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The radial-hedgehog solution in Landau–de Gennes' theory for nematic liquid crystals

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We study the radial-hedgehog solution in a three-dimensional spherical droplet, with homeotropic boundary conditions, within the Landau–de Gennes theory for nematic liquid crystals. The radial-hedgehog solution is a candidate for a global Landau–de Gennes minimiser in this model framework and is also a prototype configuration for studying isolated point defects in condensed matter physics. The static properties of the radial-hedgehog solution are governed by a non-linear singular ordinary differential equation. We study the analogies between *Ginzburg–Landau* vortices and the radial-hedgehog solution and demonstrate a Ginzburg–Landau limit for the Landau–de Gennes theory. We prove that the radial-hedgehog solution is not the global Landau–de Gennes minimiser for droplets of finite radius and sufficiently low temperatures and prove the stability of the radial-hedgehog solution in other parameter regimes. These results contain quantitative information about the effect of geometry and temperature on the properties of the radial-hedgehog solution and the associated biaxial instabilities.

Key words: Defects; Landau–de Gennes; Ginzburg–Landau

1 Introduction

Defect structures have attracted a lot of interest in the liquid crystal community [23, 25–27]. 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 **Q**-tensor order parameter [7]. The **Q**-tensor can be written in terms of its eigenvalues and eigenvectors as shown below

$$\mathbf{Q} = \sum_{i=1}^{3} \lambda_i \mathbf{e}_i \otimes \mathbf{e}_i, \quad \sum_i \lambda_i = 0, \tag{1.1}$$

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 $i = 1 \ldots 3$, (ii) uniaxial state when **Q** has a pair of equal non-zero eigenvalues and (iii) biaxial state when **Q** has three distinct eigenvalues [22].

A prototype example of such a confined system is a spherical droplet with *strong radial anchoring* or *homeotropic* (normal) boundary conditions. This example has been widely studied in the literature, especially from a numerical point of view, and it is generally believed that there are two competing equilibria: (a) the *radial-hedgehog* solution that has a single isolated point defect at the droplet centre and (b) the *biaxial-torus* solution where the point defect broadens out to a ring-like structure around the droplet centre [10,16,26,27]. The radial-hedgehog solution 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. The isotropic point in the radial-hedgehog solution and the biaxial ring in the torus solution are interpreted as being *defect structures* since they are localised regions of abrupt changes in the eigenvalue structure.

This paper aims to build a self-contained mathematical description of the radial-hedgehog solution within the Landau–de Gennes framework. Firstly, this is an interesting mathematical problem in its own right since the radial-hedgehog solution is a rare example of an explicit solution of the Landau–de Gennes Euler–Lagrange equations in (2.12). Moreover, the corresponding scalar order parameter is a solution of an ordinary differential equation (see (2.17)) and hence has a tractable and yet non-trivial mathematical structure. Indeed, this is the first step in the mathematical theory of defects in liquid crystalline systems. Secondly, a systematic mathematical analysis of the radial-hedgehog solution is crucial for understanding the structure and locations of point defects in liquid crystalline systems, the multiplicity of uniaxial solutions and the characterisation of the competing biaxial structures.

This paper has two main themes: (i) rigorously study the effect of the droplet radius, R, and the reduced temperature, t (see (2.7) for definition) on the stability of the radial-hedgehog solution and (ii) identify the analogies and differences between the radial-hedgehog solution and Ginzburg–Landau vortices. We work with low temperatures for which the isotropic phase is a locally unstable critical point of the bulk Landau–de Gennes potential and $t > 0$ in this parameter regime, by our definition of the model variables (see (2.3) and (2.7)). The stability of the radial-hedgehog solution has been studied in a batch of papers [10, 23, 25–27]. In [10], the authors demonstrate instability of the radial-hedgehog solution in the limit $R \to \infty$ and $t \to +\infty$ (in terms of our definition of t from (2.3) and (2.7)). An important ingredient of their proof is the construction of explicit lower and upper bounds for the scalar order parameter of the radial-hedgehog solution. However, their bounds are only valid in the $R \to \infty$ limit. In this paper, we go a step further by constructing lower and upper bounds for the corresponding scalar order parameter that are valid for finite but sufficiently large values of R. We use these bounds to demonstrate that the radial-hedgehog solution cannot be a global Landau–de Gennes energy minimiser for finite t and for droplets with finite R. Numerical simulations indicate that the radial-hedgehog solution cannot be globally energy minimising for modest values of R and t, i.e. $R \sim 10, t \sim 5$ (see [17]). Secondly, we consider the second variation of the Landau–de Gennes functional and show that the radial-hedgehog solution is locally stable for droplets of sufficiently small radius, of the order of the biaxial correlation length [17]. The condition for local stability prescribes a curve in the (R, t)-plane and this curve is in qualitative agreement with the numerical bifurcations reported in the literature [10,11,27]. We have generalised the local stability results to include the effect of elastic anisotropy.

