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Abstract

We study the radial-hedgehog solution on a unit ball in three dimensions, with homeotropic boundary conditions, within the Landau-de Gennes theory for nematic liquid crystals. The radial-hedgehog solution is a candidate for a globally stable configuration in this model framework and is also a prototype configuration for studying isolated point defects in condensed matter physics. We use a combination of Ginzburg-Landau techniques, perturbation methods and stability analyses to study the qualitative properties of the radial-hedgehog solution, the structure of its defect core, its stability and instability with respect to biaxial perturbations. Our results complement previous work in the field, are rigorous in nature, give information about the role of geometry, elastic constants and temperature on the properties of the radial-hedgehog solution and the associated biaxial instabilities.

1 Introduction

Defect structures have attracted a lot of interest in the liquid crystal community [23, 24, 22, 20]. Defect structures in liquid crystalline systems are usually modelled within the Landau-de Gennes framework, whereby the liquid crystal configuration is mathematically described by a symmetric, traceless 3×3 matrix, known as the $\mathbf{Q}$-tensor order parameter [5]. The $\mathbf{Q}$-tensor can be written in terms of its eigenvalues and eigenvectors as shown below -

$$\mathbf{Q} = \sum_{i=1}^{3} \lambda_i \mathbf{e}_i \otimes \mathbf{e}_i, \quad \sum_i \lambda_i = 0 \tag{1}$$

where λ_i are the eigenvalues and $\mathbf{e}_i$ are the corresponding orthonormal eigenvectors. The liquid crystal is said to be in the (i) isotropic state when $\lambda_i = 0$ for $i = 1 \dots 3$, (ii) uniaxial state when $\mathbf{Q}$ has a pair of equal non-zero eigenvalues and (iii) biaxial state when $\mathbf{Q}$ has three distinct non-zero eigenvalues [19]. There is a lot of debate regarding the uniaxial versus biaxial structure of defects in confined liquid crystalline systems and which structure is energetically favourable.

A prototype example of such a confined system is a spherical droplet with *strong radial anchoring* or *homeotropic* (normal) boundary conditions. This system has been widely studied in the literature and it is generally believed that there are two competing equilibrium configurations - (a)the *radial-hedgehog* configuration which has a single isolated point defect at the droplet centre and (b) the *biaxial-torus* configuration where the point defect broadens out to a ring-like structure around the droplet centre [23, 24, 12, 16, 8]. The radial-hedgehog configuration is purely uniaxial everywhere except for an isotropic point at the droplet centre whereas the biaxial-torus configuration exhibits a high degree of biaxiality around the droplet centre. One would like to understand which structure is energetically favourable and the structural dependence on material parameters, absolute temperature and droplet size. The isotropic core of a radial-hedgehog configuration and the localized biaxial region of the biaxial-torus configuration are interpreted as *defect* structures. Secondly, the *radial-hedgehog* configuration is prototypical of vortices in the Ginzburg-Landau theory for superconductors [1]. There is a very well-developed theory for vortices in Ginzburg-Landau theory, especially in two dimensions but generalizations to higher dimensions are non-trivial [2, 17]. For example, in two dimensions, it is known that vortices of degree $+1$ or -1 are locally stable on a disc with normal boundary conditions, in the sense of the positivity of the second variation of the associated Ginzburg-Landau energy functional. In some cases, degree $+1$ vortices can also be global energy minimizers within the two-dimensional Ginzburg-Landau framework [18, 1]. The radial-hedgehog solution can be interpreted as being a degree $+1$ vortex in three dimensions. Vortices have been studied in three dimensions, within the Ginzburg-Landau framework [9, 17, 7]. For example, the existence and qualitative properties of degree $+1$ three-dimensional vortices have been studied in [7] and their local stability has been established in [9]. However, there are no higher-degree vortices in three dimensions, within the Ginzburg-Landau framework [9].

There are mathematical and physical differences between the Landau-de Gennes theory for liquid crystals and the Ginzburg-Landau theory for superconductors. The study of uniaxial liquid crystal configurations can be viewed as a generalized Ginzburg-Landau theory from $\mathbb{R}^3 \to \mathbb{R}^3$ [15], even though the nonlinearities of the governing equations are different from the nonlinearities encountered in the Ginzburg-Landau framework (see (28) and (30) for an example). This, in turn, implies that not all of the techniques from Ginzburg-Landau theory readily generalize to the theory of uniaxial configurations within the Landau-de Gennes framework. On the other hand, the study of general biaxial configurations presents a whole host of new mathematical challenges, outside the scope of Ginzburg-Landau theory [13]. In particular, there is no analogue of a biaxial instability in the current Ginzburg-Landau literature. It is important to systematically study the analogies and differences between the Landau-de Gennes and Ginzburg-Landau theoretical frameworks to bridge the two communities and effectively use the existing mathematical tools in the context of liquid crystals. In this paper, we carry out an analytic study of the radial-hedgehog configuration on a three-dimensional unit ball subject to homeotropic boundary conditions, using a combination of Ginzburg-Landau techniques, perturbation methods and stability analysis. These methods will contribute to a complete characterization of uniaxial stable configurations in three dimensions and a characterization of the competing low-energy biaxial configurations, such as the biaxial-torus configuration. In Section 2, we recall useful results from [13] and prove the existence of a radial-hedgehog configuration in the Landau-de Gennes framework and study its qualitative properties. In Sections 3 and 4, we use Ginzburg-Landau techniques to study the structure of the radial-hedgehog configuration near its isotropic core and away from the isotropic core. Our results are rigorous and are established in a physically relevant limit involving the material-dependent constants. In Section 5, we explicitly demonstrate the instability of the radial-hedgehog configuration with respect to localized biaxial perturbations for sufficiently low temperatures. This result is qualitatively similar to a result reported in [8] but our method of proof is different and we use information about the isotropic core. In Section 6, we perform a linear stability analysis of the radial-hedgehog configuration and this stability analysis gives insight into the effect of the ball radius on the associated equilibrium structure. In Section 7, we discuss our results and how they complement previous work in this area.

2 Preliminaries

We are interested in studying the qualitative properties of radial-hedgehog solutions on a unit ball, $B(0,1) \subset \mathbb{R}^3$, subject to strong radial anchoring conditions, within the Landau-de Gennes theory for nematic liquid crystals, in the low-temperature regime.

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

$$\bar{S} \stackrel{def}{=} \left\{ \mathbf{Q} \in \mathbb{M}^{3\times 3}; \mathbf{Q}_{ij} = \mathbf{Q}_{ji},\ \mathbf{Q}_{ii} = 0 \right\}$$

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

$$|\mathbf{Q}| \stackrel{def}{=} \sqrt{\mathrm{tr}\mathbf{Q}^2} = \sqrt{\mathbf{Q}_{ij}\mathbf{Q}_{ij}} \quad i,j = 1\ldots 3.$$

We recall from [13, 19] that an arbitrary $\mathbf{Q} \in \bar{S}$ can be written as

$$\mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right) + r\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}\mathbf{I}\right)$$

where $\mathbf{n}, \mathbf{m}$ are orthonormal eigenvectors of $\mathbf{Q}$, s, r are scalar order parameters and we either have $0 \leq r \leq \frac{s}{2}$ or $\frac{s}{2} \leq r \leq 0$. If $\mathbf{Q} \in \bar{S}$ is uniaxial, then this representation formula can be simplified to

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

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

We take our domain Ω to be the unit ball $B(0,1) \subset \mathbb{R}^3$ in three-dimensional Euclidean space i.e.

$$B(0,1) = \left\{\mathbf{r} \in \mathbb{R}^3; |\mathbf{r}| \leq 1\right\}.$$

The Landau-de Gennes energy functional is given by [5, 19]

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}] = \int_{B(0,1)} \frac{1}{2}\left|\nabla\mathbf{Q}\right|^2 + \frac{f_B(\mathbf{Q})}{L}\, dV \tag{2}$$

where $\left|\nabla\mathbf{Q}\right|^2 = \sum_{i,j,k=1}^{3}\left(\frac{\partial\mathbf{Q}_{ij}}{\partial\mathbf{x}_k}\right)^2$ is the elastic energy density, L is a small material-dependent elastic constant and f_B is the bulk energy density given by

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

The form (3) is the simplest form of the bulk energy density that allows for a first-order nematic-isotropic phase transition; here b^2, c^2 are material-dependent positive constants and $a^2 > 0$ is a temperature-dependent parameter. We note that the $\mathrm{tr}\mathbf{Q}^2$-term in (3) has a negative coefficient; this represents the low-temperature regime where the bulk energy density attains its global minimum on the set of uniaxial $\mathbf{Q}$-tensors given by [14]

$$\mathbf{Q}_{min} = \left\{\mathbf{Q} \in \bar{S},\ \mathbf{Q} = s_+\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right)\ \right\} \tag{4}$$

with $\mathbf{n} \in \mathbb{S}^2$ and

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \tag{5}$$

In particular, as a^2 increases, we move to lower temperatures *deep* in the nematic phase. The additive constant $C\left(a^2, b^2, c^2\right)$ in (3) ensures that $f_B(\mathbf{Q}) \geq 0$ for all $\mathbf{Q} \in \bar{S}$. The admissible space is defined to be

$$\mathcal{A}_{\mathbf{Q}} = \left\{\mathbf{Q} \in W^{1,2}\left(B(0,1); \bar{S}\right); \mathbf{Q} = \mathbf{Q}_b \text{ on } \partial B(0,1)\right\}. \tag{6}$$

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

$$\mathbf{Q}_b = s_+\left(\frac{\mathbf{r}}{|\mathbf{r}|}\otimes\frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I}\right) \tag{7}$$

and this is referred to as *strong radial anchoring* in the liquid crystal literature [16, 8]. The physically observable, equilibrium configurations correspond to either global or local minimizers of $\mathcal{I}_{\mathcal{LG}}$ in $\mathcal{A}_{\mathbf{Q}}$. For completeness, we recall that $W^{1,2}\left(B(0,1);\bar{S}\right)$ is the Sobolev space of square-integrable $\mathbf{Q}$-tensors with square-integrable first derivatives [6]. The corresponding $W^{1,2}$-norm is given by $\|\mathbf{Q}\|_{W^{1,2}(B(0,1))} = \left(\int_{B(0,1)} |\mathbf{Q}|^2 + |\nabla\mathbf{Q}|^2 \, dx\right)^{1/2}$. In addition to the $W^{1,2}$-norm, we also use the L^∞-norm in this paper, defined to be $\|\mathbf{Q}\|_{L^\infty(B(0,1))} = \text{ess sup}_{\mathbf{x}\in B(0,1)}|\mathbf{Q}(\mathbf{x})|$.

