tilde{\mathbf{Q}}^t(\tilde{\mathbf{x}}+\tilde{\mathbf{x}}_j^*)}{h_t(|\tilde{\mathbf{x}}|)}$ converges to $\sqrt{\frac{3}{2}}(\frac{\tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|} \otimes \frac{\tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|} - \frac{\mathbf{I}}{3})$, where h_t is the solution of an explicit boundary-value problem as stated in Proposition 5 and $h = \lim_{t\to\infty} h_t$. (This would make the statement that minimizers of $\tilde{\mathcal{I}}_{LG}$ in the restricted class of uniaxial maps look "almost" like the radial-hedgehog solution more rigorous.) Finally, it remains open to determine whether the radial symmetry result in Theorem 2 holds not only in the $a^2 \to \infty$ limit but also for sufficiently large but finite a^2.

3. Preliminaries.

LEMMA 1 (uniaxiality). *For every* $\mathbf{Q} \in S_0$*, the following are equivalent:*

(i) $\mathbf{Q}$ *has two equal eigenvalues,*

(ii) $\mathbf{Q}$ *can be written in the form* $\mathbf{Q} = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I})$ *for some* $s \in \mathbb{R}$ *and some* $\mathbf{n} \in \mathbb{S}^2$*,*

(iii) $(\operatorname{tr} \mathbf{Q}^2)^3 = 6(\operatorname{tr} \mathbf{Q}^3)^2$.

Proof. If $\mathbf{Q} \in S_0$ has two equal eigenvalues, then there exists an orthonormal frame $\mathbf{e}$, $\mathbf{f}$, $\mathbf{n}$ such that

$$\mathbf{Q} = \lambda\,(\mathbf{e} \otimes \mathbf{e} + \mathbf{f} \otimes \mathbf{f}) - 2\lambda\mathbf{n} \otimes \mathbf{n}.$$

Since $\mathbf{n}\otimes\mathbf{n} + \mathbf{e}\otimes\mathbf{e} + \mathbf{f}\otimes\mathbf{f} = \mathbf{I}$, we may write $\mathbf{Q}$ in the simpler form $\mathbf{Q} = -3\lambda(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I})$, where $s = -3\lambda$ and $\mathbf{n}$ is the distinguished eigenvector with the nondegenerate eigenvalue. Let us now show that (iii) implies (ii). Let $\mathbf{Q} \in S_0$ with eigenvalues $\lambda_1, \lambda_2, \lambda_3$. The fact that $\operatorname{tr}\mathbf{Q} = 0$ implies that

$$\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 = \frac{(\operatorname{tr}\mathbf{Q})^2 - \operatorname{tr}\mathbf{Q}^2}{2} = -\frac{1}{2}\operatorname{tr}\mathbf{Q}^2,$$

$$\operatorname{tr}\mathbf{Q}^3 = \lambda_1^3 + \lambda_2^3 + \lambda_3^3 = \frac{6\lambda_1\lambda_2\lambda_3 - (\lambda_1 + \lambda_2 + \lambda_3)^3}{2} = 3\det\mathbf{Q}.$$

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Thus, as in [1, Prop. 1], if $(\operatorname{tr}\mathbf{Q}^2)^3 = 6(\operatorname{tr}\mathbf{Q}^3)^2$, then $\det(\lambda\mathbf{I}-\mathbf{Q})$ can be factorized as

$$\lambda^3 + (\lambda_1\lambda_2+\lambda_2\lambda_3+\lambda_3\lambda_1)\lambda - \lambda_1\lambda_2\lambda_3 = \left(\lambda + \sqrt{\frac{\operatorname{tr}\mathbf{Q}^2}{6}}\right)^2\left(\lambda - 2\sqrt{\frac{\operatorname{tr}\mathbf{Q}^2}{6}}\right),$$

completing the proof. ∎

Note. If s in the above representation is such that $s \geq 0$, it is clear that we can also write

$$\mathbf{Q} = \sqrt{\frac{3}{2}}|\mathbf{Q}|\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right). \tag{29}$$

LEMMA 2 (orientability). *Let $\Omega \subset \mathbb{R}^3$ be a bounded simply-connected domain with continuous boundary. If $\mathbf{Q} \in W^{1,2}(\Omega, S_0)$ and $|\mathbf{Q}(\mathbf{x})| = \sqrt{\frac{2}{3}}s$ a.e. in Ω for some fixed $s \neq 0$, then $\mathbf{Q}$ admits a representation of the form* (11) *for some unit-vector field $\mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2)$ if and only if*

$$(\operatorname{tr}\mathbf{Q}(\mathbf{x})^2)^3 = 6(\operatorname{tr}\mathbf{Q}(\mathbf{x})^3)^2 \quad \textit{for a.e. } \mathbf{x} \in \Omega. \tag{30}$$

Proof. By Lemma 1, property (30) holds if and only if for a.e. $\mathbf{x} \in \Omega$ the tensor $\mathbf{Q}(\mathbf{x})$ belongs to the manifold

$$\boldsymbol{\mathcal{Q}} := \left\{\mathbf{Q} \in S_0 : \ \mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right) \text{ for some } \mathbf{n} \in \mathbb{S}^2\right\}. \tag{31}$$

However, it is difficult to determine if for each $\mathbf{x}$ the unit vector $\mathbf{n}(\mathbf{x})$ can be chosen in such a way that the resulting map $\mathbf{n} : \Omega \to \mathbb{S}^2$ has the desired regularity ($\mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2)$). The main difficulty is that the topology of $\boldsymbol{\mathcal{Q}}$ is that of $\mathbb{RP}^2$, and in fact it is possible to construct $\mathbf{Q}$-tensors that cannot be oriented (for which it is not possible to find $\mathbf{n} \in W^{1,2}$) if the domain Ω is not simply connected or if we only know that $\mathbf{Q} \in W^{1,p}(\Omega, S_0)$ for some $p < 2$ (see Ball and Zarnescu [1]). For the case at hand of a simply-connected domain and a $\mathbf{Q}$-tensor in $W^{1,2}(\Omega; S_0)$, there exists a lifting $\mathbf{n} \in W^{1,2}(\Omega; \mathbb{S}^2)$ as required (this is proved in [1, Th. 2]). ∎

PROPOSITION 1. *For every $a^2 > 0$, the infimum of the Landau–de Gennes energy $\mathbf{I_{LG}}$ in* (3) *on the restricted class $\mathcal{A}_u$ in* (12) *is attained. Moreover, the minimizers of $\mathbf{I_{LG}}$ on $\mathcal{A}_u$ are smooth and real analytic on $B(0, R_0)$ and solve the same system* (10) *of Euler–Lagrange equations as do the minimizers of $\mathbf{I_{LG}}$ on the unrestricted class $\mathcal{A}$.*

Proof. For consistency with the rest of the paper, we use the dimensionless variables introduced in (15) and consider the equivalent problem of minimizing the functional $\tilde{\mathcal{I}}_{LG}$ defined in (20) on the admissible class $\mathcal{A}_{\mathbf{Q}}$ of (23) with $t > 0$ fixed. In what follows, we drop the tilde on the dimensionless variables for brevity, and all subsequent results in the proof of this proposition are to be understood in terms of the dimensionless variables. In what follows, we prove the existence of minimizers in the restricted class $\mathcal{A}_{\mathbf{Q}}$ and show that they solve the corresponding system of Euler–Lagrange equations in (24).

Fix $t > 0$ and let $\{\mathbf{Q}_k\}_{k\in\mathbb{N}}$ be a minimizing sequence for $\tilde{\mathcal{I}}_{LG}$ in $\mathcal{A}_{\mathbf{Q}}$. Since the boundary condition is fixed, $\{\mathbf{Q}_k\}$ is bounded in $W^{1,2}(B(0, R_t); S_0)$, hence there exists a subsequence (not relabeled) converging weakly in $W^{1,2}(B(0, R_t); S_0)$ to some $\mathbf{Q}^t \in W^{1,2}(B(0, R_t); S_0)$. By the trace theorem, $\mathbf{Q}^t = \mathbf{Q}_b$ on $\partial B(0, R_t)$. Since

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$W^{1,2} \hookrightarrow L^4$ and the bulk energy density (21) is a quartic polynomial in $\mathbf{Q}$, it follows that $\tilde{\mathcal{I}}_{LG}[\mathbf{Q}^t] \leq \inf_{\mathcal{A}_\mathbf{Q}} \tilde{\mathcal{I}}_{LG}$. We only need to show that $\mathbf{Q}^t \in \mathcal{A}_\mathbf{Q}$. This can be seen by extracting a subsequence of $\{\mathbf{Q}_k\}_{k\in\mathbb{N}}$ converging a.e. in $B(0,R_t)$ to $\mathbf{Q}^t$, recalling that $\mathbf{Q}$ is uniaxial if and only if $(\operatorname{tr}\mathbf{Q}^2)^3 = 6(\operatorname{tr}\mathbf{Q}^3)^2$ (Lemma 1) and noting that this constraint is preserved under weak convergence.

If $\mathbf{Q}$ is a minimizer of $\tilde{\mathcal{I}}_{LG}$ on $\mathcal{A}_\mathbf{Q}$, then

$$\int_{B(0,R_t)} \nabla\mathbf{Q}\cdot\nabla\mathbf{H} - \left(\mathbf{Q} + \frac{3\sqrt{6}h_+}{t}\mathbf{Q}^2 - \frac{2h_+^2}{t}(\operatorname{tr}\mathbf{Q}^2)\mathbf{Q}\right)\cdot\mathbf{H}\,dV = 0 \tag{32}$$

for every $\mathbf{H} \in C_c^\infty(B(0,R_t);S_0)$ satisfying

$$6\big((\operatorname{tr}\mathbf{Q}^2)^2\mathbf{Q} - 6(\operatorname{tr}\mathbf{Q}^3)\mathbf{Q}^2\big)\cdot\mathbf{H} = 0 \tag{33}$$

(condition coming from the uniaxiality constraint $(\operatorname{tr}\mathbf{Q}^2)^3 = 6(\operatorname{tr}\mathbf{Q}^3)^2$). However, one can immediately check that if $\mathbf{Q} = s(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3})$, then $(\operatorname{tr}\mathbf{Q}^2)^2\mathbf{Q} - 6(\operatorname{tr}\mathbf{Q}^3)\mathbf{Q}^2 = -\frac{8}{27}s^5\mathbf{I}$. Since $\operatorname{tr}\mathbf{H} = 0$ for all $\mathbf{H} \in C_c^\infty(B(0,R_t);S_0)$, we find that (33) is satisfied for every $\mathbf{H} \in C_c^\infty(B(0,R_t);S_0)$.