Thirdly, we identify a Ginzburg–Landau limit for the Landau–de Gennes theory. The radial-hedgehog solutions can be thought of as being prototypical vortices in the

Ginzburg–Landau theory for superconductors [2]. More precisely, the radial-hedgehog solution can be interpreted as being a degree $+1$ vortex in three dimensions. There is a very well-developed theory for the structure, location, multiplicity and stability of vortices in Ginzburg–Landau theory, especially in two dimensions but generalisations to higher dimensions are non-trivial [2, 9, 12, 21]. We show that for sufficiently low temperatures, the non-linearities in the Landau–de Gennes Euler–Lagrange equations *effectively* reduce to the non-linearities in the Ginzburg–Landau equations although there are technical differences. For sufficiently low temperatures, we exploit Ginzburg–Landau methods and shooting methods to prove uniqueness of the radial-hedgehog solution and to study its qualitative properties, e.g. far-field expansions. More generally, although the study of uniaxial states can be viewed as a generalised Ginzburg–Landau theory from $\mathbb{R}^3 \to \mathbb{R}^3$ (see [20] for a Ginzburg–Landau description of uniaxiality), biaxiality presents a whole host of new mathematical challenges, outside the scope of Ginzburg–Landau theory [18]. In particular, there is no analogue of a biaxial instability in the current Ginzburg–Landau literature and such instabilities play a pivotal role in Landau–de Gennes theory.

The paper is organised as follows. In Section 2, we prove the existence of a radial-hedgehog solution in spherical droplets with radial anchoring in the Landau–de Gennes framework and establish bounds for the corresponding scalar order parameter. In Section 3, we derive a series expansion for the radial-hedgehog solution near its isotropic core and demonstrate its similarity with three-dimensional vortices in Ginzburg–Landau theory [9]. We then prove that the radial-hedgehog solution cannot be a global Landau–de Gennes energy minimiser for sufficiently large (but finite) droplets and for sufficiently low (but finite) temperatures by means of an explicit comparison argument. We perform a parallel linear stability analysis and obtain quantitative information about the effect of geometry and temperature on the stability of the radial-hedgehog solution. In Section 4, we focus on the low-temperature regime and the resulting Ginzburg–Landau structure of the governing ordinary differential equation. We demonstrate the applications of Ginzburg–Landau techniques and shooting methods to the radial-hedgehog solution in this regime. In Section 5, we discuss our results and how they complement previous work in this area.

2 Preliminaries

We study the qualitative properties of radial-hedgehog solutions on spherical droplets, $B(0,R_o) \subset \mathbb{R}^3$, where

$$B(0,R_o) = \left\{ \mathbf{r} \in \mathbb{R}^3; |\mathbf{r}| \leqslant R_o \right\} \tag{2.1}$$

and $R_o > 0$ is independent of any model parameters, subject to strong radial anchoring conditions. We work within the Landau–de Gennes theory for nematic liquid crystals, in the low-temperature regime where the isotropic phase is locally unstable.

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

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

where we have used the Einstein summation convention and the Einstein convention will

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be used in the rest of the paper. The corresponding matrix norm is defined to be

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

We recall from [18, 22] 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 $\mathbf{Q}$ and s, r are real scalar order parameters. 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 eigenvector of $\mathbf{Q}$ with the non-degenerate eigenvalue and s is a scalar order parameter that measures the degree of orientational ordering about $\mathbf{n}$.