One can readily compute the Euler-Lagrange equations associated with the energy functional, $\mathcal{I}_{\mathcal{LG}}$, as shown below [14, 13] -

$$\Delta\mathbf{Q}_{ij} = \frac{1}{L}\left\{-a^2\mathbf{Q}_{ij} - b^2\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \frac{\delta_{ij}}{3}\text{tr}(\mathbf{Q}^2)\right) + c^2\mathbf{Q}_{ij}\text{tr}(\mathbf{Q}^2)\right\} \quad i,j = 1,2,3, \tag{8}$$

where the term $b^2\frac{\delta_{ij}}{3}\text{tr}(\mathbf{Q}^2)$ is a Lagrange multiplier associated with the tracelessness constraint. It follows from standard arguments in elliptic regularity that any solution $\mathbf{Q}^L$ of the nonlinear elliptic system (8) is smooth and real analytic on $B(0,1)$, up to the boundary [13]. In particular, all global and local energy minimizers in $\mathcal{A}_{\mathbf{Q}}$ are classical solutions of (8).

Radial-hedgehog solutions are examples of spherically-symmetric uniaxial solutions of the system (8) in the admissible space $\mathcal{A}_{\mathbf{Q}}$ and have the form

$$\mathbf{Q} = s(r)\left(\frac{\mathbf{r}}{|\mathbf{r}|}\otimes\frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I}\right). \tag{9}$$

Here the scalar order parameter s only depends on the radial distance $r = |\mathbf{r}|$ from the origin and the corresponding admissible space is defined to be

$$\mathcal{A}_s = \left\{s \in W^{1,2}\left([0,1],\mathbb{R}\right); s(1) = s_+\right\}. \tag{10}$$

We note that $\mathbf{Q} \in W^{1,2}\left(B(0,1);\bar{S}\right)$ necessarily implies that $s \in W^{1,2}\left([0,1];\mathbb{R}\right)$ since the eigenvalues of a symmetric matrix are Lipschitz functions of the matrix components [26] and hence, $\mathcal{A}_s$ is a natural choice for the admissible space. There may be multiple spherically-symmetric solutions of (8) but we define a radial-hedgehog solution to be an energy-minimizing spherically-symmetric solution in the sense described below:

Proposition 2.1. *(a) Let*

$$\mathbf{Q}_h^L(\mathbf{r}) = s_h^L(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right) \tag{11}$$

be a radially-symmetric solution of the system (8) in the admissible space $\mathcal{A}_{\mathbf{Q}}$ defined in (6). Then $s_h^L \in \mathcal{A}_s$, where $\mathcal{A}_s$ has been defined in (10), is a solution of the following singular nonlinear ordinary differential equation

$$\frac{d^2s}{dr^2} + \frac{2}{r}\frac{ds}{dr} - \frac{6s}{r^2} = \frac{1}{3L}\left(2c^2s^3 - b^2s^2 - 3a^2s\right) \tag{12}$$

subject to the boundary conditions

$$s(0) = 0 \text{ and } s(1) = s_+. \tag{13}$$

Moreover, s_h^L is analytic for all $r > 0$.
(b) The radially-symmetric solutions $\mathbf{Q}_h^L$ in (11) have the associated energy functional.

$$I[s] = \int_0^1 \left(\frac{1}{3}\left(\frac{ds}{dr}\right)^2 + \frac{2s^2}{r^2}\right)r^2 + \frac{r^2}{L}\left(-\frac{a^2}{3}s^2 - \frac{2b^2}{27}s^3 + \frac{c^2}{9}s^4 + C(a^2,b^2,c^2)\right)\, dr \tag{14}$$

There exists *a global minimizer $s_H^L \in \mathcal{A}_s$ for I in (14), for each $L > 0$. The function s_H^L is a solution of the ordinary differential equation (12) subject to the boundary conditions (13).*

(c) Define the radial-hedgehog solution by

$$\mathbf{Q}_H^L(\mathbf{r}) = s_H^L(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right) \tag{15}$$

where s_H^L is a global minimizer of I, in the admissible space $\mathcal{A}_s$. Then $\mathbf{Q}_H^L$ is a solution of the Euler-Lagrange equations (8) and these solutions $\left\{\mathbf{Q}_H^L\right\}$ have bounded energies for all values of the elastic constant L i.e.

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_H^L] = \int_{B(0,1)} \frac{1}{2}\left|\nabla \mathbf{Q}\right|^2 + \frac{f_B(\mathbf{Q})}{L}\, dV \le 8\pi s_+^2 \quad \forall L > 0. \tag{16}$$

(d) The function s_H^L satisfies the following bounds for $r \in [0,1]$ -

$$0 \le s_H^L(r) \le s_+ \quad r \in [0,1]. \tag{17}$$

Proof

(a) Let

$$\mathbf{Q}_h^L(\mathbf{r}) = s_h^L(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)$$

be a radially-symmetric solution of the Euler-Lagrange equations for $\mathcal{I}_{\mathcal{LG}}$, given by (8). Then $s_h^L \in \mathcal{A}_s$ as mentioned above and one can substitute this ansatz into (8) to find that s_h^L is necessarily a solution of the singular, nonlinear ordinary differential equation (12). Further, since all solutions of the system (8) are analytic, and

$$\left(\mathbf{Q}_h^L\right)_{ij} = s_h^L(r)\left(\frac{\mathbf{r}_i\mathbf{r}_j}{r^2} - \frac{1}{3}\delta_{ij}\right),$$

we deduce that $\mathbf{Q}_h^L = 0$ at $r = 0$ and $s_h^L(0) = 0$ since $\frac{\mathbf{r}}{|\mathbf{r}|}$ is not defined at $r = 0$. The boundary condition $s = s_+$ at $r = 1$ follows from our choice of the boundary condition $\mathbf{Q}_b$ in (7). Thus, s_h^L is a solution of the ordinary differential equation (12) subject to the boundary conditions (13). Secondly,

$$s_h^L = \frac{3}{2}\left(\mathbf{Q}_h^L\right)_{ij}\left(\frac{\mathbf{r}_i\mathbf{r}_j}{r^2} - \frac{1}{3}\delta_{ij}\right) \quad i,j = 1\ldots 3$$

i.e. s_h^L is the product of two analytic matrices everywhere away from $r = 0$. Thus, s_h^L is continuous for $r \in [0,1]$, since $s \in W^{1,2}\left([0,1];\mathbb{R}\right)$ necessarily implies that $s \in C^{0,\alpha}([0,1];\mathbb{R})$ for $0 < \alpha < \frac{1}{2}$ (for definition of Holder spaces $C^{0,\alpha}$, see [6]) and is additionally analytic for $r \neq 0$.

(b) Let $\mathbf{Q}_h^L$ be a radially-symmetric configuration of the form (11). One can substitute (11) into the Landau-de Gennes energy functional, $\mathcal{I}_{\mathcal{LG}}$, (see (2)) and check that

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_h^L] = I[s_h^L]$$

where I has been defined in (14).

Next, we address the question of *existence* of global minimizers for I in the admissible space $\mathcal{A}_s$. Firstly, we note that the admissible space $\mathcal{A}_s$ is non-empty. Indeed, the constant function $s(r) = s_+$ for $r \in [0,1]$ belongs to $\mathcal{A}_s$. Secondly, the functional I in (14) is bounded from below i.e. $I[s] \ge 0$ for $s \in \mathcal{A}_s$ and is weakly lower semicontinuous on our admissible space, for each $L > 0$ (since the integrand is convex in ds/dr). The existence of a global minimizer s_H^L now follows from the direct methods in the calculus of variations [6].

It is straightforward to compute the Euler-Lagrange equations associated with the functional I in (14) i.e.

$$\frac{d}{dr}\left(\frac{\partial e(s,s')}{\partial s'}\right) = \frac{\partial e(s,s')}{\partial s}$$

where $s' = ds/dr$, $e(s,s') = \left(\frac{1}{3}\left(s'(r)\right)^2 + \frac{2s^2}{r^2}\right)r^2 + \frac{r^2}{L}\left(-\frac{a^2}{3}s^2 - \frac{2b^2}{27}s^3 + \frac{c^2}{9}s^4 + C(a^2,b^2,c^2)\right)$. One can check that the corresponding Euler-Lagrange equations are indeed given by (12).

The boundary condition $s(1) = s_+$ follows from our definition of the admissible space $\mathcal{A}_s$. The boundary condition $s(0) = 0$ follows from the continuity of $s_H^L(r)$ for $r \in [0,1]$. We proceed by contradiction and assume that $|s(r)| \geq s_0$ for $r \in [0, r_0]$, for some fixed $s_0 > 0$ and $0 < r_0 << 1$. Since $s \in C^{0,\alpha}([0,1],\mathbb{R})$ for $0 < \alpha < 1/2$, we deduce that s has a fixed sign near the origin and we further assume that $s(r) > s_0 > 0$ for $r \in [0, r_0]$. Consider the governing equation (12); it can be re-written as

$$\frac{d}{dr}\left(r^2\frac{ds}{dr}\right) = 6s + \frac{r^2}{3L}\left(2c^2s^3 - b^2s^2 - 3a^2s\right). \tag{18}$$

Then for a fixed $L > 0$, we have

$$r^2\frac{ds}{dr} \geq \int_\epsilon^r 6s(r')dr' + Cr^3 + \epsilon^2 s^{'}(\epsilon) \quad for\ r \in (0, r_0) \tag{19}$$

where $0 < \epsilon < r/10$ is fixed, $s^{'}(\epsilon) = \frac{ds}{dr}|_{r=\epsilon}$ and C is a constant independent of ϵ. We note that $s^{'}(\epsilon)$ can be bounded independently of ϵ i.e. $\left|\frac{ds}{dr}\right| \leq C(a^2,b^2,c^2,L)$ for $r \in [0,1]$ from [13]. Squaring both sides of (19) and integrating from ϵ to r, we obtain

$$\int_\epsilon^r \left(\frac{ds}{dr'}\right)^2 dr' \geq \int_\epsilon^r \frac{\gamma s_0^2}{t^2}\, dt + C^{''}r^2 + \epsilon^2 s^{'}(\epsilon)\int_\epsilon^r \frac{1}{t^3}dt \quad for\ r \in (0, r_0), \tag{20}$$

where $C^{''}$ is a constant independent of ϵ. In the limit $\epsilon \to 0$, (20) contradicts the hypothesis that $s \in W^{1,2}([0,1];\mathbb{R})$ from which we must have

$$\int_0^1 \left(\frac{ds}{dr}\right)^2 dr < \infty.$$

Therefore, we deduce that $s(0) = 0$ for any solution of (12) in $\mathcal{A}_s$ and $s_H^L \in \mathcal{A}_s$ is a solution of (12), subject to the boundary conditions (13). The analyticity of s_H^L, away from $r = 0$, now follows from standard arguments in the theory of ordinary differential equations [10]. Given s_H^L, we can then construct a radially-symmetric solution $\mathbf{Q}_H^L = s_H^L(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)$ of the Euler-Lagrange equations (8).