Given $\mathbf{H} \in C_c^\infty(B(0,R_t),M^{3\times3})$ satisfying $\mathbf{H} = \mathbf{H}^T$, it is clear that $\bar{\mathbf{H}} = \mathbf{H} - \frac{\operatorname{tr}\mathbf{H}}{3}\mathbf{I}$ belongs to $C_c^\infty(B(0,R_t),S_0)$ and hence we can apply (32) to $\bar{\mathbf{H}}$. We have $\mathbf{Q}\cdot\mathbf{I} = 0$ and $\nabla\mathbf{Q}\cdot\mathbf{I} = 0$; therefore

$$\begin{aligned}&\int_{B(0,R_t)} \nabla\mathbf{Q}\cdot\nabla\mathbf{H} - \left(\mathbf{Q} + \frac{3\sqrt{6}h_+}{t}\left(\mathbf{Q}^2 - \frac{\operatorname{tr}\mathbf{Q}^2}{3}\mathbf{I}\right) - \frac{2h_+^2}{t}(\operatorname{tr}\mathbf{Q}^2)\mathbf{Q}\right)\cdot\mathbf{H}\,dV\\ &= \int_{B(0,R_t)} \nabla\mathbf{Q}\cdot\nabla\bar{\mathbf{H}} - \left(\mathbf{Q} + \frac{3\sqrt{6}h_+}{t}\mathbf{Q}^2 - \frac{2h_+^2}{t}(\operatorname{tr}\mathbf{Q}^2)\mathbf{Q}\right)\cdot\bar{\mathbf{H}}\,dV = 0\end{aligned} \tag{34}$$

for all symmetric $\mathbf{H} \in C_c^\infty(B(0,R_t),M^{3\times3})$. If $\mathbf{H}$ is not symmetric, we can apply the previous argument to $\tilde{\mathbf{H}} = \frac{\mathbf{H}+\mathbf{H}^T}{2}$ and since $\mathbf{Q}\cdot\tilde{\mathbf{H}} = \mathbf{Q}\cdot\mathbf{H}$ and $\mathbf{Q}^2\cdot\tilde{\mathbf{H}} = \mathbf{Q}^2\cdot\mathbf{H}$, we conclude that (34) is valid for all tensor-valued test functions $\mathbf{H} \in C_c^\infty(B(0,R_t),M^{3\times3})$. Therefore, $\mathbf{Q}$ satisfies the weak form of the Euler–Lagrange equations (24). Proposition 1 now follows from standard elliptic regularity theory. ∎

PROPOSITION 2. *For each $a^2 > 0$, let $\mathbf{Q}^a \in W^{1,2}(B(0,R_0);S_0)$ be a minimizer of the Landau–de Gennes energy $\mathbf{I_{LG}}$ in the space $\mathcal{A}_u$ (the existence of which is guaranteed by Proposition* 1). *Define*

$$\bar{\mathbf{Q}}^a_{ij}(\mathbf{x}) = \frac{1}{h_+}\sqrt{\frac{27c^4}{2b^4}}\mathbf{Q}^a_{ij}(\mathbf{x}), \quad \mathbf{x} \in B(0,R_0). \tag{35}$$

Then

(i) $\bar{\mathbf{Q}}^a = \sqrt{\frac{3}{2}}|\bar{\mathbf{Q}}^a|(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I})$ *for some* $\mathbf{n} : B(0,R_0) \to S^2$*;*

(ii) $|\bar{\mathbf{Q}}^a(\mathbf{x})| \leq 1$ *for all* $\mathbf{x} \in B(0,R_0)$*;*

(iii) $\bar{\mathbf{Q}}^a$ *converges to* $\bar{\mathbf{Q}}^0(\mathbf{x}) = \sqrt{\frac{3}{2}}(\frac{\mathbf{x}\otimes\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3})$ *strongly in* $W^{1,2}(B(0,R_0);S_0)$ *as* $a^2 \to \infty$*;*

(iv) *for any compact $K \subset B(0,R_0)$ such that K does not contain any singularities of $\bar{\mathbf{Q}}^0$, i.e., does not contain the origin, we have*

$$\lim_{a^2\to\infty} |\bar{\mathbf{Q}}^a(\mathbf{x})| = 1 \quad \forall\mathbf{x} \in K, \tag{36}$$

the limit being uniform on K;

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(v) *for every* $a^2 > 0$, *there exists* $\mathbf{x}_a^* \in B(0,R_0)$ *such that* $\bar{\mathbf{Q}}^a(\mathbf{x}_a^*) = 0$ *with* $|\mathbf{x}_a^*| \to 0$ *as* $a^2 \to \infty$.

Proof of (i). The proof of [15, Lem. 2] shows that if $\mathbf{Q}^a$ is a Landau–de Gennes minimizer in $\mathcal{A}_u$, then s in the representation $\mathbf{Q}^a = s(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3})$ must necessarily be nonnegative. As mentioned in the note after Lemma 1, this implies that $s = \sqrt{\frac{3}{2}}|\mathbf{Q}^a|$, i.e., that $\bar{\mathbf{Q}}^a = \sqrt{\frac{3}{2}}|\bar{\mathbf{Q}}^a|(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I})$ for some $\mathbf{n} : B(0,R_0) \to S^2$.

Proof of (ii). From (10) and (35) and recalling Proposition 1, we have that

$$\bar{L}\Delta\bar{\mathbf{Q}}^a_{ij} = -\frac{t}{2}\bar{\mathbf{Q}}^a_{ij} - \sqrt{\frac{27}{2}}h_+\left(\bar{\mathbf{Q}}^a_{ik}\bar{\mathbf{Q}}^a_{kj} - \frac{\delta_{ij}}{3}\mathrm{tr}(\bar{\mathbf{Q}}^a)^2\right) + h_+^2\bar{\mathbf{Q}}^a_{ij}\mathrm{tr}(\bar{\mathbf{Q}}^a)^2, \quad i,j = 1,2,3, \tag{37}$$

with $\bar{L} = \frac{27c^2L}{2b^4}$ and $t = \frac{27a^2c^2}{b^4}$. We substitute the representation formula in (i) into the above to obtain

$$\bar{L}\Delta\bar{\mathbf{Q}}^a_{ij} = \frac{t}{2}(|\bar{\mathbf{Q}}^a|^2 - 1)\bar{\mathbf{Q}}^a_{ij} + \frac{3h_+}{2}(|\bar{\mathbf{Q}}^a|^2 - |\bar{\mathbf{Q}}^a|)\bar{\mathbf{Q}}^a_{ij}. \tag{38}$$

The proof of (ii) follows from multiplying both sides of the above by $\bar{\mathbf{Q}}^a_{ij}$ and applying a standard maximum principle argument for $|\bar{\mathbf{Q}}^a|^2$; the details are omitted for brevity.

Proof of (iii). We follow the proof of [16, Lem. 3], noting first that the Landau–de Gennes energy functional corresponding to the rescaled variables $\bar{\mathbf{Q}}$ is given by

$$\frac{27^2c^6}{4h_+^2b^8}\hat{\mathbf{I}}_{\mathbf{LG}}[\bar{\mathbf{Q}}] = \int_{B(0,R_0)} \frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}|^2 + \frac{t}{8}\left[\left(1 - |\bar{\mathbf{Q}}|^2\right)^2 + \bar{f}(t,\bar{\mathbf{Q}})\right]\, dV, \tag{39}$$

where $\bar{L}$ and t are as defined above,

$$\bar{f}(t,\bar{\mathbf{Q}}) = \left(1 + 3|\bar{\mathbf{Q}}|^4 - 4\sqrt{6}\,\mathrm{tr}\,\bar{\mathbf{Q}}^3\right)\frac{h_+}{t}, \tag{40}$$

and $(1 - |\bar{\mathbf{Q}}|^2)^2 + \bar{f}(t,\bar{\mathbf{Q}}) \geq 0$ for all $\mathbf{Q} \in S_0$ (see definition of $\hat{\mathbf{I}}_{\mathbf{LG}}$ in (18)). Since $\frac{h_+}{t} \sim \frac{1}{\sqrt{2t}}$ as $t \to \infty$, then

$$|\bar{f}(t,\bar{\mathbf{Q}})| \leq (1 + |\bar{\mathbf{Q}}|)^4\frac{\gamma_1}{\sqrt{t}} \tag{41}$$

for some constant γ_1 (independent of a, b, c, L, and t) in the limit $t \to \infty$.

Our aim is to show that for every sequence $\{a_k\}_{k\in\mathbb{N}}$ with $a_k \to \infty$ and every sequence $\{\bar{\mathbf{Q}}^{a_k}\}_{k\in\mathbb{N}}$ satisfying $\hat{\mathbf{I}}_{\mathbf{LG}}[\bar{\mathbf{Q}}^{a_k}] \leq \hat{\mathbf{I}}_{\mathbf{LG}}\left[\bar{\mathbf{Q}}^0\right]$ for all $k \in \mathbb{N}$, there exists a subsequence converging weakly to $\bar{\mathbf{Q}}^0$. Then we prove that the convergence is, in fact, strong in $W^{1,2}(B(0,R_0);S_0)$.

From (39) and the fact that $\mathbf{Q}^0 \in \mathcal{A}_u$, we obtain

$$\int_{B(0,R_0)} \frac{\bar{L}}{2}|\nabla\bar{\mathbf{Q}}^{a_k}|^2 + \frac{t_k}{8}\left[\left(1 - |\bar{\mathbf{Q}}^{a_k}|^2\right)^2 + \bar{f}(t_k,\bar{\mathbf{Q}}^{a_k})\right]\, dV \leq \frac{\bar{L}}{2}\|\nabla\bar{\mathbf{Q}}^0\|^2_{L^2(B(0,R_0))} \tag{42}$$

(recall that the bulk energy density f_B attains its minimum in $\mathbf{Q}_{\min}$ and that $\mathbf{Q}^0(\mathbf{x}) \in \mathbf{Q}_{\min}$ for every $\mathbf{x} \in B(0,R_0)$). The right-hand side is bounded independently of t, hence $\{\nabla\bar{\mathbf{Q}}^{a_k}\}_{k\in\mathbb{N}}$ is bounded in L^2. Moreover, $\bar{\mathbf{Q}}^{a_k} = \bar{\mathbf{Q}}_b$ on $\partial B(0,R_0)$ for

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every $k \in \mathbb{N}$; using Poincaré's inequality it follows that $\{\bar{\mathbf{Q}}^{a_k}\}_{k\in\mathbb{N}}$ is bounded in $W^{1,2}(B(0,R_0);S_0)$. By the Banach–Alaoglu theorem, we may extract a subsequence (not relabeled) converging weakly to a map $\mathbf{Q}^\infty \in W^{1,2}(B(0,R_0);S_0)$.

As in Proposition 1, we can verify that the limit map $\mathbf{Q}^\infty$ is uniaxial by taking a subsequence converging pointwise a.e. and by using the characterization of uniaxial maps in Lemma 1. By virtue of (42), (41), and part (ii),

$$\int_{B(0,R_0)} (1-|\mathbf{Q}^\infty|^2)^2 \, dV \le \lim_{t\to\infty} \left(\frac{4\bar{L}}{t} \|\nabla \bar{\mathbf{Q}}^0\|_{L^2}^2 + \frac{4\pi}{3} R_0^3 \cdot \frac{2^4\gamma_1}{\sqrt{t}} \right) = 0, \tag{43}$$

so $\mathbf{Q}^\infty$ is of the form $\mathbf{Q}^\infty = \sqrt{\frac{3}{2}}(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3})$ for some $\mathbf{n} \in W^{1,2}(B(0,R_0);\mathbb{S}^2)$ (see Lemma 2). From (42) and the lower semicontinuity of the Dirichlet energy, we obtain

$$\begin{aligned} 3\int_{B(0,R_0)} |\nabla \mathbf{n}|^2 \, dV &= \int_{B(0,R_0)} |\nabla \mathbf{Q}^\infty|^2 \, dV \\ &\le \int_{B(0,R_0)} |\nabla \bar{\mathbf{Q}}^0|^2 \, dV = 3\int_{B(0,R_0)} \left| \nabla \left(\frac{\mathbf{x}}{|\mathbf{x}|} \right) \right|^2 \, dV. \end{aligned} \tag{44}$$

By the definition of a limiting harmonic map (see (14)), we conclude that $\mathbf{n}(\mathbf{x}) = \frac{\mathbf{x}}{|\mathbf{x}|}$, that $\mathbf{Q}^\infty = \bar{\mathbf{Q}}^0$, and that the inequality above is in fact an equality. The fact that the convergence is strong follows from the convergence of the L^2-norm of the gradient. Since the limit is the same for every subsequence $\{\bar{\mathbf{Q}}^{a_k}\}_{k\in\mathbb{N}}$, we conclude that the entire sequence $\{\bar{\mathbf{Q}}^a\}_{a>0}$ converges strongly in $W^{1,2}$ to $\bar{\mathbf{Q}}^0$ as $a^2 \to \infty$.