The Landau–de Gennes energy functional is given by [7, 22]

$$\mathscr{I}_{\mathscr{L}\mathscr{G}}[\mathbf{Q}] = \int_{B(0,R)} \frac{L}{2}|\nabla\mathbf{Q}|^2 + f_B(\mathbf{Q})\, dV, \tag{2.2}$$

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

$$f_B(\mathbf{Q}) = -\frac{a^2}{2}\operatorname{tr}\mathbf{Q}^2 - \frac{b^2}{3}\operatorname{tr}\mathbf{Q}^3 + \frac{c^2}{4}\left(\operatorname{tr}\mathbf{Q}^2\right)^2. \tag{2.3}$$

The form (2.3) 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. For the commonly used liquid crystal material MBBA, typical values of these characteristic constants are $a^2 = 0.042\times 10^6(T^* - T)N/m^2, b^2 = 0.64\times 10^6 N/m^2, c^2 = 0.35\times 10^6 N/m^2$, where T is the absolute temperature and T^* is a characteristic temperature below which the isotropic phase $\mathbf{Q} = 0$ ceases to be a locally stable stationary point of f_B in (2.3) [22, 24]. We work in the temperature regime $T < T^*$, or equivalently $a^2 > 0$, where the bulk energy density attains its global minimum on the set of uniaxial $\mathbf{Q}$-tensors given by [20]

$$\mathbf{Q}_{\min} = \left\{\mathbf{Q} \in \bar{S},\ \mathbf{Q} = s_+\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right)\right\}, \tag{2.4}$$

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

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \tag{2.5}$$

In particular, as a^2 increases, we move to lower temperatures *deep* in the nematic phase. We work with strong radial anchoring/homeotropic boundary conditions [10, 27]; this is mathematically described by the Dirichlet boundary condition $\mathbf{Q}_b \in \mathbf{Q}_{\min}$ given below -

$$\mathbf{Q}_b = s_+ \left(\frac{\mathbf{r}}{|\mathbf{r}|} \otimes \frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I} \right), \tag{2.6}$$

where $\frac{\mathbf{r}}{|\mathbf{r}|}$ is the unit vector in the radial direction. The physically observable, equilibrium configurations correspond to either global or local minimisers of $\mathscr{I}_{\mathscr{L}\mathscr{G}}$ in our admissible space. For completeness, we recall that $W^{1,2}(B(0,R_o);\bar{S})$ is the Sobolev space of square-integrable $\mathbf{Q}$-tensors with square-integrable first derivatives [8]. The corresponding $W^{1,2}$-norm is given by $\|\mathbf{Q}\|_{W^{1,2}(B(0,R_o))} = (\int_{B(0,R_o)} |\mathbf{Q}|^2 + |\nabla \mathbf{Q}|^2 \, dx)^{1/2}$. In addition to the $W^{1,2}$-norm, we also use the L^∞-norm in this paper, defined to be $\|\mathbf{Q}\|_{L^\infty(B(0,R_o))} = \text{ess sup}_{\mathbf{x} \in B(0,R_o)} |\mathbf{Q}(\mathbf{x})|$.

We work in a dimensionless framework and as outlined in [10, 17], we introduce the following dimensionless variables:

$$\tilde{\mathbf{r}} = \frac{\mathbf{r}}{\xi_b}, \quad \tilde{\mathbf{Q}} = \frac{1}{h_+}\sqrt{\frac{27c^4}{2b^4}}\mathbf{Q}, \quad \widetilde{\mathscr{I}_{\mathscr{L}\mathscr{G}}} = \frac{h_+^2}{\sqrt{t}}\sqrt{\frac{27c^6}{4b^4L^3}}\mathscr{I}_{\mathscr{L}\mathscr{G}}, \tag{2.7}$$

where $t = \frac{27a^2c^2}{b^4} > 0$ is the *reduced temperature* [10], $t > 1$ throughout the paper and

$$h_+ = \frac{3 + \sqrt{9 + 8t}}{4}. \tag{2.8}$$

The length scale $\xi_b = \frac{\xi}{\sqrt{t}}$, where $\xi = \sqrt{\frac{27c^2L}{b^4}}$, is referred to as the *biaxial correlation length* in the literature [17]. The corresponding dimensionless Landau–de Gennes energy density is

$$\tilde{e}(\tilde{\mathbf{Q}}, \nabla\tilde{\mathbf{Q}}) = \frac{1}{2}|\nabla\tilde{\mathbf{Q}}|^2 - \frac{1}{2}\text{tr}\tilde{\mathbf{Q}}^2 - \frac{\sqrt{6}h_+}{t}\text{tr}\tilde{\mathbf{Q}}^3 + \frac{h_+^2}{2t}(\text{tr}\tilde{\mathbf{Q}}^2)^2 \tag{2.9}$$