(c) The function s_H^L has been defined to be the global minimizer of the functional I in (14), in the admissible space $\mathcal{A}_s$. However, the constant function, $\bar{s}(r) = s_+$ for $r \in [0,1]$, belongs to $\mathcal{A}_s$ and hence

$$I[s_H^L] \leq I[\bar{s}] = 8\pi s_+^2 \quad for\ each\ L > 0. \tag{21}$$

As mentioned above,

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_H^L] = I[s_H^L]$$

for each $L > 0$, where $\mathbf{Q}_H^L$ and s_H^L are related by $\mathbf{Q}_H^L = s_H^L(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)$. Therefore, $\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_H^L] \leq 8\pi s_+^2$ for each $L > 0$.

(d) The upper bound $|s_H^L(r)| \leq s_+$ follows directly from a result in [14] where we establish that every solution $\mathbf{Q}$ of the system (8) in the admissible space $\mathcal{A}_\mathbf{Q}$ satisfies the global upper bound

$$|\mathbf{Q}(\mathbf{r})| \leq \sqrt{\frac{2}{3}}s_+$$

where s_+ has been defined in (5). The radial-hedgehog solution $\mathbf{Q}_H^L$ is a solution of the system (8) and

$$\left|\mathbf{Q}_H^L(\mathbf{r})\right| = \sqrt{\frac{2}{3}}|s_H^L(r)|$$

where $r = |\mathbf{r}|$. The upper bound $|s_H^L(r)| \leq s_+$ follows immediately.

The lower bound $s_H^L(r) \geq 0$ follows from the energy minimality condition. We assume that there exists an interior measurable subset

$$\tilde{\Omega} = \left\{\mathbf{r} \in \Omega;\ s_H^L(r) < 0\right\} \subset B(0,1)$$

with $s_H^L(r) = 0$ on $\partial\tilde{\Omega}$. We note that $\tilde{\Omega}$ must be an interior subset because of the boundary condition $\mathbf{Q}_b$ in (7). We define the perturbation

$$\bar{s}_H^L(r) = \begin{cases} s_H^L(r), & \mathbf{r} \in B(0,1) \setminus \tilde{\Omega}, \\ -s_H^L(r), & \mathbf{r} \in \tilde{\Omega}. \end{cases} \tag{22}$$

One can then easily check that

$$I[\bar{s}_H^L] - I[s_H^L] = \int_{\tilde{\Omega}} -\frac{2b^2}{27}\left(\bar{s}_H^L\right)^3 + \frac{2b^2}{27}\left(s_H^L\right)^3\ dV = \int_{\tilde{\Omega}} \frac{4b^2}{27}\left(s_H^L\right)^3\ dV < 0 \tag{23}$$

since $s_H^L(r) < 0$ on $\tilde{\Omega}$ by assumption. The inequality (23) contradicts the global minimality of s_H^L in $\mathcal{A}_s$ and hence, we deduce that $s_H^L(r) \geq 0$ for $r \in [0,1]$. The inequalities (17) now follow. $\square$

In summary, in Proposition 2.1, we prove the existence of a radial-hedgehog solution of the form (15) for each $L > 0$, that can be interpreted as being a Landau-de Gennes energy minimizer within the class of radially-symmetric configurations. This radial-hedgehog solution satisfies the energy bound (16) for each $L > 0$ and the corresponding scalar order parameter s_H^L is bounded from both above and below as shown in (17). Next, we quote some relevant results from [13] in the limit of vanishing elastic constant $L \to 0^+$ and the subsequent results in this paper will be established in the limit of vanishing elastic constant. The limit $L \to 0^+$ is a mathematically interesting and physically relevant limit since the elastic constant L is typically several orders of magnitude smaller than the other material-dependent constants in $\mathcal{I}_{\mathcal{LG}}$ [5, 21]. Further, this limit elucidates the analogies between the study of radial-hedgehog solutions in the Landau-de Gennes theory for nematic liquid crystals and the study of vortices in the Ginzburg-Landau theory of superconductors [1] where we are typically interested in studying the qualitative properties of solutions of the following system of partial differential equations for a vector field $\mathbf{u} \in W^{1,2}\left(\Omega; \mathbb{R}^2\right)$ with $\Omega \subset \mathbb{R}^2$ and

$$-\Delta\mathbf{u} = \frac{1}{\epsilon^2}\left(1 - |\mathbf{u}|^2\right)\mathbf{u}, \tag{24}$$

in the limit $\epsilon \to 0^+$. The Ginzburg-Landau theory for superconductors has been thoroughly studied in two dimensions and there has been related work in higher dimensions too [17, 2].

Maximum principle [14]: Let $\mathbf{Q}$ be an arbitrary solution of the Euler-Lagrange equations (8) in the space $\mathcal{A}_{\mathbf{Q}}$. Then

$$\|\mathbf{Q}\|_{L^\infty(B(0,1))} \leq \sqrt{\frac{2}{3}}s_+ \tag{25}$$

where s_+ has been defined in (5).

Strong convergence to $\mathbf{Q}^0$ [13]: Let $\left\{\mathbf{Q}_H^{L_k}\right\}$ be a sequence of radial-hedgehog solutions of (8), where $\mathbf{Q}_H^{L_k}$ has been defined in (15) and $L_k \to 0^+$ as $k \to \infty$. Then $\mathbf{Q}_H^{L_k} \to \mathbf{Q}^0$ strongly in $W^{1,2}\left(B(0,1); \bar{S}\right)$ (upto a subsequence) as $k \to \infty$, and $\mathbf{Q}^0$ is given by

$$\mathbf{Q}^0 = s_+ \left(\frac{\mathbf{r} \otimes \mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I} \right). \tag{26}$$

The proof of the strong convergence result can be found in [13]. It is essentially a consequence of the fact that the radial-hedgehog solutions $\{\mathbf{Q}_H^L\}$ have bounded energy in the limit $L \to 0$ from (16). We note that $\mathbf{Q}^0$ is a global minimizer of $\mathcal{I}_{\mathcal{LG}}$ in the restricted space, $\mathcal{A}_{\mathbf{Q}} \cap \mathbf{Q}_{min}$, where $\mathcal{A}_{\mathbf{Q}}$ and $\mathbf{Q}_{min}$ have been defined in (6) and (4) respectively. The limiting map $\mathbf{Q}^0$ is referred to as the *limiting harmonic map* in [13] and $\mathbf{Q}^0$ has an isolated point defect at the origin i.e. the singular set, S_0, of $\mathbf{Q}^0$ is given by

$$S_0 = \{\mathbf{r} \in B(0,1); \mathbf{r} = \mathbf{0}\}.$$

Interior and boundary monotonicity lemmas [13]: Let $\mathbf{Q}$ be an arbitrary solution of the Euler-Lagrange equations (8). Define the normalized energy on balls $B(\mathbf{x}, r) = \{\mathbf{y} \in \Omega : |\mathbf{x} - \mathbf{y}| \leq r\} \subset \Omega$:

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

Then we have the following interior monotonicity lemma:

$$\mathcal{F}(\mathbf{Q}, \mathbf{x}, r) \leq \mathcal{F}(\mathbf{Q}, \mathbf{x}, R) \quad \forall \mathbf{x} \in \Omega;\ r \leq R \text{ and } B(\mathbf{x}, R) \subset \Omega. \tag{27}$$

Similarly, for $\mathbf{x}^0 \in \partial\Omega$, we define the region $\Omega_r = \overline{\Omega} \cap B(\mathbf{x}^0, r)$ with $r > 0$, and the corresponding normalized energy to be $\mathcal{E}(\mathbf{Q}, \mathbf{x}^0, r) = \frac{1}{r}\int_{\Omega_r} \frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{f_B(\mathbf{Q})}{L} \, dV$. Then there exists $r_0 > 0$ so that

$$\frac{d}{dr}\mathcal{E} \geq -C\left(a^2, b^2, c^2, \mathbf{Q}_b, r_0, \Omega\right) \quad 0 < r < r_0$$

where the positive constant C is independent of L.

Applying the strong convergence result and monotonicity lemmas to the radial-hedgehog solutions $\{\mathbf{Q}_H^L\}$ in (15), we find that -

Convergence of s_H^L in (15) [13]: Let $\left\{\mathbf{Q}_H^{L_k}\right\}$ be a sequence of radial-hedgehog solutions of (8), where $L_k \to 0$ as $k \to \infty$. Then $s_H^{L_k} \to s_+$ uniformly as $k \to \infty$, everywhere away from the origin. This uniform convergence holds in the interior and up to the boundary.

This uniform convergence result states that s_H^L can deviate from the equilibrium value s_+ in (5) only in a small neighbourhood of the origin and in the next section, we quantify the size of this neighbourhood which is referred to as the *isotropic core* of the radial-hedgehog solution.

3 The Isotropic Core

In this section, we study the qualitative properties of the function s_H^L in (15), as $r \to 0^+$, in the limit of vanishing elastic constant $L \to 0^+$. From the results in Section 2, we have that s_H^L is continuous for $r \in [0,1]$, is analytic away from $r = 0$ and is a solution of the nonlinear singular ordinary differential equation (12) subject to the boundary conditions (13). We introduce the scaled coordinate

$$\bar{r} = \frac{r}{\sqrt{L}}$$

and we are interested in solutions of the following limiting problem as $L \to 0^+$

$$\frac{d^2 s}{d\bar{r}^2} + \frac{2}{\bar{r}}\frac{ds}{d\bar{r}} - \frac{6s}{\bar{r}^2} = \frac{1}{3}\left(2c^2 s^3 - b^2 s^2 - 3a^2 s\right)$$
$$s(0) = 0 \quad \text{and } s \to s_+ \textit{ as } \bar{r} \to \infty, \tag{28}$$

where $0 \leq s(r) \leq s_+$ for all $r \in [0, \infty)$ from (17).

Proposition 3.1. *[7, 17] Let $s_H^* = \lim_{L\to 0^+} s_H^L$, where s_H^L has been defined in (15). Then $s_H^* : [0,\infty) \to [0, s_+)$ is a montonically increasing solution of the problem (28). In addition, s_H^* has the expansion*

$$s_H^*(r) = \sum_{n=0}^{\infty} a_n r^n = a_2 r^2 \left[1 - \frac{a^2}{14} r^2 + o(r^2)\right] \quad \textit{as } r \to 0 \tag{29}$$

where $a_n = 0$ for n odd and $a_2 > 0$ is a constant that satisfies the bounds $A \leq a_2 \leq B$, for positive constants A, B independent of a^2, b^2, c^2.