Proof of (iv). This is a consequence of the pointwise uniform convergence

$$\lim_{a^2\to\infty} \left[\left(1 - |\bar{\mathbf{Q}}^a|\right)^2 + \bar{f}(t, \bar{\mathbf{Q}}^a) \right] = 0$$

everywhere away from the singular set of $\bar{\mathbf{Q}}^0$, i.e., away from the origin (recall from (40) the definition of $\bar{f}$). This uniform convergence result holds in the interior and up to the boundary. The proof can be found in [16, Prop. 4 and 6].

Proof of (v). This follows from (iv). We have a topologically nontrivial boundary condition $\bar{\mathbf{Q}}_b = \frac{1}{h_+}\sqrt{\frac{27c^4}{2b^4}}\mathbf{Q}_b$ in (9) and hence every interior extension of $\frac{\mathbf{x}}{|\mathbf{x}|}$ must have interior discontinuities. The extension $\mathbf{n}$ in (i) has interior discontinuities and at every such point of discontinuity $\mathbf{x}_a^*$, $\bar{\mathbf{Q}}^a(\mathbf{x}_a^*) = 0$ (see [18] for further discussion on these lines; $\bar{\mathbf{Q}}^a$ is analytic at $\mathbf{x}_a^*$, whereas $\mathbf{n}$ is not, and $\mathbf{n}$ can lose regularity only when the number of distinct eigenvalues of $\bar{\mathbf{Q}}^a$ changes. Since $\mathbf{Q}^a \in \mathcal{A}_u$, the number of distinct eigenvalues of $\bar{\mathbf{Q}}^a$ can change only when $\bar{\mathbf{Q}}^a$ relaxes into the isotropic phase, i.e., $\bar{\mathbf{Q}}^a(\mathbf{x}_a^*) = 0$). From (iv), as $a^2 \to \infty$, all isotropic points are concentrated near the singular set of $\bar{\mathbf{Q}}^0$ and the singular set of $\bar{\mathbf{Q}}^0$ merely consists of the origin. Hence, $\mathbf{x}_a^* \to 0$ as $a^2 \to \infty$. ∎

PROPOSITION 3 (see [16, Lem. 2]). *For each $t > 0$, let $\tilde{\mathbf{Q}}^t$ denote a global minimizer of $\tilde{\mathcal{I}}_{LG}$ in* (20)*, in the admissible space $\mathcal{A}_{\mathbf{Q}}$ defined in* (23)*. Define*

$$e\left(\tilde{\mathbf{Q}}, \nabla\tilde{\mathbf{Q}}\right) = \frac{1}{2}|\nabla\tilde{\mathbf{Q}}|^2 - \frac{\operatorname{tr}\tilde{\mathbf{Q}}^2}{2} - \frac{\sqrt{6}h_+}{t}\operatorname{tr}\tilde{\mathbf{Q}}^3 + \frac{h_+^2}{2t}\left(\operatorname{tr}\tilde{\mathbf{Q}}^2\right)^2 + C(t)$$

with $C(t)$ defined as in (20)*. Then*

$$\frac{1}{r}\int_{B(\mathbf{x},r)} e\left(\tilde{\mathbf{Q}}^t, \nabla\tilde{\mathbf{Q}}^t\right) \, dV \le \frac{1}{R}\int_{B(\mathbf{x},R)} e\left(\tilde{\mathbf{Q}}^t, \nabla\tilde{\mathbf{Q}}^t\right) \, dV \tag{45}$$

for all $\mathbf{x} \in B(0,\tilde{R}_t)$ and $r \le R$ such that $B(\mathbf{x},R) \subset B(0,\tilde{R}_t)$.

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Proof. The proof can be found in [16, Lem. 2]. An analogous boundary monotonicity formula can be found in [16, Lem. 9]. ∎

PROPOSITION 4. *For each $t > 0$, let $\tilde{\mathbf{Q}}^t \in W^{1,2}(B(0,\tilde{R}_t); S_0)$ be a minimizer of the dimensionless Landau–de Gennes energy $\tilde{\mathcal{I}}_{LG}$ defined in* (20) *on the admissible class $\mathcal{A}_{\mathbf{Q}}$ of* (23)*. 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) $s(\mathbf{x})$ *in the representation* (11) *for $\tilde{\mathbf{Q}}^{t_j}$ is nonnegative for a.e. $\mathbf{x} \in B(0,\tilde{R}_{t_j})$,*

(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, in $C^k_{\mathrm{loc}}(\mathbb{R}^3; S_0)$ for every $k \in \mathbb{N}$, to a uniaxial solution $\tilde{\mathbf{Q}}^\infty \in C^\infty(\mathbb{R}^3; S_0)$ of the Ginzburg–Landau equations* (28) *satisfying $\tilde{\mathbf{Q}}^\infty(0) = 0$ and*

$$\frac{1}{R}\int_{B(0,R)} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}^\infty|^2 + \frac{(1-|\tilde{\mathbf{Q}}^\infty|^2)^2}{4}\, dV \le 12\pi \tag{46}$$

for all $R > 0$.

Proof. Define $\tilde{\mathbf{x}}_t^* = \frac{\mathbf{x}_a^*}{\xi_b}$, with $\mathbf{x}_a^*$ as in Proposition 2(v) and ξ_b as in (15). Note first that

$$\tilde{\mathcal{I}}_{LG}[\tilde{\mathbf{Q}}] = \int_{B(0,\tilde{R}_t)} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}|^2 + \frac{1}{4}\left[(1-|\tilde{\mathbf{Q}}|^2)^2 + \bar{f}(t,\tilde{\mathbf{Q}})\right]\, dV$$

with $\bar{f}(t,\tilde{\mathbf{Q}})$ given by (40). Since $\tilde{\mathbf{Q}}^t$ is uniaxial and $|\tilde{\mathbf{Q}}^t| \le 1$ (by Proposition 2(ii)), we have

$$\frac{t}{h_+} f(t,\tilde{\mathbf{Q}}^t) = (1-|\tilde{\mathbf{Q}}^t|)\left[(1-|\tilde{\mathbf{Q}}^t|^3) + |\tilde{\mathbf{Q}}^t|(1-|\tilde{\mathbf{Q}}^t|^2) + |\tilde{\mathbf{Q}}^t|^2(1-|\tilde{\mathbf{Q}}^t|)\right] \ge 0. \tag{47}$$

(It is easy to check that $\sqrt{6}\,\mathrm{tr}\,\mathbf{Q}^3 = |\mathbf{Q}|^3$ for uniaxial tensors.) Let $\tilde{R}_t^* = \tilde{R}_t - |\tilde{\mathbf{x}}_t^*|$. Combining (47) with Proposition 3 and with the fact that $\tilde{\mathcal{I}}_{LG}[\tilde{\mathbf{Q}}^t] \le \tilde{\mathcal{I}}_{LG}[\tilde{\mathbf{Q}}^0] = 12\pi\tilde{R}_t$ (which comes from the energy minimality of $\tilde{\mathbf{Q}}^t$ on $\mathcal{A}_{\mathbf{Q}}$, the fact that $\tilde{\mathbf{Q}}^0 \in \mathcal{A}_{\mathbf{Q}}$, and that f_B attains its minimum in $\mathbf{Q}_{\min}$), we obtain

$$\begin{aligned}
&\frac{1}{R}\int_{B(\tilde{\mathbf{x}}_t^*,R)} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}^t|^2 + \frac{(1-|\tilde{\mathbf{Q}}^t|^2)^2}{4}\, dV \\
&\quad\le \frac{1}{\tilde{R}_t^*}\int_{B(\tilde{\mathbf{x}}_t^*,\tilde{R}_t^*)} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}^t|^2 + \frac{(1-|\tilde{\mathbf{Q}}^t|^2)^2}{4}\, dV \\
&\quad\le \frac{1}{\tilde{R}_t^*}\int_{B(0,\tilde{R}_t)} \frac{1}{2}|\nabla\tilde{\mathbf{Q}}^t|^2 + \frac{(1-|\tilde{\mathbf{Q}}^t|^2)^2}{4}\, dV \le 12\pi\frac{\tilde{R}_t}{\tilde{R}_t^*}
\end{aligned} \tag{48}$$

for every $t > 0$ and every $R < \tilde{R}_t^*$. From this energy bound, it is easy to obtain the existence of a diagonal sequence (for the "shifted" maps $\tilde{\mathbf{x}} \mapsto \tilde{\mathbf{Q}}^t(\tilde{\mathbf{x}}+\tilde{\mathbf{x}}_t^*)$) converging weakly in $W^{1,2}_{\mathrm{loc}} \cap L^4_{\mathrm{loc}}(\mathbb{R}^3; S_0)$ to a limit map $\tilde{\mathbf{Q}}^\infty$ belonging to this functional space and satisfying (46) (note that $\lim_{t\to\infty} \frac{\tilde{R}_t}{\tilde{R}_t^*} = 1$ by Proposition 2(v)). From (34) and (17), one can check that $\tilde{\mathbf{Q}}^\infty$ solves the weak form of the Ginzburg–Landau equations (28) in $\mathbb{R}^3$. The fact that $\tilde{\mathbf{Q}}^\infty$ is smooth and a classical solution of (28), and that the diagonal sequence converges not only weakly in $W^{1,2}$ to $\tilde{\mathbf{Q}}^\infty$ but also in $C^k_{\mathrm{loc}}(\mathbb{R}^3; S_0)$

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for all $k \in \mathbb{N}$, follows by elliptic regularity theory. The proof of (iii) can be found in [15, Lem. 2]. Finally, $\tilde{\mathbf{Q}}^{\infty}(0) = 0$ since the map $\tilde{\mathbf{x}} \mapsto \tilde{\mathbf{Q}}^t(\tilde{\mathbf{x}} + \tilde{\mathbf{x}}_t^*)$ satisfies $\tilde{\mathbf{Q}}^t(\tilde{\mathbf{x}}_t^*) = 0$ for every $t > 0$. ∎

The following proposition has been proved in [9], [18], and [12].

PROPOSITION 5 (radial-hedgehog solution). *For every t sufficiently large, there exists a unique solution $h : [0, R_t] \to \mathbb{R}$ for the ordinary differential equation*

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h^3 - h + \frac{3h_+}{t}\left(h^3 - h^2\right) \tag{49}$$

subject to the boundary conditions

$$h(0) = 0, \qquad h(R_t) = 1. \tag{50}$$

(Recall the definition of h_+ in (17) *and $R_t = R_0\sqrt{\frac{b^4 t}{27c^2L}}$; for $t = \infty$, the boundary-value problem is to be understood as in* (26)*.) The corresponding solution $h_t : [0, R_t] \to \mathbb{R}$ is analytic and monotonically increasing and satisfies*

$$h_t(0) = h_t^{'}(0) = 0; \qquad h_t^{''}(0) > 0. \tag{51}$$

Let $h(r) = \lim_{t\to\infty} h_t(r)$; then $h(0) = h^{'}(0) = 0$, $h^{''}(0) > 0$, $h^{'}(r) > 0$ for $r > 0$ and we have the following explicit bounds:

$$0 < \frac{r^2}{r^2 + 14} \le h(r) \le \frac{r^2}{r^2 + 3} < 1 \quad \forall\, r \in (0, \infty). \tag{52}$$

4. Symmetry of uniaxial Ginzburg–Landau minimizers. As explained in the introduction, this section is based on and follows the exposition in the recent paper by Pisante [23] on the radial symmetry of critical points for the vector-valued Ginzburg–Landau equations in $\mathbb{R}^N$, $N \ge 3$. Our goal here is to adapt the division trick of Mironescu [20] to the Landau–de Gennes framework for nematic liquid crystals.