and the associated Landau–de Gennes energy functional is given by

$$\tilde{\mathscr{I}}_{LG}[\tilde{\mathbf{Q}}] = \int_{B(0,\tilde{R})} \tilde{e}(\tilde{\mathbf{Q}}, \nabla\tilde{\mathbf{Q}}) \, dV, \tag{2.10}$$

where $\tilde{R} = \sqrt{t}\frac{R_o}{\xi}$. In what follows, we drop the *tilde* on the dimensionless variables for brevity and all subsequent results are to be understood in terms of the dimensionless variables. We take the admissible $\mathbf{Q}$-tensors to belong to the space

$$\mathscr{A}_{\mathbf{Q}} = \left\{ \mathbf{Q} \in W^{1,2}\left(B(0,R);\bar{S}\right); \mathbf{Q} = \sqrt{\frac{3}{2}}\left(\frac{\mathbf{r}}{|\mathbf{r}|} \otimes \frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I}\right) \text{ on } \partial B(0,R) \right\}. \tag{2.11}$$

The associated Euler–Lagrange equations are [18, 20]

$$\Delta \mathbf{Q}_{ij} = -\mathbf{Q}_{ij} - \frac{3\sqrt{6}h_+}{t}\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \frac{\delta_{ij}}{3}\text{tr}(\mathbf{Q}^2)\right) + \frac{2h_+^2}{t}\mathbf{Q}_{ij}\text{tr}(\mathbf{Q}^2), \quad i,j = 1,2,3, \tag{2.12}$$

where the term $\frac{\delta_{ij}}{3}\text{tr}(\mathbf{Q}^2)$ is a Lagrange multiplier associated with the tracelessness constraint. It follows from standard arguments in elliptic regularity that any solution $\mathbf{Q}$ of

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the non-linear elliptic system (2.12) is smooth and real analytic on $B(0,R)$ [6, 18]. In particular, all global and local energy minimisers in $\mathscr{A}_{\mathbf{Q}}$ are classical solutions of (2.12).

Radial-hedgehog solutions are examples of spherically symmetric uniaxial solutions of the system (2.12) in the admissible space $\mathscr{A}_{\mathbf{Q}}$ and have the form

$$\mathbf{Q} = \sqrt{\frac{3}{2}} h(r) \left(\frac{\mathbf{r}}{|\mathbf{r}|} \otimes \frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I} \right). \tag{2.13}$$

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

$$\mathscr{A}_h = \left\{ h \in W^{1,2}\left([0,R], \mathbb{R}\right); h(R) = 1 \right\}. \tag{2.14}$$

We note that $\mathbf{Q} \in W^{1,2}\left(B(0,R); \bar{S}\right)$ necessarily implies that $h \in W^{1,2}\left([0,R]; \mathbb{R}\right)$ since the eigenvalues of a symmetric matrix are Lipschitz functions of the matrix components [28], and hence, $\mathscr{A}_h$ is a natural choice for the admissible space. There may be multiple spherically symmetric solutions of (2.12) but we define a radial-hedgehog solution to be an energy-minimising spherically symmetric solution as described below.

Proposition 2.1 *(a) Consider the energy functional*

$$I[h] = \int_0^R r^2 \left(\frac{1}{2}\left(\frac{dh}{dr}\right)^2 + \frac{3h^2}{r^2} + f(h) \right) dr \tag{2.15}$$

defined for functions $h \in \mathscr{A}_h$, where

$$f(h) = -\frac{h^2}{2} - \frac{h_+}{t} h^3 + \frac{h_+^2}{2t} h^4. \tag{2.16}$$

For each $t > 1$, there exists *a global minimiser $h^* \in \mathscr{A}_h$ for I in (2.15). The function h^* is a solution of the following singular non-linear ordinary differential equation:*

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = -h + h^3 + \frac{3h_+}{t}\left(h^3 - h^2\right) \tag{2.17}$$

subject to the boundary conditions

$$h(0) = 0 \text{ and } h(R) = 1. \tag{2.18}$$

Moreover, h^* is analytic for all $r \geqslant 0$.