Sketch of Proof: The proof of Proposition 3.1 parallels that of analogous results for radial solutions of the Ginzburg-Landau equations in three dimensions and follows from a standard shooting argument [7]. Namely, for any $a_2 > 0$, the problem (28) has a unique solution $s(a_2, r)$ in a neighbourhood of $r = 0$. However, if a_2 is "too" small, then the corresponding solution $s(a_2, r)$ changes sign and converges to 0 at infinity. On the other hand, if a_2 is "too" large, then the corresponding solution $s(a_2, r)$ blows up for some $R_{a_2} < \infty$. Therefore, for solutions satisfying the bounds (17), we must have $A \leq a_2 \leq B$, for positive constants A and B independent of a^2, b^2, c^2. In particular, this means that a_2 can be bounded independently of a^2, b^2, c^2 in the limit $a^2 \to \infty$. The monotonicity of s i.e. $\frac{ds}{dr} > 0$ for all $r > 0$, follows immediately from arguments in [7] and hence, s_H^* has an isolated isotropic point at the origin and is strictly positive everywhere else.

We briefly comment on why the shooting techniques for vortices in the three-dimensional Ginzburg-Landau theory readily generalize to the problem (28). Whilst studying vortices within the Ginzburg-Landau theory for superconductors in three dimensions, we seek solutions of the following singular ordinary differential equation for a scalar function $u : \mathbb{R} \to \mathbb{R}$

$$\frac{d^2 u}{dr^2} + \frac{2}{r}\frac{du}{dr} - \frac{6}{r^2}u = u(u^2 - 1) \tag{30}$$

subject to $u(0) = 0$, $u(r) \to 1$ as $r \to \infty$. It can be shown that all solutions of this ordinary differential equation satisfy the bounds $0 \leq u(r) \leq 1$ for all $r \geq 0$. It is evident that (30) and (28) have the same structure. The shooting techniques generalize because the nonlinearities on the right-hand side of (30) and (28) are non-positive for all $0 \leq u(r) \leq 1$ and $0 \leq s(r) \leq s_+$ respectively.

On the other hand, we cannot readily establish that the problem (28) has a unique solution. For (30), this has been done in [7, 17, 9] since $(1 - u^2)$ is a decreasing function of u for all $0 \leq u(r) \leq 1$. However, for (28), the function $(3a^2 + b^2 s - 2c^2 s^2)$ is *not* a decreasing function of s for $0 \leq s \leq s_+$ i.e. this function has a local maximum at $s_{\max} = \frac{b^2}{4c^2} < s_+$. However, we do not need uniqueness of the radial-hedgehog solution for the subsequent results. The interested reader is referred to [1, 7, 17, 9] for additional details. $\square$

Proposition 3.2. *Consider the radial-hedgehog solution $\mathbf{Q}_H^L$ in (15). Then in the limit $L \to 0^+$, s_H^L has the following expansion in a neighbourhood of $r = 0$:*

$$s_H^L(r) = \frac{a_2}{L}\left[r^2 - \frac{a^2}{14}\frac{r^4}{L} + \left(\frac{a^4}{14} - \frac{b^2 a_2}{3}\right)\frac{r^6}{36L^2} + \dots\right] \tag{31}$$

where $a_2 > 0$ is the constant in (29). In particular, a_2 can be bounded independently of a^2, b^2, c^2 and the elastic constant L. The expansion (31) is valid for

$$r^2 < \frac{14L}{a^2} \tag{32}$$

provided a^2 is sufficiently large i.e.

$$a^6 > \gamma_1 c^2 + \gamma_2 b^2 a^2 \tag{33}$$

where γ_1, γ_2 are explicitly computable positive constants independent of a^2, b^2, c^2 and L. Under the hypothesis (33), we have that

$$s_H^L(r) \leq 2\frac{a_2}{L} r^2 \quad \textit{for } r^2 < \frac{14L}{a^2}. \tag{34}$$

Proof: From Proposition 2.1, we have that s_H^L is analytic for $r > 0$. Hence, we seek a power series expansion of s around the origin with $s(0) = 0$, of the form

$$s_H^L(r) = \sum_{n=1}^{\infty} a_n r^n \quad 0 < r \leq R_0 \tag{35}$$

where R_0 will be specified later.

We work with the scaled coordinate

$$\bar{r} = \frac{r}{\sqrt{L}}$$

and recover the limiting problem (28) in the limit $L \to 0^+$. We substitute the ansatz $s_H^L(\bar{r}) = \sum_{n=1}^{\infty} b_n \bar{r}^n$ into (28) and equate the coefficients of $\bar{r}^n$ on both sides of the ordinary differential equation

$$\frac{d^2 s}{d\bar{r}^2} + \frac{2}{\bar{r}}\frac{ds}{d\bar{r}} - \frac{6s}{\bar{r}^2} = \frac{1}{3}\left(2c^2 s^3 - b^2 s^2 - 3a^2 s\right)$$

for each $n = 1, 2, 3 \ldots$. Straightforward computations show that

$$s_H^L(\bar{r}) = a_2\left[\bar{r}^2 - \frac{a^2}{14}\bar{r}^4 + \left(\frac{a^4}{14} - \frac{b^2 a_2}{3}\right)\frac{\bar{r}^6}{36} + \ldots\right] \tag{36}$$

where $a_2 > 0$ is independent of the model parameters. We note that a_2 is determined by Proposition 3.1 and there are no terms involving odd powers of r. It now remains to use the substitution $\bar{r} = \frac{r}{\sqrt{L}}$ and the expansion (31) readily follows.

Next, we consider a simplified but related problem. We look for power series expansions of regular solutions of the following singular ordinary differential equation around $r = 0$: -

$$\frac{d^2 s}{dr^2} + \frac{2}{r}\frac{ds}{dr} - \frac{6s}{r^2} = -\frac{a^2 s}{L} \tag{37}$$

where $s(0) = 0$. Let $s(r) = \sum_{n=1}^{\infty} b_n r^n$. Then one can readily check that

$$b_1 = 0; b_2 = \frac{b^*}{L};\ b_{n+2} = -\frac{a^2}{(n^2 + 5n)L} b_n \tag{38}$$

for some arbitrary constant b^*, so that we have an alternating series with no odd powers of r involved. This expansion will converge for all values of r such that [25]

$$\left|\frac{b_{n+2} r^2}{b_n}\right| < 1.$$

This condition is equivalent to

$$\left|\frac{b_{n+2}r^2}{b_n}\right| = \frac{r^2}{L}\frac{a^2}{n^2+5n} \leq \frac{a^2r^2}{14L} \tag{39}$$

for all $n \geq 2$ and hence, the expansion will converge for $r^2 < \frac{14L}{a^2}$. Further, this is an alternating series so that

$$\sum_{n=1}^{\infty} b_{2n}r^{2n} \leq \frac{b^* r^2}{L} - \left(|b_4|r^4 - \left(|b_6|r^6 - |b_8|r^8\right) - \dots\right) < \frac{b^*r^2}{L} - |b_4|r^4 < \frac{b^*r^2}{L}$$

since $b_4 = -\frac{a^2}{14L}\frac{b^*}{L}$ and $r^2 < \frac{14L}{a^2}$.

We can apply the same reasoning to the series in (31) with the constant b^* being replaced by $a_2 > 0$ in (36), when we work in a small neighbourhood of the origin and a^2 is sufficiently large, as in the hypothesis (33). The inequalities, (32) and (34), now readily follow. The proof of Proposition 3.2 is now complete. □

4 Estimates away from the isotropic core

Our first result closely follows the proof of Lemma 2.1 in [17] with some technical differences.

Proposition 4.1. *Let $\mathbf{Q}_H^L$ be the radial-hedgehog solution defined in (15). Then $s_H^L : [0,1] \to [0, s_+]$ is a non-negative and monotonically increasing solution of the following singular ordinary differential equation*

$$\frac{d^2s}{dr^2} + \frac{2}{r}\frac{ds}{dr} - \frac{6s}{r^2} = \frac{1}{3L}\left(2c^2s^3 - b^2s^2 - 3a^2s\right) \tag{40}$$

subject to the boundary conditions

$$s(0) = 0 \quad \textit{and } s(1) = s_+. \tag{41}$$

In the limit $L \to 0^+$, we have

$$r^2\left|\frac{d^2s_H^L}{dr^2}\right| + r\left|\frac{ds_H^L}{dr}\right| + \left|6s_+ - \frac{2c^2r^2}{3L}s_H^L(s_+ - s_H^L)(s_H^L - s_-)\right| = o(1) \quad r \geq \frac{1}{10} \tag{42}$$

where $s_+ = \frac{b^2+\sqrt{b^4+24a^2c^2}}{4c^2} > 0$ and $s_- = \frac{b^2-\sqrt{b^4+24a^2c^2}}{4c^2} < 0$.

Comment: Proposition 4.1 gives us estimates for s_H^L and its derivatives everywhere away from the origin in the limit $L \to 0^+$.

Proof: In what follows, we denote s_H^L by s_L for brevity. Consider the ordinary differential equation (40) and multiply both sides by $r^2\frac{ds}{dr}$. Then (40) simplifies to

$$\frac{d}{dr}\left[\frac{r^2}{2}\left(\frac{ds}{dr}\right)^2\right] + r\left(\frac{ds}{dr}\right)^2 - \frac{d}{dr}3s^2(r) - \frac{2c^2r^2}{3L}\frac{ds}{dr}s(s-s_+)(s-s_-) = 0. \tag{43}$$

We integrate (43) over $r \in [0, r_0]$ where $r_0 > \frac{1}{10}$ is fixed and obtain

$$\frac{r_0^2}{2}s'(r_0)^2 + \int_0^{r_0} r\left[s'(r)\right]^2\, dr + \frac{2c^2}{3L}\int_0^{r_0} r^2 s'(r)s(r)(s_+ - s)(s - s_-)dr = 3s^2(r_0) \leq 3s_+^2 \tag{44}$$

where $s'(r) = ds/dr$ and we have used $s(0) = 0$ and the bounds (17) in our computations.