As in the proof of Proposition 1, we drop the tilde on the dimensionless variables in (15) and all subsequent results are to be understood in terms of the dimensionless variables.

PROPOSITION 6. *Let $\mathbf{Q} : \mathbb{R}^3 \to S_0$ be a classical and uniaxial solution of* (28) *satisfying* (46)*. Suppose that $\mathbf{Q}(0) = 0$ and that*

$$s(\mathbf{x}) \text{ in the representation (11) is nonnegative.} \tag{53}$$

Define

$$\mathbf{S}_{ij}(\mathbf{x}) = \frac{\mathbf{Q}_{ij}(\mathbf{x})}{h(|\mathbf{x}|)}, \tag{54}$$

where h is the unique solution of the boundary-value problem (26)*. Then $\frac{\partial \mathbf{S}}{\partial |\mathbf{x}|} = 0$ and $|\mathbf{S}(\mathbf{x})| = 1$ for all $\mathbf{x} \in \mathbb{R}^3$.*

The proof of Proposition 6 is postponed. The first step is to compute the system of partial differential equations satisfied by $\mathbf{S}$:

$$\Delta \mathbf{S}_{ij} + h^2\left(1 - |\mathbf{S}|^2\right)\mathbf{S}_{ij} = -2\frac{h^{'}}{h}\mathbf{S}_{ij,k}\frac{\mathbf{x}_k}{|\mathbf{x}|} - \frac{6\mathbf{S}_{ij}}{|\mathbf{x}|^2}, \quad i, j = 1, 2, 3. \tag{55}$$

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Following the methods in [23], we proceed by multiplying both sides of (55) with $\mathbf{S}_{ij,k}\frac{\mathbf{x}_k}{|\mathbf{x}|}$,

$$\mathbf{S}_{ij,k}\frac{\mathbf{x}_k}{|\mathbf{x}|}\Delta\mathbf{S}_{ij} = \frac{1}{|\mathbf{x}|}\left(\frac{\partial\mathbf{S}_{ij}}{\partial|\mathbf{x}|}\right)^2 + \frac{\partial}{\partial\mathbf{x}_p}\left[-\frac{1}{2}|\nabla\mathbf{S}|^2\frac{\mathbf{x}_p}{|\mathbf{x}|} + \mathbf{S}_{ij,k}\frac{\mathbf{x}_k}{|\mathbf{x}|}\mathbf{S}_{ij,p}\right], \tag{56}$$

(57)

$$h^2(|\mathbf{x}|)(1-|\mathbf{S}|^2)\mathbf{S}_{ij}\mathbf{S}_{ij,k}\frac{\mathbf{x}_k}{|\mathbf{x}|} = \left[\frac{(1-|\mathbf{S}|^2)^2}{4}\left[2hh^{'} + \frac{2h^2}{r}\right] - \frac{\partial}{\partial\mathbf{x}_p}\left(\frac{\mathbf{x}_p}{|\mathbf{x}|}\frac{h^2\left(1-|\mathbf{S}|^2\right)^2}{4}\right)\right],$$

$$-2\frac{h^{'}}{h}\mathbf{S}_{ij,k}\frac{\mathbf{x}_k}{|\mathbf{x}|}\mathbf{S}_{ij,p}\frac{\mathbf{x}_p}{|\mathbf{x}|} = -2\frac{h^{'}}{h}\left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2, \text{ and} \tag{58}$$

$$-6\frac{\mathbf{S}_{ij}}{|\mathbf{x}|^2}\mathbf{S}_{ij,p}\frac{\mathbf{x}_p}{|\mathbf{x}|} = \frac{\partial}{\partial\mathbf{x}_p}\left[\frac{3\mathbf{x}_p}{|\mathbf{x}|^3}(1-|\mathbf{S}|^2)\right]. \tag{59}$$

Using (56)–(59), we obtain

$$\frac{\partial\mathbf{\Phi}_p}{\partial\mathbf{x}_p} = \frac{1}{|\mathbf{x}|}\left(\frac{\partial\mathbf{S}_{ij}}{\partial|\mathbf{x}|}\right)^2 + \frac{(1-|\mathbf{S}|^2)^2}{4}\left[2hh^{'} + \frac{2h^2}{r}\right] + 2\frac{h^{'}}{h}\left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2 \tag{60}$$

with

(61)

$$\mathbf{\Phi}_p = \frac{1}{2}|\nabla\mathbf{S}|^2\frac{\mathbf{x}_p}{|\mathbf{x}|} - \frac{\mathbf{S}_{ij,k}\mathbf{x}_k}{|\mathbf{x}|}\mathbf{S}_{ij,p} + \frac{\mathbf{x}_p}{|\mathbf{x}|}\frac{h^2\left(1-|\mathbf{S}|^2\right)^2}{4} + \frac{3\mathbf{x}_p(1-|\mathbf{S}|^2)}{|\mathbf{x}|^3}, \quad p = 1,2,3.$$

For the proof of Proposition 6, we need the following lemmas.

LEMMA 3. *Let $\mathbf{Q} : B(0,\delta) \subset \mathbb{R}^3 \to S_0$ be a traceless, symmetric, uniaxial tensor-valued map defined in a neighborhood $B(0,\delta) \subset \mathbb{R}^3$ of $\mathbf{x} = 0$. Suppose that $\mathbf{Q}(0) = 0$ and that $\mathbf{Q}$ is differentiable at $\mathbf{x} = 0$. Suppose further that $s(\mathbf{x})$ in the representation* (11) *is nonnegative. Then $\nabla\mathbf{Q}(0) = 0$.*

Proof. Suppose, for a contradiction, that $\nabla\mathbf{Q}(0)\,\mathbf{e} \neq 0$ for some $\mathbf{e} \in \mathbb{S}^2$. We have

$$\lim_{t\to 0^+}\frac{|\mathbf{Q}(t\mathbf{e})|}{t} = \left|\lim_{t\to 0^+}\frac{\mathbf{Q}(t\mathbf{e})}{t}\right| = |\nabla\mathbf{Q}(0)\,\mathbf{e}|. \tag{62}$$

In particular, $\mathbf{Q}(t\mathbf{e}) \neq \mathbf{0}$ for all t in a neighborhood of $t = 0$. Let $\mathbf{n}(t\mathbf{e})$ denote either of the two unit vectors in the representation (see the note after Lemma 1)

$$\mathbf{Q}(t\mathbf{e}) = \sqrt{\frac{3}{2}}|\mathbf{Q}(t\mathbf{e})|\left(\mathbf{n}\otimes\mathbf{n} - \frac{\mathbf{I}}{3}\right). \tag{63}$$

Since $\mathbf{Q}(t\mathbf{e}) \neq 0$ for all t close to $t = 0$, we can say that

$$\lim_{t\to 0^+}\sqrt{\frac{3}{2}}\left(\mathbf{n}(t\mathbf{e})\otimes\mathbf{n}(t\mathbf{e}) - \frac{\mathbf{I}}{3}\right) = \lim_{t\to 0^+}\frac{\frac{\mathbf{Q}(t\mathbf{e})}{t}}{\frac{|\mathbf{Q}(t\mathbf{e})|}{t}} = \frac{\nabla\mathbf{Q}(0)\,\mathbf{e}}{|\nabla\mathbf{Q}(0)\,\mathbf{e}|}. \tag{64}$$

By the same argument, also

$$\lim_{t\to 0^+}\sqrt{\frac{3}{2}}\left(\mathbf{n}(-t\mathbf{e})\otimes\mathbf{n}(-t\mathbf{e}) - \frac{\mathbf{I}}{3}\right) = \lim_{t\to 0^+}\frac{\frac{\mathbf{Q}(-t\mathbf{e})}{t}}{\frac{|\mathbf{Q}(-t\mathbf{e})|}{t}} = -\frac{\nabla\mathbf{Q}(0)\,\mathbf{e}}{|\nabla\mathbf{Q}(0)\,\mathbf{e}|}. \tag{65}$$

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We would then have that

$$\lim_{t\to 0^+} \det\left(\mathbf{n}(-t\mathbf{e})\otimes\mathbf{n}(-t\mathbf{e})-\frac{\mathbf{I}}{3}\right) = -\lim_{t\to 0^+}\det\left(\mathbf{n}(t\mathbf{e})\otimes\mathbf{n}(t\mathbf{e})-\frac{\mathbf{I}}{3}\right), \tag{66}$$

but the determinant of a tensor of the form $\mathbf{n}\otimes\mathbf{n}-\frac{\mathbf{I}}{3}$ is always equal to $2/27$, yielding a contradiction. This finishes the proof. ∎

LEMMA 4. *Let $\mathbf{Q}\in C^\infty(\mathbb{R}^3;S_0)$ be a uniaxial solution of* (28) *satisfying* (53) *and* $\mathbf{Q}(0)=0$. *Define*

$$\mathbf{B}_{ij\alpha\beta} = \frac{\mathbf{Q}_{ij,\alpha\beta}(0)}{h''(0)}, \quad i,j,\alpha,\beta = 1\dots 3. \tag{67}$$

Then $\mathbf{B}_{ij\alpha\beta}=\mathbf{B}_{ji\alpha\beta}$, $\mathbf{B}_{ij\alpha\beta}=\mathbf{B}_{ij\beta\alpha}$, $\mathbf{B}_{ij\alpha\alpha}=0$, *and* $\mathbf{B}_{ii\alpha\beta}=0$ *for all* $i,j,\alpha,\beta = 1\dots 3$, *and*

$$\mathbf{S}_{ij}(\mathbf{x}) = \mathbf{B}_{ij\alpha\beta}\frac{\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}+o(1) \quad \textit{and} \quad \frac{\partial \mathbf{S}_{ij}}{\partial \mathbf{x}_\gamma} = \frac{\partial}{\partial \mathbf{x}_\gamma}\left[\mathbf{B}_{ij\alpha\beta}\frac{\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right]+O(1) \tag{68}$$

as $\mathbf{x}\to 0$, *where S is defined as in* (54).

Proof. From equality of mixed partial derivatives, we have that $\mathbf{Q}_{ij,\alpha\beta}=\mathbf{Q}_{ij,\beta\alpha}$. The relations $\mathbf{B}_{ij\alpha\beta}=\mathbf{B}_{ji\alpha\beta}$ and $\mathbf{B}_{ii\alpha\beta}=0$ follow by recalling that $\mathbf{Q}(0)\in S_0$. Finally $\mathbf{B}_{ij\alpha\alpha}=0$ since $\Delta\mathbf{Q}=(|\mathbf{Q}|^2-1)\mathbf{Q}$ and $\mathbf{Q}(0)=0$. The estimates in (68) readily follow from Lemma 3, the fact that $h(0)=h'(0)=0$, and by computing the Taylor expansion of $\mathbf{Q}$ and h near the origin. ∎

LEMMA 5. *The integral*

$$\int_{|\mathbf{x}|=1}\frac{1}{2}\left|\nabla\left(\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right)\right|^2-\frac{3}{|\mathbf{x}|^2}\left|\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right|^2 dA = 0 \tag{69}$$

for any constant $\mathbf{B}_{ij\alpha\beta}$ *such that* $\mathbf{B}_{ij\alpha\beta}=\mathbf{B}_{ji\alpha\beta}$, $\mathbf{B}_{ij\alpha\beta}=\mathbf{B}_{ij\beta\alpha}$, *and* $\mathbf{B}_{ij\alpha\alpha}=\mathbf{B}_{ii\alpha\beta}=0$.