(b) Define the radial-hedgehog solution by

$$\mathbf{Q}^*(\mathbf{r}) = \sqrt{\frac{3}{2}} h^*(r) \left(\frac{\mathbf{r} \otimes \mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I} \right), \tag{2.19}$$

where h^* is a global minimiser of $I[h]$ in (2.15), in the admissible space $\mathscr{A}_h$. Then $\mathbf{Q}^* \in \mathscr{A}_{\mathbf{Q}}$ is a solution of the Landau–de Gennes Euler–Lagrange equation (2.12), i.e. is a stationary point of the Landau–de Gennes energy functional. Moreover, these solutions satisfy the *following energy bound:*

$$\mathcal{I}_{LG}[\mathbf{Q}^*] \leqslant 12\pi R, \tag{2.20}$$

where $\tilde{\mathcal{I}}$ *has been defined in (2.10).*

(c) The function h^* *satisfies the following bounds for* $r \in [0, R]$*:*

$$0 \leqslant h^*(r) \leqslant 1 \quad r \in [0, R]. \tag{2.21}$$

Proof

(a) Consider the energy functional $I[h]$ defined for $h \in \mathscr{A}_h$. Firstly, we note that the admissible space $\mathscr{A}_h$ is non-empty. Indeed, the constant function $h(r) = 1$ for $r \in [0, R]$ belongs to $\mathscr{A}_h$. Secondly, the functional I in (2.15) is bounded from below and is weakly lower semi-continuous on our admissible space (since the integrand is convex in dh/dr). The existence of a global minimiser $h^* \in \mathscr{A}_h$ now follows from the direct methods in the calculus of variations [8].

It is straightforward to compute the Euler–Lagrange equations associated with the functional I in (2.15), i.e.

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

where $h' = dh/dr$, $e(h, h') = r^2\left(\frac{1}{2}\left(\frac{dh}{dr}\right)^2 + \frac{3h^2}{r^2} - \frac{h^2}{2} - \frac{h_+}{t}h^3 + \frac{h_+^2}{2t}h^4\right)$. One can check that the corresponding Euler–Lagrange equation is indeed the ordinary differential equation in (2.17) and a global minimiser h^* is necessarily a solution of these Euler–Lagrange equations.

The boundary condition $h^*(R) = 1$ follows from our definition of the admissible space $\mathscr{A}_h$. All functions $h \in \mathscr{A}_h$ are necessarily continuous since $h \in W^{1,2}([0, R], \mathbb{R}) \implies h \in C^{0,\alpha}([0, R], \mathbb{R})$ for some $0 < \alpha < 1/2$ from the Sobolev embedding theorem [8]. The boundary condition $h(0) = 0$ follows from the continuity of $h^*(r)$ for $r \in [0, R]$. We proceed by contradiction and assume that $|h^*(r)| \geqslant h_0$ for $r \in [0, r_0]$, for some fixed $h_0 > 0$ and $0 < r_0 \ll 1$. Since h^* is continuous, we deduce that h^* has a fixed sign near the origin and we further assume that $h^*(r) > h_0 > 0$ for $r \in [0, r_0]$. Consider the governing equation (2.17); it can be re-written as

$$\frac{d}{dr}\left(r^2\frac{dh}{dr}\right) = 6h + r^2\left(h^3 - h + \frac{3h_+}{t}\left(h^3 - h^2\right)\right), \tag{2.22}$$

where h_+ has been defined in (2.8). Then we have

$$r^2\frac{dh}{dr} \geqslant \int_\epsilon^r 6h(r')dr' + Cr^3 + \epsilon^2 h'(\epsilon) \quad for\ r \in (0, r_0), \tag{2.23}$$

where $0 < \epsilon < r/10$ is fixed, $h'(\epsilon) = \frac{dh}{dr}|_{r=\epsilon}$ and C is a constant. We note that $h'(\epsilon)$ can be bounded independently of ϵ, i.e. $\left|\frac{dh}{dr}\right| \leqslant C(t)$ for $r \in [0, R]$ from [18]. Squaring both sides of (2.23) and integrating from ϵ to r, we obtain

$$\int_\epsilon^r \left(\frac{dh}{dr'}\right)^2 dr' \geqslant \int_\epsilon^r \frac{\gamma h_0^2}{t^2}\, dt + C'' r^3 + \epsilon^2 h'(\epsilon)\int_\epsilon^r \frac{1}{t^3}dt \quad for\ r \in (0, r_0), \tag{2.24}$$

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where γ and C'' are constants independent of ϵ. In the limit $\epsilon \to 0$, (2.24) contradicts the hypothesis that $h \in W^{1,2}([0,R];\mathbb{R})$ from which we must have

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

Therefore, we deduce that $h(0) = 0$ for any solution of (2.17) in $\mathscr{A}_h$ and $h^* \in \mathscr{A}_h$ is a solution of (2.17), subject to the boundary conditions (2.18). The analyticity of h^* now follows from standard arguments in the theory of ordinary differential equations (see [14] for a proof of the analyticity statement).