Next, we use a change of variable

$$\bar{r} = \frac{r}{\sqrt{L}}$$

and let $\bar{r_0} = \frac{r_0}{\sqrt{L}}$. Then (44) is transformed to

$$\frac{\bar{r_0}^2}{2} s'(\bar{r_0})^2 + \int_0^{\bar{r_0}} \bar{r} \left[s'(\bar{r}) \right]^2 \, d\bar{r} + \frac{2c^2}{3} \int_0^{\bar{r_0}} \bar{r}^2 s'(\bar{r}) s(\bar{r})(s_+ - s(\bar{r}))(s(\bar{r}) - s_-) d\bar{r} = 3s^2(r_0) \leq 3s_+^2. \tag{45}$$

Noting that $s_L'(\bar{r}) > 0$ for $\bar{r} > 0$ and $0 \leq s_L(\bar{r}) \leq s_+$ from (17), we have that

$$\int_0^{\bar{r_0}} \bar{r} \left[s_L'(\bar{r}) \right]^2 \, d\bar{r} \leq 3s_+^2.$$

This necessarily implies that given sequences $\{L_k\} \to 0^+$ and $\bar{r_k} = \frac{r_0}{\sqrt{L_k}} \to \infty$ as $k \to \infty$, we must have

$$\bar{r_k} s_L'(\bar{r}_k) \to 0^+ \ as \ k \to \infty.$$

(If $\bar{r_k} s_L'(\bar{r}_k) > C$ for some positive constant C as $k \to \infty$, we would contradict the finite energy condition $\int_0^{\bar{r_0}} \bar{r} \left[s_L'(\bar{r}) \right]^2 \, d\bar{r} \leq 3s_+^2$.) On the other hand, the integral terms in (45) admit a limit as $L \to 0^+$. Therefore,

$$\bar{r} \frac{ds_L}{d\bar{r}} = r \frac{ds_L}{dr} \to 0 \quad \text{as } L \to 0 \text{ for } r \geq \frac{1}{10}. \tag{46}$$

For any $k \in (0,1)$ fixed, we multiply the re-scaled equation

$$\frac{d^2 s_L}{d\bar{r}^2} + \frac{2}{\bar{r}} \frac{ds_L}{d\bar{r}} - 6 \frac{s_L}{\bar{r}^2} = \frac{1}{3} \left(2c^2 s_L^3 - b^2 s_L^2 - 3a^2 s_L \right)$$

by $\bar{r}^2$ and average over $(k\bar{r_0}, \bar{r_0})$ to obtain

$$\frac{1}{(1-k)\bar{r_0}} \int_{k\bar{r_0}}^{\bar{r_0}} \frac{d}{d\bar{r}} \left(\bar{r}^2 \frac{ds_L}{d\bar{r}} \right) d\bar{r} + \frac{2c^2}{3(1-k)\bar{r_0}} \int_{k\bar{r_0}}^{\bar{r_0}} \bar{r}^2 s_L(\bar{r}) \left(s_+ - s_L(\bar{r}) \right) \left(s_L(\bar{r}) - s_- \right) d\bar{r} = \frac{6}{(1-k)\bar{r_0}} \int_{k\bar{r_0}}^{\bar{r_0}} s_L(\bar{r}) d\bar{r}. \tag{47}$$

In the limit $L \to 0^+$, $s_L \to s_+$ uniformly everywhere away from the origin (refer to the convergence results quoted from [13] in Section 2) and using (46), we obtain the following sequence of inequalities

$$\frac{2c^2}{3} \limsup_{L \to 0^+} k^2 \bar{r_0}^2 \left(s_+ - s_L(\bar{r_0}) \right) \left(s_L(\bar{r_0}) - s_- \right) \leq 6 \leq \frac{2c^2}{3} \liminf_{L \to 0^+} \bar{r_0}^2 \left(s_+ - s_L(k\bar{r_0}) \right) \left(s_L(k\bar{r_0}) - s_- \right). \tag{48}$$

It immediately follows that

$$\frac{2c^2}{3} \frac{r^2}{L} (s_+ - s_L(r))(s_L(r) - s_-) \to 6 \tag{49}$$

uniformly in the limit $L \to 0^+$, everywhere away from the origin (in (49), we use the substitution $\bar{r} = r/\sqrt{L}$).

Finally, using the estimates (46) and (49) in (40), we deduce that

$$r^2 \left| \frac{d^2 s_L}{dr^2} \right| \to 0 \tag{50}$$

uniformly in the limit $L \to 0^+$, everywhere away from the origin. Proposition 4.1 now follows. $\square$

One immediate consequence of (42) is that

$$s_H^L(r) = s_+ - \frac{18L}{r^2\sqrt{b^4 + 24a^2c^2}} + \sigma(r, a^2, b^2, c^2, L) \quad where \ \sigma(r, a^2, b^2, c^2, L) = o(L) \tag{51}$$

for $r > r_0$ with r_0 independent of L, in the limit $L \to 0^+$. Therefore, we can obtain an upper bound for $\left|\mathbf{Q}_H^L - \mathbf{Q}^0\right|$ in the limit $L \to 0^+$, where $\mathbf{Q}^0$ is defined in (26) i.e.

$$\left|\mathbf{Q}_H^L(\mathbf{r}) - \mathbf{Q}^0(\mathbf{r})\right| = \left|s_H^L(r) - s_+\right| \left|\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)\right| \leq \frac{CL}{r^2\sqrt{b^4 + 24a^2c^2}}$$

where $r > r_0$ and C is a constant independent of a^2, b^2, c^2, L. This explicitly estimates the rate of convergence of the radial-hedgehog solution to the limiting harmonic map, everywhere away from the origin, in the limit $L \to 0^+$.

We can refine this estimate further by a simple analysis of the ordinary differential equation (40). We substitute (51) into (40) and find the following equality

$$-\frac{6s_+}{r^2} + \frac{72L}{r^4\sqrt{b^4 + 24a^2c^2}} + C(a^2, b^2, c^2, r, L) = -\frac{6s_+}{r^2} + D(a^2, b^2, c^2, r)L + F(a^2, b^2, c^2, r)\frac{\sigma}{L} \tag{52}$$

for $r > r_0$, where $C(a^2, b^2, c^2, r, L) = o(L)$ in the limit $L \to 0^+$ and D and F are positive, bounded functions independent of L. We can see straightaway from (52) that

$$\frac{\sigma}{L} \leq G(a^2, b^2, c^2, r)L \tag{53}$$

for a positive bounded function G independent of L. In other words, the expansion (51) can be further refined to

$$s_H^L(r) = s_+ - \frac{18L}{r^2\sqrt{b^4 + 24a^2c^2}} + O(L^2) \tag{54}$$

in the limit $L \to 0^+$, everywhere away from the origin. The expansion (54) will be useful for people interested in quantitative estimates for the energy of the radial-hedgehog solution $\mathbf{Q}_H^L$ as a function of the elastic constant L.

5 Instability with respect to biaxial perturbations

Proposition 5.1. *We define the radial-hedgehog solution to be*

$$\mathbf{Q}_H^L(\mathbf{r}) = s_H^L(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)$$

where s_H^L is a global minimizer of I in (14) in the admissible space $\mathcal{A}_s$. Then $\mathbf{Q}_H^L$ is not the global minimizer of $\mathcal{I}_{\mathcal{LG}}$ in (2) in the admissible space $\mathcal{A}_{\mathbf{Q}}$ defined in (6), in the limit $L \to 0^+$, for sufficiently low temperatures i.e. for

$$a^2 > \max\left\{28a_2, \frac{55}{42}c^2 - \frac{11}{9}b^2, \left(\gamma_1 c^2 + \gamma_2 b^2 a^2\right)^{1/3}\right\} \tag{55}$$

where a_2 is the constant in (29) and γ_1, γ_2 are the positive constants in (33).

Proof: We explicitly construct a biaxial perturbation which has lower free energy than $\mathbf{Q}_H^L$ in the low-temperature regime specified by (55), for sufficiently small values of the elastic constant L. This biaxial perturbation is localised in a small ball $B(0,\sigma) = \{\mathbf{r} \in B(0,1); |\mathbf{r}| \leq \sigma\}$ where $\sigma^2 < \frac{14L}{a^2}$.

We define this perturbation to be

$$\begin{aligned}\mathbf{Q}_{ij} &= \left(\mathbf{Q}_H^L\right)_{ij} + \left(1 - \frac{r}{\sigma}\right)\left(\mathbf{z}_i\mathbf{z}_j - \frac{\delta_{ij}}{3}\right) = \\ &= s_H^L(r)\left(\frac{\mathbf{r}_i\mathbf{r}_j}{r^2} - \frac{\delta_{ij}}{3}\right) + \left(1 - \frac{r}{\sigma}\right)\left(\mathbf{z}_i\mathbf{z}_j - \frac{\delta_{ij}}{3}\right) \quad r \leq \sigma\end{aligned} \tag{56}$$

where $\mathbf{r} = (x, y, z)$ is the position vector, $\mathbf{z} = (0, 0, 1)$ is the unit-vector in the z-direction and δ_{ij} is the Kronecker delta symbol. For $r^2 \leq \sigma^2 < \frac{14L}{a^2}$ and for sufficiently small values of L, we have

$$s_H^L(r) \leq 2\frac{a_2}{L} r^2$$

from (34), where $a_2 > 0$ can be bounded independently of a^2, b^2, c^2 and is independent of L (see Proposition 3.1).

Straightforward computations show that

$$\begin{aligned}
|\nabla \mathbf{Q}|^2 &= \left|\nabla \mathbf{Q}_H^L\right|^2 + \frac{2}{3\sigma^2} - \frac{2}{\sigma}\frac{ds_H^L}{dr}\left(\cos^2\theta - \frac{1}{3}\right) \\
|\mathbf{Q}|^2 &= |\mathbf{Q}_H^L|^2 + \frac{2}{3}\left(1 - \frac{r}{\sigma}\right)^2 + 2s_H^L(r)\left(1 - \frac{r}{\sigma}\right)\left(\cos^2\theta - \frac{1}{3}\right) \\
\mathrm{tr}\mathbf{Q}^3 &= \mathrm{tr}\left(\mathbf{Q}_H^L\right)^3 + \frac{2}{9}\left(1 - \frac{r}{\sigma}\right)^3 + \left[\left(s_H^L(r)\right)^2\left(1 - \frac{r}{\sigma}\right) + s_H^L(r)\left(1 - \frac{r}{\sigma}\right)^2\right]\left(\cos^2\theta - \frac{1}{3}\right) \\
\left(\mathrm{tr}\mathbf{Q}^2\right)^2 &= |\mathbf{Q}|^4 = \left|\mathbf{Q}_H^L\right|^4 + \frac{4}{9}\left(1 - \frac{r}{\sigma}\right)^4 + \left(s_H^L(r)\right)^2\left(1 - \frac{r}{\sigma}\right)^2\left[4\left(\cos^2\theta - \frac{1}{3}\right)^2 + \frac{8}{9}\right] + \\
&\quad + \frac{8}{3}\left[s_H^L(r)\left(1 - \frac{r}{\sigma}\right)^3 + \left(s_H^L(r)\right)^3\left(1 - \frac{r}{\sigma}\right)\right]\left(\cos^2\theta - \frac{1}{3}\right) \qquad (57)
\end{aligned}$$

where $\mathbf{r} = r(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is the position vector in spherical polar coordinates and $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$.