Proof. A direct computation shows that

$$\frac{1}{2}\left|\nabla\left(\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right)\right|^2 = \frac{2}{|\mathbf{x}|^4}\mathbf{B}_{ijpq}\mathbf{B}_{ijrs}\mathbf{x}_q\mathbf{x}_s\left(\delta_{rp}-\frac{\mathbf{x}_r\mathbf{x}_p}{|\mathbf{x}|^2}\right) \tag{70}$$

and

$$\frac{3}{|\mathbf{x}|^2}\left|\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right|^2 = \frac{3}{|\mathbf{x}|^6}\mathbf{B}_{ijpq}\mathbf{B}_{ijrs}\mathbf{x}_p\mathbf{x}_q\mathbf{x}_r\mathbf{x}_s \tag{71}$$

so that

$$\begin{aligned}&\int_{|\mathbf{x}|=1}\frac{1}{2}\left|\nabla\left(\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right)\right|^2-\frac{3}{|\mathbf{x}|^2}\left|\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right|^2 dA\\ &= \mathbf{B}_{ijpq}\mathbf{B}_{ijrs}\left[2\delta_{rp}\int_{|\mathbf{x}|=1}\mathbf{x}_q\mathbf{x}_s dA - 5\int_{|\mathbf{x}|=1}\mathbf{x}_p\mathbf{x}_q\mathbf{x}_r\mathbf{x}_s dA\right]\end{aligned} \tag{72}$$

for $i,j,p,q,r,s=1,2,3$.

Using spherical coordinate representation, we can check that

$$\int_{|\mathbf{x}|=1}\mathbf{x}_q\mathbf{x}_s dA = \frac{4\pi}{3}\delta_{qs} \tag{73}$$

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and

$$\int_{|\mathbf{x}|=1} \mathbf{x}_p\mathbf{x}_q\mathbf{x}_r\mathbf{x}_s dA = \frac{4\pi}{15}\left[\delta_{pq}\delta_{rs} + \delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr}\right]. \tag{74}$$

Substituting (73) and (74) into (72), we obtain

$$\begin{aligned}&\int_{|\mathbf{x}|=1} \frac{1}{2}\left|\nabla\left(\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right)\right|^2 - \frac{3}{|\mathbf{x}|^2}\left|\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right|^2 dA \\ &= \frac{4\pi}{3}\left[2\mathbf{B}_{ijrs}\mathbf{B}_{ijrs} - \mathbf{B}_{ijpp}\mathbf{B}_{ijss} - \mathbf{B}_{ijqr}\mathbf{B}_{ijrq} - \mathbf{B}_{ijsr}\mathbf{B}_{ijrs}\right]\end{aligned} \tag{75}$$

and the right-hand side vanishes since $\mathbf{B}_{ijss} = 0$ and $\mathbf{B}_{ijsr} = \mathbf{B}_{ijrs}$. The integral equality (69) now follows. ∎

LEMMA 6. *Let* $\mathbf{Q} \in C^\infty(\mathbb{R}^3; S_0)$ *be a uniaxial solution of* (28) *satisfying* (53) *and* $\mathbf{Q}(0) = 0$. *Then*

$$\int_{|\mathbf{x}|=\delta} \Phi_p \frac{\mathbf{x}_p}{|\mathbf{x}|} dA \to 12\pi \quad \text{as } \delta \to 0, \tag{76}$$

where Φ_p *is defined in* (61) *and* dA *is the surface area element on* $\partial B(0,\delta)$.

Proof. By the definition of Φ_p in (61), we have

$$\begin{aligned}&\int_{|\mathbf{x}|=\delta} \Phi_p \frac{\mathbf{x}_p}{|\mathbf{x}|} dA \\ &= \int_{|\mathbf{x}|=\delta} \frac{1}{2}|\nabla\mathbf{S}|^2 - \left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2 + \frac{h^2(1-|\mathbf{S}|^2)^2}{4} + \frac{3\left(1-|\mathbf{S}|^2\right)}{|\mathbf{x}|^2} dA.\end{aligned} \tag{77}$$

By Lemma 4, we have that

$$\left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2 = o(|\mathbf{x}|^{-2}) \quad \text{and} \quad 1 - |\mathbf{S}|^2 = \frac{|\mathbf{x}|^4 - |\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta|^2}{|\mathbf{x}|^4} + o(1). \tag{78}$$

Substituting (78) into (77), we get

$$\begin{aligned}\int_{|\mathbf{x}|=\delta} \Phi_p \frac{\mathbf{x}_p}{|\mathbf{x}|} dA &= \int_{|\mathbf{x}|=\delta} \frac{1}{2}\left|\nabla\left(\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right)\right|^2 \\ &\quad + 3\left(\frac{|\mathbf{x}|^4 - |\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta|^2}{|\mathbf{x}|^6}\right) + o(|\mathbf{x}|^{-2})\, dA \\ &= 12\pi + o(1) + \int_{|\mathbf{x}|=\delta} \frac{1}{2}\left|\nabla\left(\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right)\right|^2 \\ &\quad - \frac{3}{|\mathbf{x}|^2}\left|\frac{\mathbf{B}_{ij\alpha\beta}\mathbf{x}_\alpha\mathbf{x}_\beta}{|\mathbf{x}|^2}\right|^2 dA.\end{aligned} \tag{79}$$

The conclusion of Lemma 6 then follows by Lemma 5. ∎

PROPOSITION 7. *Let* $\mathbf{Q} \in C^2(\mathbb{R}^3; S_0)$ *be a uniaxial solution of* (28) *satisfying* (46), (53), *and* $\mathbf{Q}(0) = 0$. *Then*

$$\begin{aligned}&\lim_{R\to\infty} \frac{1}{R}\int_{B(0,R)} \frac{1}{2}|\nabla\mathbf{S}|^2 + \frac{\left(1-|\mathbf{S}|^2\right)^2}{4}\, dV \le 12\pi \\ &\lim_{R\to\infty} \frac{1}{R}\int_{B(0,R)} \frac{|1-|\mathbf{S}|^2|}{|\mathbf{x}|^2}\, dV = 0,\end{aligned} \tag{80}$$

where $\mathbf{S}$ *is defined as in* (54).

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Proof. As in [16, Lem. 2], it is possible to prove that if $\Delta\mathbf{Q} = (|\mathbf{Q}|^2 - 1)\mathbf{Q}$, then

$$\begin{aligned}\frac{1}{R}\int_{B(0,R)} e(\mathbf{Q},\nabla\mathbf{Q})\ dV - \frac{1}{r}\int_{B(0,r)} e(\mathbf{Q},\nabla\mathbf{Q})\ dV \\ \geq \int_r^R \frac{1}{2t^2}\int_{B(0,t)} (1-|\mathbf{Q}|^2)^2\ dV\ dt \\ \geq \frac{1}{2}\left(\frac{1}{r}-\frac{1}{R}\right)\int_{B(0,r)} (1-|\mathbf{Q}|^2)^2\ dV\end{aligned} \tag{81}$$

with $e(\mathbf{Q},\nabla\mathbf{Q}) = \frac{1}{2}|\nabla\mathbf{Q}|^2 + \frac{(1-|\mathbf{Q}|^2)^2}{4}$ for all r and R such that $r < R$. In particular, $\frac{1}{R}\int_{B(0,R)} e(\mathbf{Q},\nabla\mathbf{Q})\ dV$ is monotone and bounded. Hence, as in [19, Lem. 4.1], if we set $r = R/2$, the left-hand side of (81) tends to zero as $R \to \infty$ (by virtue of (46)). Therefore,

$$\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)} (1-|\mathbf{Q}|^2)^2\ dV = 0. \tag{82}$$

Note that

$$\left|1-|\mathbf{S}|^2\right|^2 \leq 2\left(\left|1-\frac{1}{h^2}\right|^2 + \frac{\left|1-|\mathbf{Q}|^2\right|^2}{h^4}\right). \tag{83}$$

By (68), it is clear that $|\mathbf{S}|$ is bounded as $\mathbf{x} \to 0$. For $|\mathbf{x}|^2 \geq 1$, we recall the bounds in (52) to find

$$\left|1-\frac{1}{h^2}\right|^2 \leq \frac{\delta_1}{|\mathbf{x}|^4} \quad \text{and} \quad \frac{\left|1-|\mathbf{Q}|^2\right|^2}{h^4} \leq \delta_2\left|1-|\mathbf{Q}|^2\right|^2 \quad \text{for } |\mathbf{x}|^2 \geq 1 \tag{84}$$

for some constants $\delta_1, \delta_2 > 0$. Combining the inequalities (83) and (84), we obtain

$$\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)} \left|1-|\mathbf{S}|^2\right|^2\ dV \leq 2\delta_2 \lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)} \left(1-|\mathbf{Q}|^2\right)^2\ dV = 0. \tag{85}$$

Next, we turn to the elastic term, $|\nabla\mathbf{S}|^2$. For $\mathbf{x}$ close to the origin, we have that $|\nabla\mathbf{S}| = O(|\mathbf{x}|^{-1})$ by virtue of (68). Hence

$$\int_{B(0,r_0)} \frac{1}{2}|\nabla\mathbf{S}|^2\ dV \leq \delta_4 r_0^3 \tag{86}$$

for all r_0 small and some $\delta_4 > 0$. On $B(0,R)\setminus B(0,r_0)$, an explicit computation shows that

$$|\nabla\mathbf{S}|^2 = \frac{|\nabla\mathbf{Q}|^2}{h^2} + |\mathbf{Q}|^2\left(\frac{h'}{h^2}\right)^2 - 2\mathbf{Q}_{ij}\mathbf{Q}_{ij,k}\frac{\mathbf{x}_k}{|\mathbf{x}|}\frac{h'}{h^3}, \quad i,j,k = 1\ldots 3. \tag{87}$$

For $|\mathbf{x}| \geq r_0$, we recall from [18] that

$$\left|h'(|\mathbf{x}|)\right| \leq \frac{\delta_5}{|\mathbf{x}|^3} \quad \text{and} \quad \frac{|\nabla\mathbf{Q}|^2}{h^2} = |\nabla\mathbf{Q}|^2\left(1+\frac{\delta_6}{|\mathbf{x}|^2}\right) \tag{88}$$

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for some constants δ_5 and $\delta_6 > 0$. Combining (85)–(88), we deduce the following chain of inequalities:

$$\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{1}{2}|\nabla\mathbf{S}|^2+\frac{\left|1-|\mathbf{S}|^2\right|^2}{4}\,dV=\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{1}{2}|\nabla\mathbf{S}|^2\,dV$$
$$\leq\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{1}{2}|\nabla\mathbf{Q}|^2\,dV\leq 12\pi, \tag{89}$$

where the last inequality follows from (46).