(b) Given a global minimiser h^* of $I[h]$ in (2.15) , define a radial-hedgehog solution as follows:

$$\mathbf{Q}^* = \sqrt{\frac{3}{2}} h^*(r) \left(\frac{\mathbf{r} \otimes \mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right).$$

It is clear that $\mathbf{Q}^* \in \mathscr{A}_{\mathbf{Q}}$ since $h^* \in W^{1,2}([0,R];\mathbb{R})$ by definition. One can directly check that

$$\mathscr{I}_{\mathscr{L}\mathscr{G}}[\mathbf{Q}^*] = 4\pi I[h^*] \tag{2.25}$$

and that $\mathbf{Q}^*$ is a solution of the Euler–Lagrange equation (2.12), since h^* is a solution of the ordinary differential equation (2.17), subject to the boundary conditions (2.18).

The function h^* has been defined to be the global minimiser of the functional I in (2.15), in the admissible space $\mathscr{A}_h$. However, the constant function, $\bar{h}(r) = 1$ for $r \in [0,R]$, belongs to $\mathscr{A}_h$ and hence

$$I[h^*] \leqslant I[\bar{h}] = 3R. \tag{2.26}$$

The energy bound on $\mathscr{I}_{\mathscr{L}\mathscr{G}}[\mathbf{Q}^*]$, where $\mathbf{Q}^*$ is as in (2.19), follows from (2.25).

(c) The upper bound $|h^*(r)| \leqslant 1$ follows directly from a result in [19] where we establish that every solution $\mathbf{Q}$ of the system (2.12) in the admissible space $\mathscr{A}_{\mathbf{Q}} = \{\mathbf{Q} \in W^{1,2}(B(0,R);\bar{S}); \mathbf{Q} = \sqrt{\frac{3}{2}}\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2} - \frac{1}{3}\mathbf{I}\right) \text{ on } \partial B(0,R)\}$ satisfies the global upper bound

$$|\mathbf{Q}(\mathbf{r})| \leqslant 1.$$

The radial-hedgehog solution $\mathbf{Q}^*$ is a solution of the system (2.12) and

$$|\mathbf{Q}^*(\mathbf{r})| = |h^*(r)|.$$

The upper bound $|h^*(r)| \leqslant 1$ follows immediately.

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

$$\tilde{\Omega} = \{\mathbf{r} \in B(0,R);\ h^*(r) < 0\} \subset B(0,R),$$

with $h^*(r) = 0$ on $\partial\tilde{\Omega}$. We note that $\tilde{\Omega}$ must be an interior subset because of the boundary condition $\mathbf{Q}_b$ in (2.6). We define the perturbation

$$\bar{h}^*(r) = \begin{cases} h^*(r), & \mathbf{r} \in B(0,R) \setminus \tilde{\Omega}, \\ -h^*(r), & \mathbf{r} \in \tilde{\Omega}. \end{cases} \tag{2.27}$$

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One can then easily check that

$$I[\bar{h}^*] - I[h^*] = \int_{\tilde{\Omega}} -\frac{h_+}{t}\left(\bar{h}^*\right)^3 + \frac{h_+}{t} h^{*3}\, dV = \int_{\tilde{\Omega}} \frac{2h_+}{t} h^{*3}\, dV < 0, \tag{2.28}$$

since $h^*(r) < 0$ on $\tilde{\Omega}$ by assumption. The inequality (2.28) contradicts the global minimality of h^* in $\mathscr{A}_h$, and hence, we deduce that $h^*(r) \geqslant 0$ for $r \in [0, R]$. The inequalities (2.21) now follow. □

Corollary *For h^* as defined in Proposition 2.1, we have $h^*(r) > 0$ for $r > 0$.*