Noting that

$$\int_0^\pi \left(\cos^2\theta - \frac{1}{3}\right)\sin\theta d\theta = 0$$

and

$$\int_0^\pi \left(\cos^2\theta - \frac{1}{3}\right)^2 \sin\theta d\theta = \frac{8}{45},$$

we obtain the following estimates -

$$\int_{B(0,\sigma)} \frac{1}{2}\left\{|\nabla\mathbf{Q}|^2 - \left|\nabla\mathbf{Q}_H^L\right|^2\right\} dV = \frac{4\pi\sigma}{9} \qquad (58)$$

$$\int_{B(0,\sigma)} \frac{-a^2}{L}\left(|\mathbf{Q}|^2 - |\mathbf{Q}_H^L|^2\right) dV = -\frac{4\pi a^2\sigma^3}{90L} \qquad (59)$$

$$\int_{B(0,\sigma)} \frac{-b^2}{3L}\left(\mathrm{tr}\mathbf{Q}^3 - \mathrm{tr}\left(\mathbf{Q}_H^L\right)^3\right) dV = -\frac{8\pi b^2\sigma^3}{1620L} \qquad (60)$$

$$\int_{B(0,\sigma)} \frac{c^2}{4L}\left(\left(\mathrm{tr}\mathbf{Q}^2\right)^2 - \left(\mathrm{tr}\left(\mathbf{Q}_H^L\right)^2\right)^2\right) dV \leq \frac{5\pi c^2\sigma^3}{945L} \qquad (61)$$

where we have used the inequality (34) and the hypothesis $a^2 > 28a_2$ in estimating (61).

Combining (58)-(61), we obtain an upper bound for the free energy difference, $\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}] - \mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_H^L]$, as shown below -

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}] - \mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_H^L] \leq \frac{\sigma}{L}\left(\frac{4\pi L}{9} - \frac{4\pi a^2\sigma^2}{90} - \frac{8\pi b^2\sigma^2}{1620} + \frac{5\pi c^2\sigma^2}{945}\right) \qquad (62)$$

and $\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}] - \mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_H^L]$ will be negative whenever

$$\sigma^2 > L \frac{4\pi/9}{\frac{4\pi a^2}{90} + \frac{8\pi b^2}{1620} - \frac{5\pi c^2}{945}}. \tag{63}$$

In what follows, we set $\sigma^2 = \frac{11L}{a^2}$ (note that this is within the range of validity for the expansion (31)). Then

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}] - \mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_H^L] < 0$$

for

$$a^2 > \frac{55}{42}c^2 - \frac{11}{9}b^2$$

as stated in the hypothesis (55). Thus, we can construct an explicit biaxial perturbation in a ball of radius σ, where $\sigma^2 = \frac{11L}{a^2}$, which has lower free energy than the radial-hedgehog solution in the low-temperature regime specified by (55), for sufficiently small values of the elastic constant L. Proposition 5.1 now follows. $\square$

We make some comments about Proposition 5.1. Firstly, the constraint

$$a^2 > \frac{55}{42}c^2 - \frac{11}{9}b^2$$

will be satisfied for all $a^2 > 0$ provided that $b^2 > \frac{3}{2}c^2$. The constants b^2 and c^2 are generally taken to be material-dependent constants and from the quoted values in the literature [16, 19], we expect that $b^2 > \frac{3}{2}c^2$ for most commonly used liquid crystal materials such as MBBA.

Secondly, our result is qualitatively similar to a result on the instability of the radial-hedgehog solution in [8]. The authors in [8] demonstrate that the radial-hedgehog solution will be unstable with respect to biaxial perturbations for sufficiently low temperatures, in balls of sufficiently large radius. They consider the second variation of the Landau-de Gennes energy functional and treat the instability condition as a Schrodinger eigenvalue problem. On the other hand, we construct an explicit biaxial perturbation, localized near the isotropic core of the radial-hedgehog solution and use explicit estimates for s_H^L near $r = 0$ from Proposition 3.2 to show that this biaxial perturbation will have lower free energy than the radial-hedgehog solution, for sufficiently low temperatures and for sufficiently small values of the elastic constant L. However, if we use scaled coordinates, $\bar{r} = \frac{r}{\sqrt{L}}$ in the limit $L \to 0^+$, then Proposition 5.1 would be equivalent to the statement in [8] where the authors demonstrate instability for sufficiently low temperatures and balls of sufficiently large radius. Our approach is different to the methods used in [8] and our approach gives insight into how to quantify the instability regime analytically.

6 Stability of Radial-Hedgehog Solution

In the previous section, we demonstrated that the radial-hedgehog solution cannot be a global Landau-de Gennes energy minimizer in the low-temperature regime and for sufficiently small values of the elastic constant. However, this does not tell us anything about the local stability or metastability of the radial-hedgehog solution. In this section, we demonstrate that the radial-hedgehog solution is locally stable with respect to certain kinds of perturbations for all $a^2 > 0$ (whenever we work with temperatures for which the bulk energy density f_B in (3) has an ordered nematic minimum). The following results are therefore, more general in nature.

Proposition 6.1. *Let $\mathbf{Q}_H^L$ denote the radial-hedgehog solution in (15) for a fixed $L > 0$. Then $\left\{\mathbf{Q}_H^L\right\} \to \mathbf{Q}^0$ in $W^{1,2}\left(B(0,1); \bar{S}\right)$ as $L \to 0^+$, where $\mathbf{Q}^0 = s_+\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)$ [13]. As $L \to 0^+$, the radial-hedgehog solution*

$\mathbf{Q}^L_H$ *is stable against all small perturbations,* $\epsilon\mathbf{P} \in \bar{S}$ *with* $\epsilon \in \mathbb{R}$, $|\epsilon| << 1$, $\mathbf{P}$ *independent of* L, $\mathbf{P} = \mathbf{0}$ *on* $\partial B(0,1)$ *and*

$$\mathbf{P}(\mathbf{r}) = 0 \quad \mathbf{r} \in B(0, r_0), \tag{64}$$

where $0 < r_0 < 1$ *is independent of* ϵ *and* L. *In other words,* $\mathbf{Q}^L_H$ *is locally stable against perturbations which are localized outside the isotropic core around the origin, in the limit* $L \to 0^+$.

Comment: We are considering perturbations $\mathbf{P} \in \bar{S}$*, which are symmetric, traceless* 3×3 *matrices that vanish on the boundary. These perturbations are completely general; they can be either uniaxial or biaxial and we take them to vanish on the boundary since we are dealing with a Dirichlet boundary-value problem. Proposition 6.1 states that the radial-hedgehog solution is stable against* all *such small perturbations which are spread outside the defect core, in the limit* $L \to 0^+$. *Note that this is consistent with Proposition 5.1 where we demonstrate instability of the radial-hedgehog solution against biaxial perturbations localized in the isotropic core of size* $O(\sqrt{\frac{L}{a^2}})$. *In particular, these biaxial perturbations do not satisfy the hypothesis (64).*

The strong convergence result $\left\{\mathbf{Q}^L_H\right\} \to \mathbf{Q}^0$ *in* $W^{1,2}\left(B(0,1); \bar{S}\right)$ *as* $L \to 0^+$ *has already been established in [13]; interested readers are referred to [13] for details.*

Proof: We consider perturbations of the radial-hedgehog solution of the form

$$\left(\mathbf{Q}^\epsilon_L\right)_{ij} = \left(\mathbf{Q}^L_H\right)_{ij} + \epsilon \mathbf{P}_{ij} \quad i,j = 1\dots 3 \tag{65}$$

where $\epsilon \in \mathbb{R}$, $|\epsilon| << 1$, $\mathbf{P} \in \bar{S}$, $\mathbf{P} = \mathbf{0}$ inside the ball $B(0, r_0)$, where r_0 is independent of L and $\mathbf{P} = \mathbf{0}$ on the boundary, $\partial B(0,1)$.

We compute the second variation of $\mathcal{I}_{\mathcal{LG}}$ in (2) i.e. we compute

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^\epsilon_L]\right]_{\epsilon=0}.$$

Direct computations show that

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^\epsilon_L]\right]_{\epsilon=0} = \int_{B(0,1)\setminus B(0,r_0)} |\nabla \mathbf{P}|^2 + \frac{1}{L}\left(-a^2|\mathbf{P}|^2 - 2b^2\left(\mathbf{Q}^L_H\right)_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} + c^2\left|\mathbf{Q}^L_H\right|^2|\mathbf{P}|^2 + 2c^2\left[\mathbf{P}_{ij}\left(\mathbf{Q}^L_H\right)_{ij}\right]^2\right) dV. \tag{66}$$

In the limit $L \to 0^+$, $\left\{\mathbf{Q}^L_H\right\} \to \mathbf{Q}^0$ in $W^{1,2}\left(B(0,1); \bar{S}\right)$ and

$$s^L_H(r) = s_+ - \frac{18L}{r^2\sqrt{b^4 + 24a^2c^2}} + O(L^2)$$

on $B(0,1) \setminus B(0, r_0)$ from (54), so that

$$\left|\mathbf{Q}^L_H(\mathbf{r}) - \mathbf{Q}^0(\mathbf{r})\right| \leq C(a^2, b^2, c^2, \mathbf{r})L \quad \mathbf{r} \in B(0,1) \setminus B(0, r_0).$$

Substituting the above into (66), we obtain

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^\epsilon_L]\right]_{\epsilon=0} =$$
$$= \int_{B(0,1)\setminus B(0,r_0)} |\nabla \mathbf{P}|^2 + \frac{1}{L}\left(-a^2|\mathbf{P}|^2 - 2b^2\mathbf{Q}^0_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} + c^2\left|\mathbf{Q}^0\right|^2|\mathbf{P}|^2 + 2c^2\left(\mathbf{P}_{ij}\mathbf{Q}^0_{ij}\right)^2 + O(L)\right) dV \tag{67}$$

Using the fact that $\mathbf{Q}^0 = s_+\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)$, we find that

$$\mathbf{Q}^0_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} = s_+\left[\left(\frac{\mathbf{r}_i\mathbf{P}_{ip}}{r}\right)^2 - \frac{|\mathbf{P}|^2}{3}\right], \quad \left(\mathbf{P}_{ij}\mathbf{Q}^0_{ij}\right)^2 = \left(\frac{\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_j}{r^2}\right)^2. \tag{68}$$