Finally, we turn to the integral $\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{|1-|\mathbf{S}|^2|}{|\mathbf{x}|^2}\,dV$. Recall that $|\mathbf{S}|$ is bounded close to the origin (see (68)); hence a direct computation shows that

$$\int_{B(0,1)}\frac{|1-|\mathbf{S}|^2|}{|\mathbf{x}|^2}\,dV\leq\delta_8 \tag{90}$$

for some constant $\delta_8>0$. On the region $B(0,R)\setminus B(0,1)$, we use Young's inequality to deduce

$$\frac{|1-|\mathbf{S}|^2|}{|\mathbf{x}|^2}\leq\frac{1}{2}\left[\frac{\left(1-|\mathbf{S}|^2\right)^2}{4}+\frac{4}{|\mathbf{x}|^4}\right]. \tag{91}$$

Combining (90)–(91) and recalling (85), we obtain

$$\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{|1-|\mathbf{S}|^2|}{|\mathbf{x}|^2}\,dV$$
$$\leq\lim_{R\to\infty}\left[\frac{\delta_8}{R}+\frac{1}{2R}\int_{B(0,R)\setminus B(0,1)}\frac{\left(1-|\mathbf{S}|^2\right)^2}{4}\,dV+\frac{1}{2R}\int_{B(0,R)\setminus B(0,1)}\frac{4}{|\mathbf{x}|^4}\,dV\right]=0 \tag{92}$$

as required. The proof of Proposition 7 is now complete. ∎

Proof of Proposition 6. We integrate both sides of (60) over the ball $B(0,r)\subset\mathbb{R}^3$, integrate again from $r=0$ to $r=R$, divide by R, use Lemma 6, and take the limit $R\to\infty$ to obtain

$$12\pi+\lim_{R\to\infty}\frac{1}{R}\int_0^R\int_{B(0,r)}\frac{1}{|\mathbf{x}|}\left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2$$
$$+\frac{\left(1-|\mathbf{S}|^2\right)^2}{4}\left[2h'h+\frac{2h^2}{|\mathbf{x}|}\right]+\frac{2h'}{h}\left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2\,dV\,dr$$
$$=\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{1}{2}|\nabla\mathbf{S}|^2-\left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2+\frac{h^2\left(1-|\mathbf{S}|^2\right)^2}{4}+\frac{3\left(1-|\mathbf{S}|^2\right)}{|\mathbf{x}|^2}\,dV. \tag{93}$$

From (80), we have that

$$\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{3\left(1-|\mathbf{S}|^2\right)}{|\mathbf{x}|^2}\,dV=0$$

and

$$\lim_{R\to\infty}\frac{1}{R}\int_{B(0,R)}\frac{1}{2}|\nabla\mathbf{S}|^2-\left(\frac{\partial\mathbf{S}}{\partial|\mathbf{x}|}\right)^2+\frac{h^2\left(1-|\mathbf{S}|^2\right)^2}{4}\leq 12\pi$$

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since $h^2(|\mathbf{x}|) \leq 1$ on $\mathbb{R}^3$. We deduce that

(94)
$$\lim_{R\to\infty} \frac{1}{R}\int_0^R \int_{B(0,r)} \frac{1}{|\mathbf{x}|}\left(\frac{\partial \mathbf{S}}{\partial |\mathbf{x}|}\right)^2 + \frac{\left(1-|\mathbf{S}|^2\right)^2}{4}\left[2h^{'}h + \frac{2h^2}{|\mathbf{x}|}\right] + \frac{2h^{'}}{h}\left(\frac{\partial \mathbf{S}}{\partial |\mathbf{x}|}\right)^2 \, dV dr = 0.$$

We note that every term in the above integrand is nonnegative (recall that h is monotonically increasing; Proposition 5). Define the function

$$A(R) = \int_{B(0,R)} \frac{1}{|\mathbf{x}|}\left(\frac{\partial \mathbf{S}}{\partial |\mathbf{x}|}\right)^2 + \frac{\left(1-|\mathbf{S}|^2\right)^2}{4}\left[2h^{'}h + \frac{2h^2}{|\mathbf{x}|}\right] + \frac{2h^{'}}{h}\left(\frac{\partial \mathbf{S}}{\partial |\mathbf{x}|}\right)^2 \, dV$$

and we note that $A(R)$ is an increasing function of R. From (94), we deduce that

$$\frac{1}{2}A\left(\frac{R}{2}\right) \leq \lim_{R\to\infty} \frac{1}{R}\int_{R/2}^R A(s)ds = 0$$

and hence,

$$\int_{B(0,R)} \frac{1}{|\mathbf{x}|}\left(\frac{\partial \mathbf{S}}{\partial |\mathbf{x}|}\right)^2 + \frac{\left(1-|\mathbf{S}|^2\right)^2}{4}\left[2h^{'}h + \frac{2h^2}{|\mathbf{x}|}\right] + \frac{2h^{'}}{h}\left(\frac{\partial \mathbf{S}}{\partial |\mathbf{x}|}\right)^2 \, dV = 0$$

for every $R > 0$. The conclusion of Proposition 6 now follows. ∎

PROPOSITION 8. *Let $\mathbf{Q} \in C^2(\mathbb{R}^3; S_0)$ be a uniaxial solution of* (28) *satisfying* (46), (53), *and $\mathbf{Q}(0) = 0$. Let h denote the unique solution for the boundary-value problem* (26). *Then there exists an orthogonal matrix $\mathbf{T} \in \mathcal{O}(3)$ such that*

$$\mathbf{Q}(\mathbf{x}) = \sqrt{\frac{3}{2}}h(|\mathbf{x}|)\left(\frac{\mathbf{T}\mathbf{x}\otimes\mathbf{T}\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3}\right), \quad \mathbf{x} \in \mathbb{R}^3. \tag{95}$$

Proof. From Proposition 6, we have that

$$\mathbf{Q}_{ij}(\mathbf{x}) = h(|\mathbf{x}|)\mathbf{M}_{ij}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right), \tag{96}$$

where $\mathbf{M}_{ij} = \sqrt{\frac{3}{2}}(\mathbf{m}\otimes\mathbf{m} - \frac{\mathbf{I}}{3})$ for some $\mathbf{m} \in W^{1,2}(\mathbb{S}^2;\mathbb{S}^2)$ (from the uniaxial character of $\mathbf{Q}$ and Lemma 2). Note that

$$|\mathbf{M}(\mathbf{x})|^2 = 1 \quad \forall\, \mathbf{x} \in \mathbb{R}^3. \tag{97}$$

Substituting (96) into (55) yields $\Delta\mathbf{S} = -6\mathbf{S}/r^2$ with $\mathbf{S}(\mathbf{x}) = \mathbf{M}(\frac{\mathbf{x}}{r})$ and $r = |\mathbf{x}|$. We write this equation in its weak form (using that $\nabla\mathbf{S}$ and $\frac{\mathbf{S}}{r^2}$ are in $L^1(B(0,1))$ and that $\frac{\partial\mathbf{S}}{\partial r} = 0$) to obtain

$$\int_{B(0,1)} \nabla\mathbf{S}\cdot\nabla\boldsymbol{\phi}\, dV = 6\int_{B(0,1)} \frac{\mathbf{S}\cdot\boldsymbol{\phi}}{r^2}\, dV \quad \forall\, \boldsymbol{\phi} \in W^{1,2}(B(0,1);\mathbb{R}^{3\times 3}). \tag{98}$$

Extend $\mathbf{m} : \mathbb{S}^2 \to \mathbb{S}^2$ to a map $\mathbf{m} \in W^{1,2}(B(0,1);\mathbb{S}^2)$ by $\mathbf{m}(\mathbf{x}) = \mathbf{m}(\frac{\mathbf{x}}{r})$. Testing against $\boldsymbol{\phi} = \boldsymbol{\varphi}\otimes\mathbf{m}$ with $\boldsymbol{\varphi} \in (L^\infty \cap W^{1,2})(B(0,1),\mathbb{R}^3)$, and using that $\mathbf{m} \perp \frac{\partial\mathbf{m}}{\partial x_k}$ for all k,

$$\int_{B(0,1)} \left(\nabla\boldsymbol{\varphi}\cdot\nabla\mathbf{m} + (\boldsymbol{\varphi}\cdot\mathbf{m})|\nabla\mathbf{m}|^2\right) dV = 4\int_{B(0,1)} \frac{\boldsymbol{\varphi}\cdot\mathbf{m}}{r^2}\, dV \tag{99}$$

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for all $\boldsymbol{\varphi} \in (L^\infty \cap W^{1,2})(B(0,1);\mathbb{R}^3)$. Specializing further to test functions of the form $\boldsymbol{\varphi} = \eta\mathbf{m}$, $\eta \in C^\infty(\overline{B(0,1)})$ and noting that $2(\nabla\mathbf{m})^T\mathbf{m} = \nabla(|\mathbf{m}|^2) = 0$, we obtain

$$\int_{B(0,1)} 2\eta|\nabla\mathbf{m}|^2\, dV = 4\int_{B(0,1)} \frac{\eta}{r^2}\, dV \quad \forall\, \eta \in C^\infty(\overline{B(0,1)}), \tag{100}$$

which, in turn, implies that $|\nabla\mathbf{m}|^2 \equiv 2r^{-2}$. Substituting the above into (99), we have

$$\int_{B(0,1)} \nabla\boldsymbol{\varphi}\cdot\nabla\mathbf{m}\, dV = 2\int_{B(0,1)} \frac{\boldsymbol{\varphi}\cdot\mathbf{m}}{r^2}\, dV \quad \forall\, \boldsymbol{\varphi} \in (L^\infty \cap W^{1,2})(B(0,1);\mathbb{R}^3) \tag{101}$$

or, equivalently,

$$\int_{\mathbb{S}^2} \nabla_0\boldsymbol{\varphi}\cdot\nabla_0\mathbf{m}\, dS = 2\int_{\mathbb{S}^2} \boldsymbol{\varphi}\cdot\mathbf{m}\, dS \quad \forall\, \boldsymbol{\varphi} \in W^{1,2}(\mathbb{S}^2,\mathbb{R}^3), \tag{102}$$

where ∇_0 denotes the tangential gradient. This is the weak form of $\Delta_0\mathbf{m} = -2\mathbf{m}$ with Δ_0 being the Laplace–Beltrami operator. It follows that the components of $\mathbf{m}$ are spherical harmonics of degree one, i.e., they are restrictions to the unit sphere of entire affine functions in $\mathbb{R}^3$ (see, e.g., [3, sect. V.8, VII.5]). Hence, $\mathbf{m}(\mathbf{x}) = \mathbf{T}\frac{\mathbf{x}}{|\mathbf{x}|}$ for some constant $\mathbf{T} \in M^{3\times 3}$. Since $\mathbf{m}$ takes values on $\mathbb{S}^2 \subset \mathbb{R}^3$, it follows that $\mathbf{T} \in \mathcal{O}(3)$, thus completing the proof. ∎

5. Instability of the radial-hedgehog solution. For a fixed $t > 0$, let $\mathbf{Q}^t \in W^{1,2}_{loc}\left(\mathbb{R}^3, S_0\right)$ be an entire solution of the Euler–Lagrange equations:

$$\begin{aligned}\Delta\mathbf{Q}_{ij} = -\mathbf{Q}_{ij} - \frac{3\sqrt{6}h_+}{t}\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \mathbf{Q}_{pq}\mathbf{Q}_{pq}\frac{\delta_{ij}}{3}\right)\\ + \frac{2h_+^2}{t}\mathbf{Q}_{ij}\mathbf{Q}_{pq}\mathbf{Q}_{pq}, \quad i,j,k,p,q = 1,2,3.\end{aligned} \tag{103}$$

Definition 2. *$\mathbf{Q}^t$ is stable if the following inequality holds for any bounded open set $\Omega \subset \mathbb{R}^3$ and for any $\mathbf{P} \in C_0^\infty(\Omega, S_0)$:*

$$\int_\Omega |\nabla\mathbf{P}|^2 - |\mathbf{P}|^2 - \frac{6\sqrt{6}h_+}{t}\mathbf{Q}^t_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} + \frac{h_+^2}{2t}\left(8\left(\mathbf{Q}^t\cdot\mathbf{P}\right)^2 + 4|\mathbf{Q}^t|^2|\mathbf{P}|^2\right)\, dV \geq 0. \tag{104}$$