Proof We proceed by contradiction. Assume that $h^*(r_0) = 0$ for some $r_0 \in (0, R]$. From the bounds in (2.21) and the boundary conditions (2.18), this implies that h^* has a minimum at r_0 so that

$$\frac{d^2 h^*}{dr^2} + \frac{2}{r}\frac{dh^*}{dr} \geqslant 0$$

at r_0 by definition of a minimum (the first derivative vanishes and the second derivative is strictly non-negative for a global minimum). Then (2.17) implies that

$$\frac{d^2 h^*}{dr^2} = 0$$

at r_0. Given that $h^*(r_0) = \frac{dh^*}{dr}|_{r=r_0} = \frac{d^2 h^*}{dr^2}|_{r=r_0} = 0$, we can repeatedly differentiate both sides of (2.17) to deduce that $\frac{d^n h^*}{dr^n}|_{r=r_0} = 0$ for all $n \geqslant 2$. This contradicts the boundary condition $h(R) = 1$, and hence, h^* is strictly positive everywhere away from the origin. □

In summary, in Proposition 2.1, we prove the existence of a radial-hedgehog solution of the form (2.19), that can be interpreted as being a Landau–de Gennes energy minimiser within the class of radially symmetric configurations. This radial-hedgehog solution satisfies the energy bound (2.20) and the corresponding scalar order parameter h^* is bounded from both above and below as shown in (2.21). The radial-hedgehog solution has a single isolated isotropic point at the origin where h^* vanishes and this isolated isotropic point is interpreted as being a defect point, since the radial-hedgehog solution is strictly uniaxial everywhere else. In the next section, we study the *isotropic core* of the radial-hedgehog solution and the manifestation of biaxial instabilities within this core.

3 The isotropic core, biaxial instabilities and local stability of the radial-hedgehog solution

Proposition 3.1 *Let h^* be a global minimiser of the energy functional I in (2.15). Then h^* is a solution of the ordinary differential equation (2.17) subject to the boundary conditions (2.18). As $r \to 0$, we have the following series expansion for h^*:*

$$h^*(r) = \sum_{n=0}^{\infty} a_n r^n = a_2 r^2 \left[1 - \frac{r^2}{14} + o(r^2)\right] \quad \text{as } r \to 0, \tag{3.1}$$

where $a_n = 0$ for all n odd and $a_2 > 0$ is an arbitrary constant. For R sufficiently large, we have the following bounds on the constant a_2 in (3.1):

$$\frac{1}{14} \leqslant a_2 \leqslant \frac{1}{3} + \frac{3}{8t} + \frac{1}{8t}\sqrt{9 + 8t}. \tag{3.2}$$

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Comment. Equation (3.1) is identical to the series expansion for three-dimensional vortices near the origin, within the Ginzburg–Landau theory for superconductivity [9].
Comment. If $a_2 = 0$ in (3.1), then h^* identically vanishes contradicting our choice of the Dirichlet boundary condition.

Proof From Proposition 2.1, we have that h^* is analytic for $r \geqslant 0$. We seek a power series expansion of h^* around the origin with $h^*(0) = 0$, of the form

$$h^*(r) = \sum_{n=1}^{\infty} a_n r^n \quad 0 < r \leqslant R_c, \tag{3.3}$$

where R_c is the radius of convergence.

We substitute the ansatz (3.3) into the ordinary differential equation (2.17) and equate the coefficients of r^n on both sides of (2.17). Straightforward computations show that

$$\begin{aligned} &a_1 = a_3 = 0,\ a_2 > 0 \text{ is arbitrary},\\ &a_4 = -\frac{a_2}{14},\\ &h^*(r) = a_2\left[r^2 - \frac{r^4}{14} + \cdots\right], \end{aligned} \tag{3.4}$$

where $a_2 > 0$ since h^* is non-negative from Proposition 2.1.

Next we show that the formal expansion (3.3) involves no odd powers of r. Direct computations show that $a_1 = a_3 = 0$, as stated in (3.4). We proceed by induction. Suppose that $a_{2n+1} = 0$ for $n = 0 \dots p$. We show that $a_{2p+3} = 0$ too. Consider the left-hand side of the ordinary differential equation (2.17), i.e.