Any $\mathbf{P} \in \bar{S}$ can be written as $\mathbf{P} = S\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right) + R\left(\mathbf{m}\otimes\mathbf{m} - \mathbf{p}\otimes\mathbf{p}\right)$ where $0 \leq R \leq \frac{S}{3}$ or $\frac{S}{3} \leq R \leq 0$, $\mathbf{n}, \mathbf{m}, \mathbf{p}$ are the orthonormal eigenvectors of $\mathbf{P}$ [13]. Then $|\mathbf{P}|^2 = \frac{2}{3}S^2 + 2R^2$, $\left(\mathbf{P}_{ip}\mathbf{e}_p\right)^2 = \frac{S^2}{3}\left[(\mathbf{n}\cdot\mathbf{e})^2 + \frac{1}{3}\right] + R^2\left[(\mathbf{m}\cdot\mathbf{e})^2 + (\mathbf{p}\cdot\mathbf{e})^2\right] - \frac{2SR}{3}\left[(\mathbf{m}\cdot\mathbf{e})^2 - (\mathbf{p}\cdot\mathbf{e})^2\right]$ and
$(\mathbf{e}_i\mathbf{P}_{ij}\mathbf{e}_j)^2 = S^2\left[(\mathbf{n}\cdot\mathbf{e})^4 - \frac{2}{3}(\mathbf{n}\cdot\mathbf{e})^2 + \frac{1}{9}\right] + R^2\left[(\mathbf{m}\cdot\mathbf{e})^4 + (\mathbf{p}\cdot\mathbf{e})^4 - 2(\mathbf{m}\cdot\mathbf{e})^2(\mathbf{p}\cdot\mathbf{e})^2\right] - \frac{2SR}{3}(1-3(\mathbf{n}\cdot\mathbf{e})^2)\left[(\mathbf{m}\cdot\mathbf{e})^2 - (\mathbf{p}\cdot\mathbf{e})^2\right.$
for any unit-vector $\mathbf{e}$. Tedious manipulations then lead to the inequality

$$2\left(\frac{\mathbf{r}_i\mathbf{P}_{ip}}{r}\right)^2 - \left(\frac{\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_j}{r^2}\right)^2 \leq |\mathbf{P}|^2 \tag{69}$$

for all $\mathbf{P} \in \bar{S}$.

Substituting (68) and (69) into (67) and using the definition of s_+ in (5) i.e. $2c^2s_+^2 = b^2s_+ + 3a^2$, we obtain the following in the limit $L \to 0^+$

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_L^\epsilon]\right]_{\epsilon=0} = \int_{B(0,1)\setminus B(0,r_0)} |\nabla\mathbf{P}|^2 + \frac{1}{L}\left(b^2s_+|\mathbf{P}|^2 + 3a^2\left(\frac{\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_j}{r^2}\right)^2 + b^2s_+\left(\left(\frac{\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_j}{r^2}\right)^2 - 2\left(\frac{\mathbf{r}_i\mathbf{P}_{ip}}{r}\right)^2\right) + O(L)\right) \tag{70}$$

Recalling (69) and noting that

$$\frac{\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_j}{r^2} = 0 \implies \frac{\mathbf{r}_i\mathbf{P}_{ip}}{r} = 0,$$

we have the following inequality in the limit $L \to 0^+$, (since $\mathbf{P}$ is independent of L)

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_L^\epsilon]\right]_{\epsilon=0} \geq \int_{B(0,1)\setminus B(0,r_0)} |\nabla\mathbf{P}|^2 + \frac{1}{L}\left(\Gamma(a^2,b^2,c^2,\mathbf{P},\mathbf{r}) + O(L)\right)\, dV > 0 \tag{71}$$

where

$$\Gamma(a^2,b^2,c^2,\mathbf{P},\mathbf{r}) = \begin{cases} 3a^2\left(\frac{\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_j}{r^2}\right)^2, & if\ \left(\frac{\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_j}{r^2}\right)^2 > 0, \\ b^2s_+|\mathbf{P}|^2, & otherwise. \end{cases} \tag{72}$$

The positivity of the second variation ensures that the radial-hedgehog solution is locally stable against all perturbations satisfying (64) in the limit $L \to 0^+$ and Proposition 6.1 now follows. □

Comment: An alternative proof for Proposition 6.1 can be obtained by performing a Taylor series expansion of the bulk energy density as follows - $f_B(\mathbf{Q}_L^\epsilon) = f_B(\mathbf{Q}_H^L) + \epsilon\frac{\partial f_B}{\partial(\mathbf{Q}_H^L)_{ij}}\mathbf{P}_{ij} + \frac{\epsilon^2}{2}\frac{\partial^2 f_B}{\partial(\mathbf{Q}_H^L)_{ij}\partial(\mathbf{Q}_H^L)_{pq}}\mathbf{P}_{ij}\mathbf{P}_{pq}$*. It then suffices to note that* $\frac{\partial^2 f_B}{\partial(\mathbf{Q}_H^L)_{ij}\partial(\mathbf{Q}_H^L)_{pq}}\mathbf{P}_{ij}\mathbf{P}_{pq} = \frac{\partial^2 f_B}{\partial\mathbf{Q}^0_{ij}\partial\mathbf{Q}^0_{pq}}\mathbf{P}_{ij}\mathbf{P}_{pq} + O(L)$ *since* $\left|\mathbf{Q}_H^L - \mathbf{Q}^0\right| \leq CL$*, everywhere away from the origin, in the limit* $L \to 0^+$*.* $\mathbf{Q}^0$ *is a global minimizer of* f_B *and hence,* $\frac{\partial^2 f_B}{\partial\mathbf{Q}^0_{ij}\partial\mathbf{Q}^0_{pq}}\mathbf{P}_{ij}\mathbf{P}_{pq} > \alpha(a^2,b^2,c^2) > 0$ *for some positive constant* α *independent of* L*. The positivity of the second variation of* $\mathcal{I}_{\mathcal{LG}}$ *then follows as in (70), (71) and (22).*

Proposition 6.2. *Let* $B(0,R)$ *denote a ball of radius* R *centered at the origin in* $\mathbb{R}^3$*. The corresponding radial-hedgehog solution* $\mathbf{Q}_H^R$ *is stable against all small perturbations of the form*

$$\mathbf{Q} = \mathbf{Q}_H^R + \epsilon\mathbf{P} \tag{73}$$

where $\epsilon \in \mathbb{R}$, $|\epsilon| << 1$ *and* $\mathbf{P} \in \bar{S}$ *is separable in the sense of (75) below provided that the radius* R *is sufficiently small i.e.*

$$R^2 < \frac{1}{4}\left(\frac{L}{a^2 + \gamma b^2 s_+}\right), \tag{74}$$

where γ is an explicitly computable positive constant. $\mathbf{P} \in \bar{S}$ is separable in the following sense -

$$\mathbf{P}_{ij} = \alpha(r)\bar{\mathbf{P}}\left(\theta,\phi\right)_{ij} \in \bar{S} \tag{75}$$

where (r,θ,ϕ) denotes a spherical coordinate system centered at the origin, the function $\alpha : \mathbb{R} \to \mathbb{R}$ only depends on the radial distance r from the origin and $\bar{\mathbf{P}} \in \bar{S}$ only depends on the polar angles (θ,ϕ) with $\theta \in [0,\pi]\,,\ \phi \in [0,2\pi)$.

Comment: Proposition 6.2 is not restricted to the limit $L \to 0^+$; it holds for all values of the elastic constant L. The perturbation in (56) is an example of a separable perturbation in (75).

Proof: We first make two elementary observations. Consider the Landau-de Gennes energy functional $\mathcal{I}_{LG}^R$ on a ball of radius R, in the admissible space $\mathcal{A}_{\mathbf{Q}}$ i.e.

$$\mathcal{I}_{LG}^R[\mathbf{Q}] = \int_{B(0,R)} \frac{1}{2}\left|\nabla \mathbf{Q}\right|^2 + \frac{f_B(\mathbf{Q})}{L}\ dV; \tag{76}$$

the corresponding Euler-Lagrange equations are given by (8) and the upper bound (25) is independent of R. The corresponding radial-hedgehog solution is given by $\mathbf{Q}_H^R = s_H^R(r)\left(\frac{\mathbf{r}}{r}\otimes\frac{\mathbf{r}}{r} - \frac{1}{3}\mathbf{I}\right)$ where s_H^R is a global minimizer of

$$I^R[s] = \int_0^R \left(\frac{1}{3}\left(\frac{ds}{dr}\right)^2 + \frac{2s^2}{r^2}\right)r^2 + \frac{r^2}{L}\left(-\frac{a^2}{3}s^2 - \frac{2b^2}{27}s^3 + \frac{c^2}{9}s^4 + C(a^2,b^2,c^2)\right)\ dr$$

in the admissible space $\mathcal{A}_s^R = \left\{s \in W^{1,2}\left([0,R],\mathbb{R}\right); s(R) = s_+\right\}$. Following the methods of Proposition 2.1, one can prove that s_H^R is a non-negative and monotonically increasing solution of (12), subject to the boundary conditions

$$s(0) = 0 \quad \text{and } s(R) = s_+, \tag{77}$$

that satisfies the energy inequality (16) and the bounds (17) i.e. a radial-hedgehog solution $\mathbf{Q}_H^R$ exists for each $R > 0$.

As in Proposition 6.1, we compute the second variation of $\mathcal{I}_{LG}^R$ and find that

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{LG}^R[\mathbf{Q}]\right]_{\epsilon=0} = \int_{B(0,R)} |\nabla\mathbf{P}|^2 + \frac{1}{L}\left(-a^2|\mathbf{P}|^2 - 2b^2\left(\mathbf{Q}_H^R\right)_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi} + c^2\left|\mathbf{Q}_H^R\right|^2|\mathbf{P}|^2 + 2c^2\left[\mathbf{P}_{ij}\left(\mathbf{Q}_H^R\right)_{ij}\right]^2\right)\ dV \tag{78}$$

where $\mathbf{Q}$ is given by (73). We use the change of variable $\tau = \frac{r}{R}$ and the inequality $\left|\nabla\mathbf{P}\right|^2 \geq \left|\frac{\partial \mathbf{P}}{\partial r}\right|^2$ to obtain the following lower bound for the second variation

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{LG}^R[\mathbf{Q}]\right]_{\epsilon=0} \geq \int_{B(0,1)} \left[R\left|\frac{\partial\mathbf{P}}{\partial\tau}\right|^2 - \frac{R^3}{L}a^2|\mathbf{P}|^2 - \frac{2b^2}{L}R^3\left(\mathbf{Q}_H^R\right)_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi}\right]\ dV. \tag{79}$$

Using the *separability* condition (75), one can verify that

$$\left|\mathbf{P}(\mathbf{r})\right|^2 = \alpha^2(r)\left|\bar{\mathbf{P}}(\theta,\phi)\right|^2, \quad \left|\frac{\partial\mathbf{P}}{\partial\tau}\right|^2 = \left|\bar{\mathbf{P}}(\theta,\phi)\right|^2\left(\frac{\partial\alpha}{\partial\tau}\right)^2.$$