Definition 3. *$\mathbf{Q}^t$ is unstable if there exists a bounded open set $\Omega \subset \mathbb{R}^3$ and $\mathbf{P} \in C_0^\infty(\Omega, S_0)$ for which*

$$\int_\Omega |\nabla\mathbf{P}|^2 - |\mathbf{P}|^2 - \frac{6\sqrt{6}h_+}{t}\mathbf{Q}^t_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} + \frac{h_+^2}{2t}\left(8\left(\mathbf{Q}^t\cdot\mathbf{P}\right)^2 + 4|\mathbf{Q}^t|^2|\mathbf{P}|^2\right)\, dV < 0. \tag{105}$$

The integral inequality in (104) follows from computing the second variation of the Landau–de Gennes energy functional, as in [23]. We sketch the details of the computation below. Consider an arbitrary $\mathbf{P} \in C_0^\infty(\Omega, S_0)$ and define perturbations

$$\mathbf{Q}^\epsilon_{ij} = \mathbf{Q}^t_{ij} + \epsilon\mathbf{P}_{ij} \quad i,j = 1,2,3,$$

for $0 < \epsilon \ll 1$. One can verify by a direct computation that

$$\begin{aligned}|\nabla\mathbf{Q}^\epsilon|^2 &= |\nabla\mathbf{Q}^t|^2 + 2\epsilon\mathbf{Q}^t_{ij,k}\mathbf{P}_{ij,k} + \epsilon^2|\nabla\mathbf{P}|^2,\\ |\mathbf{Q}^\epsilon|^2 &= \left|\mathbf{Q}^t\right|^2 + 2\epsilon\mathbf{Q}^t_{ij}\mathbf{P}_{ij} + \epsilon^2|\mathbf{P}|^2,\end{aligned} \tag{106}$$

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where $\mathbf{Q}^t_{ij,k} = \frac{\partial \mathbf{Q}^t_{ij}}{\partial \mathbf{x}_k}$ etc. and $i, j, k = 1, 2, 3$. Similarly,

$$\mathbf{Q}^\epsilon_{ij}\mathbf{Q}^\epsilon_{jp}\mathbf{Q}^\epsilon_{pi} = \mathbf{Q}^t_{ij}\mathbf{Q}^t_{jp}\mathbf{Q}^t_{pi} + 3\epsilon\mathbf{Q}^t_{ij}\mathbf{Q}^t_{jp}\mathbf{P}_{pi} + 3\epsilon^2\mathbf{Q}^t_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} + \epsilon^3\mathbf{P}_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} \tag{107}$$

$$\begin{aligned}\left(\mathbf{Q}^\epsilon_{ij}\mathbf{Q}^\epsilon_{ij}\right)^2 &= |\mathbf{Q}^t|^4 + 4\epsilon|\mathbf{Q}^t|^2\left(\mathbf{Q}^t\cdot\mathbf{P}\right) + 2\epsilon^2\left(|\mathbf{Q}^t|^2|\mathbf{P}|^2 + 2\left(\mathbf{Q}^t\cdot\mathbf{P}\right)^2\right)\\ &\quad + 4\epsilon^3|\mathbf{P}|^2\left(\mathbf{Q}^t\cdot\mathbf{P}\right) + \epsilon^4|\mathbf{P}|^4.\end{aligned} \tag{108}$$

The integral inequality in (104) now follows from the positivity of the second variation of the Landau–de Gennes energy:

$$\begin{aligned}\frac{d^2\mathcal{I}_{LG}\left[\mathbf{Q}^\epsilon\right]}{d\epsilon^2}\Big|_{\epsilon=0} &= \int_\Omega |\nabla\mathbf{P}|^2 - |\mathbf{P}|^2 - \frac{6\sqrt{6}h_+}{t}\mathbf{Q}^t_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi}\\ &\quad + \frac{h_+^2}{2t}\left(8\left(\mathbf{Q}^t\cdot\mathbf{P}\right)^2 + 4|\mathbf{Q}^t|^2|\mathbf{P}|^2\right)\, dV.\end{aligned} \tag{109}$$

For each $t > 0$, let $R_t = R_0 b^2 \frac{\sqrt{t}}{\sqrt{27c^2L}}$ as before (where R_0 is independent of t) and let $B(0, R_t) \subset \mathbb{R}^3$ denote the ball of radius R_t centered at the origin. We define $\mathbf{H}^t : B(0, R_t) \to S_0$ to be

$$\mathbf{H}^t(\mathbf{x}) = \sqrt{\frac{3}{2}}h_t(r)\left(\frac{\mathbf{x}\otimes\mathbf{x}}{|\mathbf{x}|^2} - \frac{\mathbf{I}}{3}\right), \tag{110}$$

where $r = |\mathbf{x}|$ and $h_t : [0, R_t] \to \mathbb{R}$ is a solution of the following boundary-value problem:

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h^3 - h + \frac{3h_+}{t}\left(h^3 - h^2\right) \tag{111}$$

and

$$h(0) = 0, \quad h(R_t) = 1. \tag{112}$$

We recall that the boundary-value problem (111)–(112) has a solution for all $t > 0$. There exists a $t_0 > 0$ such that for all $t > t_0$, the solution, h_t, satisfies the global bounds $0 \le h_t(r) \le 1$ for $r \in [0, R_t]$. Further, for $t > t_0$, h_t is unique and monotonically increasing for $r > 0$ [12, 18].

THEOREM 3. *The tensor-field,* $\mathbf{H}^t : B(0, R_t) \to S_0$, *as defined in* (110), *is a classical solution of the system of the Euler–Lagrange equations in* (103). *There exists a* $t^* > 0$ *such that for* $t > t^*$, $\mathbf{H}^t$ *is an unstable equilibrium of the Landau–de Gennes energy in the sense of Definition* 3 *and* (105).

Proof. One can immediately check from the definition of $\mathbf{H}^t$ in (110) and the definition of h_t in (111)–(112) that $\mathbf{H}^t$ is a solution of the system of partial differential equations in (103). The instability of the radial-hedgehog solution in the $t \to \infty$ limit has been proved in [9] and similar results have been proved for finite but large values of t in [18]. We reproduce the main details here for completeness.

To demonstrate instability, it suffices to show that the second variation of the Landau–de Gennes energy is negative for a perturbation $\mathbf{P}$ localized in a ball of radius σ, independent of the reduced temperature t such that $\sigma < R_t$.

Consider the radial-hedgehog solution $\mathbf{H}(\mathbf{x}) = \sqrt{\frac{3}{2}}h_\infty(r)(\frac{\mathbf{x}\otimes\mathbf{x}}{|\mathbf{x}|^2} - \frac{1}{3}\mathbf{I})$, where h_∞ is the unique, monotonically increasing solution of the boundary-value problem [18]:

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h^3 - h \tag{113}$$

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with $h_\infty(0) = 0$ and $h_\infty(r) \to 1$ as $r \to \infty$. From [18] and [9], it is known that $\frac{r^2}{r^2+14} \leq h_\infty(r) \leq \frac{r^2}{r^2+3}$. One can readily verify that

$$\mathbf{H}^t \to \mathbf{H} \text{ in } C^2_{loc}\left(\mathbb{R}^3, S_0\right)$$

as $t \to \infty$. In what follows, we demonstrate instability of the radial-hedgehog solution $\mathbf{H}$ in the sense of Definition 3 and use the uniform convergence, $\mathbf{H}^t \to \mathbf{H}$ as $t \to \infty$, to deduce that $\mathbf{H}^t$ is unstable for $t > t^*$, where $t^* > 0$ is sufficiently large and suitably defined.

We consider perturbations of the form

$$\mathbf{Q}^\epsilon_{ij} = \mathbf{H}_{ij} + \epsilon \mathbf{P}_{ij}, \quad 0 < \epsilon \ll 1; i, j = 1, 2, 3, \tag{114}$$

where

$$\mathbf{P}_{ij}(\mathbf{x}) = p(r)\left(\mathbf{z}_i\mathbf{z}_j - \frac{1}{3}\delta_{ij}\right), \tag{115}$$

$\mathbf{z} = (0, 0, 1)$ is the unit vector in the z-direction, $p(r) \in C^\infty_0\left(B(0, \sigma), \mathbb{R}\right) \geq 0$, and $p(r) = 0$ otherwise. We work with a spherical coordinate system (r, θ, ϕ) centered at the origin. The second variation of the Landau–de Gennes energy, for this choice of the perturbation, is bounded from above by (see (104))

$$\frac{d^2\tilde{\mathcal{I}}_{LG}[\mathbf{Q}^\epsilon]}{d\epsilon^2}|_{\epsilon=0} \leq 8\pi \int_0^\sigma \frac{r^2}{3}\left(\frac{dp}{dr}\right)^2 - \frac{r^2p^2(r)}{3} + \frac{7}{15}r^2p^2(r)\left(\frac{r^2}{r^2+3}\right)^2 dr. \tag{116}$$

We compute the integral above with

$$p(r) = \frac{1}{(r^2+12)^2}\left(1 - \frac{r}{\sigma}\right)$$

and $\sigma = 50$ to find

$$\frac{d^2\tilde{\mathcal{I}}_{LG}[\mathbf{Q}^\epsilon]}{d\epsilon^2}|_{\epsilon=0} = -4 \times 10^{-6} < 0. \tag{117}$$

From the continuous dependence of $\mathbf{H}^t$ on the reduced temperature t and the uniform convergence $\frac{h_+^2}{2t} \to \frac{1}{4}$ as $t \to \infty$, we deduce that there exists a $t^* > 0$ such that for $t > t^*$,

$$\frac{d^2\tilde{\mathcal{I}}_{LG}[\mathbf{Q}^\epsilon_t]}{d\epsilon^2}|_{\epsilon=0} < \frac{1}{2}\frac{d^2\tilde{\mathcal{I}}_{LG}[\mathbf{Q}^\epsilon]}{d\epsilon^2}|_{\epsilon=0} < 0, \quad t > t^*, \tag{118}$$

where

$$\mathbf{Q}^\epsilon_t(\mathbf{x}) = \mathbf{H}^t(\mathbf{x}) + \epsilon\mathbf{P}(\mathbf{x}),$$

$\mathbf{P}$ has been defined in (115) with $p(r) = \frac{1}{(r^2+12)^2}(1 - \frac{r}{\sigma})$ and $\sigma = 50$. We conclude that $\mathbf{H}^t$ is unstable in the sense of Definition 3 and (105) for $t > t^*$ as claimed in Theorem 3. ∎

Proof of Theorem 1. We prove Theorem 1 by contradiction. Let $\left\{t^k\right\}$ be a sequence such that $t^k \to \infty$ as $k \to \infty$ and let $\{\mathbf{Q}^{t_k}\}$ be a corresponding sequence of global Landau–de Gennes minimizers in the admissible space $\tilde{\mathcal{A}}$, where

$$\tilde{\mathcal{A}} = \left\{\mathbf{Q} \in W^{1,2}\left(B(0, \tilde{R}_{t_k}); S_0\right) : \mathbf{Q} = \tilde{\mathbf{Q}}_b \text{ on } \partial B(0, \tilde{R}_{t_k})\right\},$$

where $\tilde{R}_{t_k}$ has been defined in (19) and $\mathbf{Q}_b$ has been defined in (9).