Substituting the above into (79), noting that $\left|\left(\mathbf{Q}_H^R\right)_{ij}\mathbf{P}_{jp}\mathbf{P}_{pi}\right| \leq \gamma s_+\left|\mathbf{P}\right|^2$ from (25) for some explicitly computable positive constant $\gamma \leq 9\sqrt{6}$ and using the inequality $\tau \leq 1$, we obtain the following lower bound for the second variation

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{LG}^R[\mathbf{Q}]\right]_{\epsilon=0} \geq \int_0^{2\pi}\int_0^{\pi}\int_0^1 \sin\theta\left[R\tau^2\left|\bar{\mathbf{P}}\right|^2\left(\frac{\partial\alpha}{\partial\tau}\right)^2 - \frac{R^3}{L}a^2|\mathbf{P}|^2 - \frac{2b^2}{L}R^3\gamma s_+\left|\mathbf{P}\right|^2\right]\ d\tau\ d\theta\ d\phi. \tag{80}$$

At this point, we use the inequality [4, 11]

$$\int_0^1 \tau^2 \left(\frac{\partial \alpha}{\partial \tau}\right)^2 \, d\tau \geq \frac{1}{4}\int_0^1 \alpha(\tau)^2 \, d\tau$$

and the relation $|\mathbf{P}(\mathbf{r})|^2 = \alpha^2(r)\left|\bar{\mathbf{P}}(\theta,\phi)\right|^2$ to deduce that

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{LG}^R[\mathbf{Q}]\right]_{\epsilon=0} \geq \int_0^{2\pi}\int_0^{\pi}\int_0^1 \sin\theta \left[\frac{R}{4} - \frac{a^2R^3}{L} - \frac{\gamma' s_+ b^2}{L}R^3\right]|\mathbf{P}|^2 \, d\tau \, d\theta \, d\phi. \tag{81}$$

It follows immediately from (81) that if $\mathbf{P}$ is not identically zero everywhere in $B(0,R)$, then

$$\left[\frac{d^2}{d\epsilon^2}\mathcal{I}_{LG}^R[\mathbf{Q}]\right]_{\epsilon=0} > 0 \quad \text{for } R^2 < \frac{1}{4}\frac{L}{\gamma' b^2 s_+ + a^2}$$

for some explicitly computable positive constant γ' independent of a^2, b^2, c^2 and L. Proposition 6.2 now follows. $\Box$

7 Discussion

In this paper, we have rigorously studied the qualitative properties of the radial-hedgehog solution

$$\mathbf{Q}_H(\mathbf{r}) = s(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right)$$

on a unit ball with strong *radial* anchoring conditions. The radial-hedgehog solution is a purely uniaxial solution of the system (8) in the sense that the biaxiality parameter $\beta(\mathbf{Q}_H) = \left(|\mathbf{Q}_H|^6 - 6\left(\mathrm{tr}\mathbf{Q}_H^3\right)^2\right)$ is identically zero everywhere inside the unit ball [16, 8]. In [3], H. Brezis postulated the following problem in the context of Ginzburg-Landau theory for superconductors: for maps $\mathbf{u} : \mathbb{R}^3 \to \mathbb{R}^3$, is any solution of the system

$$\Delta \mathbf{u} + \mathbf{u}\left(1 - |\mathbf{u}|^2\right) = 0 \tag{82}$$

satisfying $|\mathbf{u}(\mathbf{r})| \to 1$ as $|\mathbf{r}| + \infty$ (possibly with a good rate of convergence) and $deg_\infty \mathbf{u} = 1$ of the form

$$\mathbf{U}(\mathbf{r}) = \frac{\mathbf{r}}{r}f(r) \tag{83}$$

for a unique function f vanishing at zero and increasing to one at infinity. In [17], the authors show that every non-constant local minimizer of the Ginzburg-Landau energy functional associated with (82),

$$E(\mathbf{u},\Omega) := \int_\Omega \frac{1}{2}|\nabla \mathbf{u}|^2 + \frac{1}{4}\left(1 - |\mathbf{u}|^2\right)^2 \, dV$$

is of the form (83), up to a translation on the domain and an orthogonal transformation on the image. For nematic liquid crystals, the corresponding problem translates to: is any uniaxial solution of (8) necessarily of the form (15) i.e. are radial-hedgehog solutions the only possible uniaxial solutions of the system (8) in $\mathbb{R}^3$? If so, then radial-hedgehog solutions are also global energy minimizers within the class of uniaxial configurations and detailed numerical investigations suggest that radial-hedgehog solutions may well be global energy minimizers within the class of uniaxial and biaxial configurations for certain temperature regimes and certain values of the elastic constants [24, 16, 8, 12].

We have studied the qualitative properties of the radial-hedgehog solution in the physically relevant limit of $L \to 0^+$ and *deep* in the nematic phase. The limit $L \to 0^+$ is equivalent to the limiting problem (28) and from the results in [17], it is likely that radial-hedgehog solutions are the only possible stable uniaxial solutions of the system (8) in this limit. We have defined the radial-hedgehog solution to be a Landau-de Gennes energy minimizer within a suitably defined restricted class of radially-symmetric configurations and then adapted arguments from Ginzburg-Landau theory [1, 7] to prove the existence of a radial-hedgehog solution and study its qualitative properties in Proposition 2.1. The radial-hedgehog solution has three characteristic length scales in the limit $L \to 0^+$: (a) *isotropic core* length scale, $0 \leq r \leq r_c$ (b) a *matching scale*, $r_c < r < r_b$ and (c) an *outer* scale $r_b \leq r \leq 1$ where $\mathbf{Q}_H(\mathbf{r}) = \mathbf{Q}^0(\mathbf{r}) + C(\mathbf{r}, a^2, b^2, c^2)L$, $\mathbf{Q}^0$ is defined in (26) and the function $C(\mathbf{r}, a^2, b^2, c^2)$ is independent of L . In Section 3, we study the *isotropic core*: we derive an expansion for s_H^L near $r = 0$ and give the maximal range of validity for this expansion under certain material and temperature-dependent constraints. This analysis also shows that $r_c^2 \sim O(\frac{L}{a^2})$, consistent with the estimates for the nematic correlation length quoted in [16, 8]. In Section 4, we study the outer regime $r_b \leq r \leq 1$ and derive an expansion for s_H^L that is valid everywhere away from the origin, in the limit $L \to 0^+$. In Section 5, we demonstrate that the radial-hedgehog solution cannot be a global Landau-de Gennes minimizer in the limit $L \to 0^+$, for sufficiently low temperatures. This result is qualitatively similar to a result in [8] but our approach utilizes information about the isotropic core and we expect that these methods may be generalized to prove instability for small, but finite values of L and for temperatures close to $a^2 = 0$ in (3). In Section 6, we perform a *linear* stability analysis of the radial-hedgehog solution with respect to certain perturbations i.e. we study the stability of the radial-hedgehog solution with respect to *small* perturbations. We demonstrate that the radial-hedgehog solution is locally stable with respect to perturbations that are localized *outside* the isotropic core, in the limit $L \to 0^+$. This is consistent with Proposition 5.1 and the results in [8], where the authors consider perturbations that do not satisfy the hypothesis (64). Further, we demonstrate that the radial-hedgehog solution is locally stable with respect to all perturbations for balls of sufficiently small radius, for all values of the elastic constant L and for all $a^2 \geq 0$. We note that Proposition 5.1 is consistent with Proposition 6.2, since (63) suggests that biaxiality can manifest itself only in balls of sufficiently large radius. In the limit $a^2 \to \infty$, (63) simplifies to

$$\sigma^2 > \frac{10L}{a^2}$$

whereas Proposition 6.2 shows that the radial-hedgehog solution is *locally* stable for

$$\sigma^2 < \frac{1}{4}\frac{L}{\gamma' b^2 s_+ + a^2}.$$

The lower bound for instability in (63) and the upper bound for local stability in (74) are consistent.

The results in this paper form a good framework for a thorough analytic study of the radial-hedgehog solution in the future. These results are interesting in their own right and will contribute to a complete understanding of the uniaxial or biaxial structure of global Landau-de Gennes energy minimizers in the future. We expect that some of these results can be readily generalized to small but finite values of the elastic constant, such as Proposition 3.2 and Proposition 5.1. Further, these results can also be used to investigate the effect of the domain radius R on the equilibrium structure of the radial-hedgehog solution. For example, consider the ordinary differential equation (12) on a ball of arbitrary radius $R > 0$. Introducing the scaling $r_* = r/R$, we get the following re-scaled version of (12) on the unit ball

$$\frac{d^2 s}{dr_*^2} + \frac{2}{r_*}\frac{ds}{dr_*} - \frac{6s}{r_*^2} = \frac{R^2}{3L}\left(2c^2 s^3 - b^2 s^2 - 3a^2 s\right) \tag{84}$$

and the methods in Sections 2,3 and 4 can be applied to (84), subject to the boundary conditions (13).

Finally, we briefly compare our results to related work in the literature. Our results are in qualitative agreement with numerical investigations of nematic droplets with *homeotropic* boundary conditions (also known as *strong radial anchoring* as in (7)) reported in [24, 12]. In [24], the authors report that a radial-hedgehog type configuration can only be observed in either very small droplets or very close to nematic-isotropic transition temperature i.e. for $a^2 \sim 0$ in (3). This is consistent with Proposition 5.1, where instability occurs deep in the nematic phase (for sufficiently large values of a^2) and the stability result in Proposition 6.2, where we show that a radial-hedgehog solution is locally stable for sufficiently small droplets. In [12], the authors examine the confining effect of the boundary conditions on the core structure and find that the defect core structure becomes universal or ceases to be affected by the far-field for balls of sufficiently large radius. One can verify that the core size $r_c^2 \sim O\left(\frac{L}{a^2 R^2}\right)$ from (84) so that the core *shrinks* as R increases and has negligible effect on any far-field properties. Further, in [22], the authors study the stability or metastability of the radial-hedgehog solution with respect to *small* biaxial perturbations and perform a linear stability analysis, similar in spirit to the analysis in Section 6. Their approach is different but they find that for the Landau-de Gennes energy functional (2), the radial-hedgehog solution is *always* locally stable. This does not contradict Proposition 5.1 where we consider a *large* and *localized* biaxial perturbation that does not satisfy the Lyuksyutov's constraint $\mathrm{tr}\mathbf{Q}^2 = \frac{2}{3}s_+^2$ employed in [22]. Finally, the analogies between our results and those reported in [16, 8] have already been mentioned in Section 5. Future work includes a theoretical study of the radial-hedgehog solution using asymptotic methods, obtaining precise bounds for its energy in terms of the elastic constant L and understanding the structure of energetically favourable biaxial configurations.

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