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Suppose, for a contradiction, that $\mathbf{Q}^{t_k}$ is purely uniaxial for every $k \in \mathbb{N}$ so that each $\mathbf{Q}^{t_k}$ is also a minimizer of $\tilde{\mathcal{I}}_{LG}$ in the restricted space $\mathcal{A}_{\mathbf{Q}}$ of purely uniaxial $\mathbf{Q}$-tensors. The sequence $\{\mathbf{Q}^{t_k}\}$ satisfies the hypotheses of Theorem 2. Then (passing to a subsequence if necessary), there exists a sequence $\{\tilde{\mathbf{x}}_k^*\}$ such that $\tilde{\mathbf{x}}_k^* \in B(0, \tilde{R}_{t_k})$, $\mathbf{Q}^{t_k}(\tilde{\mathbf{x}}_k^*) = 0$ for every $k \in \mathbb{N}$, $\frac{\tilde{\mathbf{x}}_k^*}{\tilde{R}_{t_k}} \to 0$ as $k \to \infty$ and for t_k sufficiently large,

$$\mathbf{Q}^{t_k}(\mathbf{x}) = \mathbf{H}(\mathbf{T}\mathbf{x}) + \mathbf{A}^{t_k}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \tag{119}$$

where $\mathbf{T}$ is an orthogonal transformation, $\mathbf{H}$ is the radial-hedgehog solution, and

$$\|\mathbf{A}^{t_k}\|_{L^\infty(B(0,\sigma))} \to 0$$

uniformly as $k \to \infty$, for every fixed $\sigma > 0$. We now compute the second variation of the Landau–de Gennes energy functional for purely uniaxial global minimizers $\mathbf{Q}^{t_k}$ in the limit $k \to \infty$, using the perturbation $\mathbf{P}$ defined in (115) with $p(r) = \frac{1}{(r^2+12)^2}\left(1 - \frac{r}{\sigma}\right)$ and $\sigma = 50$. Let $\mathbf{Q}_k^\epsilon(\mathbf{x}) = \mathbf{Q}^{t_k}(\mathbf{x} + \tilde{\mathbf{x}}_k^*) + \epsilon\mathbf{P}(\mathbf{T}\mathbf{x})$ as before; then

$$\begin{aligned}
&\frac{d^2\tilde{\mathcal{I}}_{LG}[\mathbf{Q}_k^\epsilon]}{d\epsilon^2}\Big|_{\epsilon=0} \\
&= \int_{B(0,\sigma)} |\nabla\mathbf{P}(\mathbf{T}\mathbf{x})|^2 - |\mathbf{P}(\mathbf{T}\mathbf{x})|^2 - \frac{6\sqrt{6}h_+}{t}\mathbf{P}_{ij}(\mathbf{T}\mathbf{x})\,\mathbf{P}_{jp}(\mathbf{T}\mathbf{x})\,\mathbf{Q}_{pi}^{t_k}(\mathbf{x} + \tilde{\mathbf{x}}_k^*)\,dV \\
&\quad + \int_{B(0,\sigma)} \frac{h_+^2}{2t}\left(8\left(\mathbf{Q}^{t_k}(\mathbf{x} + \tilde{\mathbf{x}}_k^*)\cdot\mathbf{P}(\mathbf{T}\mathbf{x})\right)^2 + 4|\mathbf{Q}^{t_k}(\mathbf{x} + \tilde{\mathbf{x}}_k^*)|^2|\mathbf{P}(\mathbf{T}\mathbf{x})|^2\right)\,dV.
\end{aligned} \tag{120}$$

Using (119) and working in the limit $k \to \infty$, we obtain the following inequalities:

$$\begin{aligned}
\mathbf{P}_{ij}(\mathbf{T}\mathbf{x})\,\mathbf{P}_{jp}(\mathbf{T}\mathbf{x})\,\mathbf{Q}_{pi}^{t_k}(\mathbf{x} + \tilde{\mathbf{x}}_k^*) &\le \mathbf{P}_{ij}(\mathbf{T}\mathbf{x})\,\mathbf{P}_{jp}(\mathbf{T}\mathbf{x})\,\mathbf{H}_{pi}(\mathbf{T}\mathbf{x}) + \gamma_0\|\mathbf{A}^{t_k}\|_{L^\infty(B(0,\sigma))}, \\
\left(\mathbf{Q}^{t_k}(\mathbf{x} + \tilde{\mathbf{x}}_k^*)\cdot\mathbf{P}(\mathbf{T}\mathbf{x})\right)^2 &\le \left(\mathbf{H}(\mathbf{T}\mathbf{x})\cdot\mathbf{P}(\mathbf{T}\mathbf{x})\right)^2 + \gamma_1\|\mathbf{A}^{t_k}\|_{L^\infty(B(0,\sigma))}, \\
|\mathbf{Q}^{t_k}(\mathbf{x} + \tilde{\mathbf{x}}_k^*)|^2|\mathbf{P}(\mathbf{T}\mathbf{x})|^2 &\le |\mathbf{H}(\mathbf{T}\mathbf{x})|^2|\mathbf{P}(\mathbf{T}\mathbf{x})|^2 + \gamma_2\|\mathbf{A}^{t_k}\|_{L^\infty(B(0,\sigma))},
\end{aligned} \tag{121}$$

where γ_0, γ_1, and γ_2 are positive constants independent of t_k as $k \to \infty$. In (121), we use the fact that $\mathbf{P}$ is supported on $B(0,\sigma)$ and that both $|\mathbf{P}|$ and $|\mathbf{H}|$ can be bounded independently of t_k as $k \to \infty$. Substituting the above into (120) and recalling (117) (which continues to hold after precomposing with the orthogonal transformation $\mathbf{T}$ and using a change of variable $\mathbf{X} = \mathbf{T}\mathbf{x}$), we have

$$\begin{aligned}
\frac{d^2\tilde{\mathcal{I}}_{LG}[\mathbf{Q}_k^\epsilon]}{d\epsilon^2}\Big|_{\epsilon=0} \le \int_{B(0,\sigma)} &|\nabla\mathbf{P}|^2 - |\mathbf{P}|^2 \\
&+ \frac{1}{4}\left(8(\mathbf{H}\cdot\mathbf{P})^2 + 4|\mathbf{H}|^2|\mathbf{P}|^2\right)\,dV + \gamma_3\|\mathbf{A}^{t_k}\|_{L^\infty} < 0
\end{aligned} \tag{122}$$

for k sufficiently large and $\gamma_3 > 0$ independent of t_k, since σ is independent of t and $\|\mathbf{A}^{t_k}\|_{L^\infty} \to 0$ uniformly as $k \to \infty$. It follows that $\mathbf{Q}^{t_k}$ is unstable in the sense of Definition 3 for t_k sufficiently large and hence cannot be a global Landau–de Gennes minimizer. Theorem 1 now follows. ∎

6. Conclusions. In this paper, we adapt the recent radial symmetry results for the vector-valued Ginzburg–Landau equations in $\mathbb{R}^N$ for $N \ge 3$ [19, 23] to the

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Landau–de Gennes framework for nematic liquid crystals. We use the division trick in [20] and Ginzburg–Landau methods to establish the universal character of uniaxial equilibria on spherical droplets with homeotropic boundary conditions in a certain distinguished limit. We show that for all sufficiently low temperatures, globally stable uniaxial equilibria (if they exist) can be approximated arbitrarily closely by the well-studied radial-hedgehog solution [9, 18, 25]. We then use the instability of the radial-hedgehog solution with respect to biaxial perturbations, in the low temperature limit, to demonstrate the nonexistence of purely uniaxial global Landau–de Gennes minimizers for this model problem. The equivariant radial-hedgehog solution is analogous to the equivariant degree +1-vortex in superconductivity theory. Our work elucidates the Ginzburg–Landau type features of the Landau–de Gennes theory, and the identification of these analogies is the first step in the development of new mathematical tools specific to Landau–de Gennes theory, including a rigorous description of the competing biaxial equilibria. A uniaxial $\mathbf{Q}$-tensor has three degrees of freedom, whereas a fully biaxial tensor has five degrees of freedom in a three-dimensional setting. Ginzburg–Landau techniques and methods from the theory of harmonic maps are useful for describing the far-field behavior of global Landau–de Gennes minimizers (away from defects) in the biaxial case, in certain asymptotic limits (see [2] and [16] for related work). However, it is not clear if Ginzburg–Landau methods can give any information about biaxial defects in $\mathbb{R}^3$ and it is a major mathematical challenge to understand how these extra biaxial degrees of freedom manifest themselves in physical phenomena.

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REFERENCES

[1] J.M. Ball and A. Zarnescu, *Orientability and energy minimization for liquid crystals*, Arch. Ration. Mech. Anal., 202 (2011), pp. 493–535.

[2] F. Bethuel, H. Brezis, and F. Hélein, *Asymptotics for the minimization of a Ginzburg-Landau functional*, Calc. Var. Partial Differential Equations, 1 (1993), pp. 123–148.

[3] R. Courant and D. Hilbert, *Methods of Mathematical Physics, Vol.* II*: Partial Differential Equations*, Interscience Publishers, New York, 1962.

[4] T. Davis and E. Gartland, *Finite element analysis of the Landau–De Gennes minimization problem for liquid crystals*, SIAM J. Numer. Anal., 35 (1998), pp. 336–362.

[5] J.L. Ericksen, *Liquid crystals with variable degree of orientation*, Arch. Ration. Mech. Anal., 113 (1990), pp. 97–120.

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

[7] F.C. Frank, *On the theory of liquid crystals*, Discuss. Faraday Soc., 25 (1958), p. 1.

[8] P.G. De Gennes, *The Physics of Liquid Crystals*, Clarendon Press, Oxford, UK, 1974.

[9] 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 (1999), pp. 563–567.

[10] D. Gilbarg and N. Trudinger, *Elliptic Partial Differential Equations of Second Order*, Classics Math. 224, Springer, Berlin, 1977.

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[11] R. Hardt, D. Kinderlehrer, and F.H. Lin, *Existence and partial regularity of static liquid crystals configurations*, Comm. Math. Phys., 105 (1986), pp. 547–570.

[12] X. Lamy, *Some properties of the nematic radial hedgehog in the Landau-de Gennes theory*, J. Math. Anal. Appl., to appear.

[13] F.H. Lin, *A remark on the map $x/|x|$*, Comptes Rendus des Séances de l'Académie des Sciences. Série I. Mathématique., 305 (1987), pp. 529–531.

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

[15] A. Majumdar, *Equilibrium order parameters of liquid crystals in the Landau–de Gennes theory*, European J. Appl. Math., 21 (2010), pp. 181–203.

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

[17] A. Majumdar, *The Landau-de Gennes theory of nematic liquid crystals: Uniaxiality versus Biaxiality*, Commun. Pure Appl. Anal., 11 (2012), pp. 1303–1337.

[18] A. Majumdar, *The Radial-Hedgehog solution in the Landau-de Gennes theory for nematic liquid crystals*, European J. Appl. Math., 23 (2012), pp. 61–97.

[19] V. Millot and A. Pisante, *Symmetry of local minimizers for the three-dimensional Ginzburg-Landau functional*, J. Eur. Math. Soc. (JEMS), 12 (2010), pp. 1069–1096.

[20] P. Mironescu, *Les minimiseurs locaux pour l'équation de Ginzburg-Landau sont à symétrie radiale*, Comptes Rendus de l'Académie des Sciences. Série I. Mathématique, 323 (1996), pp. 593–598.

[21] R. Moser, *Partial Regularity for Harmonic Maps and Related Problems*, World Scientific, Hackensack, NJ, 2005.

[22] N.J. Mottram and C. Newton, *Introduction to $\boldsymbol{Q}$-tensor Theory*, Research report 10, Department of Mathematics, University of Strathclyde, 2004.

[23] A. Pisante, *Two results on the equivariant Ginzburg–Landau vortex in arbitrary dimension*, J. Funct. Anal., 260 (2011), pp. 892–905.

[24] R. Schoen and K. Uhlenbeck, *A regularity theory for harmonic mappings*, J. Differential Geom., 17 (1982), pp. 307–335.

[25] A. Sonnet, A. Kilian, and S. Hess, *Alignment tensor versus director: Description of defects in nematic liquid crystals*, Phys. Rev. E, 52 (1995), pp. 718–722.

[26] E.G. Virga, *Variational Theories for Liquid Crystals*, Chapman and Hall, London, 1994.

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