$$\frac{d^2h^*}{dr^2} + \frac{2}{r}\frac{dh^*}{dr} - \frac{6h^*}{r^2} = \sum_{n=1}^{\infty} r^{n-2} a_n \left[n^2 + n - 6\right]$$

so that the coefficient of r^{2p+1} is $(4p+2)(p+3)a_{2p+3}$. We compute the coefficient of r^{2p+1} on the right-hand side of (2.17). One can directly show that

$$-h^* + {h^*}^3 + \frac{3h_+}{t}\left({h^*}^3 - {h^*}^2\right) = \sum_{n=1}^{\infty} b_n r^n,$$

where

$$\begin{aligned} b_{2p+1} &= -a_{2p+1} + \left(1 + \frac{3h_+}{t}\right)\left[3(a_1^2 a_{2p-1} + a_2^2 a_{2p-3} + \cdots + a_p^2 a_1) + a^3_{\frac{2p+1}{3}}\right]\\ &\quad - \frac{6h_+}{t}\left(a_1 a_{2p} + a_2 a_{2p-1} + \cdots + a_p a_{p+1}\right), \end{aligned} \tag{3.5}$$

where the term involving $a_{\frac{2p+1}{3}}$ comes into play if $\frac{2p+1}{3}$ is a positive integer. One can check (3.5) by noting that the coefficient of r^{2p+1} in the series ${h^*}^2$ is $\sum_{n=1}^{2p} 2a_n a_{2p+1-n}$ so that both $\{n, 2p+1-n\} \leqslant 2p+1$ and one of $\{n, 2p+1-n\}$ is odd. Similarly, we note that the coefficient of r^{2p+1} in the series ${h^*}^3$ is $a^3_{\frac{2p+1}{3}} + \sum_{n=1}^{p} 3a_n^2 a_{2p+1-2n}$, where

$\{n, 2p+1-2n\} < 2p+1$ and $\{\frac{2p+1}{3}, 2p+1-2n\}$ are necessarily odd. However, from the hypothesis, $a_{2n+1} = 0$ for $n = 0 \ldots p$. Therefore, $b_{2p+1} = 0$ in (3.5) and since

$$b_{2p+1} = (4p+2)(p+3)a_{2p+3},$$

we deduce that $a_{2p+3} = 0$ as required.

The following bounds have been established in [10] and are valid in the $R \to \infty$ limit:

$$\frac{r^2}{r^2+14} \leqslant h^*(r) \leqslant \frac{r^2}{r^2+t\lambda_t^2}, \tag{3.6}$$

where $\lambda_t^2 = \frac{24}{9+8t+3\sqrt{9+8t}} \leqslant \frac{3}{t} \leqslant 3$ since $t \geqslant 1$. The inequalities (3.2) follow from (3.6) and the limit

$$a_2 = \lim_{r \to 0} \frac{h^*(r)}{r^2}.$$

□

3.1 Biaxial instabilities

Proposition 3.2 *Let $R \geqslant 200$ and $t \geqslant 200$. Let h_R be the corresponding global minimiser of $I[h]$ in (2.15) in the admissible space $\mathscr{A}_h$. Then h_R is a solution of the ordinary differential equation (2.17), subject to the boundary conditions (2.18). The function h_R satisfies the following explicit bounds:*

$$\left(\frac{r}{R}\right)^2 \leqslant h_R(r) \leqslant \frac{r^2}{r^2+t\lambda_t^2}\left(1+\frac{t\lambda_t^2}{R^2}\right), \tag{3.7}$$

where λ_t has been defined in (3.6).

Proof The proof of Proposition 3.2 follows from classical arguments in the theory of differential inequalities [10]. We recall the following classical result that is adequate for our purposes. Consider the general problem

$$\begin{aligned} &N[x] := \frac{d^2x}{dt^2} - f\left(t, x, \frac{dx}{dt}\right) \quad a < t < b, \\ &x(a) = A, \ x(b) = B, \end{aligned} \tag{3.8}$$

with $-\infty < a < b < \infty$. Under reasonable hypotheses on the function f, if there exist functions $\alpha, \beta \in C^2(a,b) \cap C^0[a,b]$ such that

$$\begin{aligned} &N[\alpha] \geqslant 0, \ N[\beta] \leqslant 0, \\ &\alpha(a) \leqslant A \leqslant \beta(a), \ \alpha(b) \leqslant B \leqslant \beta(b), \end{aligned} \tag{3.9}$$

then

$$\alpha(t) \leqslant x(t) \leqslant \beta(t) \tag{3.10}$$

for a solution $x \in C^2(a,b) \cap C^0[a,b]$ of $N[x] = 0$, subject to the boundary conditions (3.8).

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We set

$$N[h] := \frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} + h - h^3 + \frac{3h_+}{t}\left(h^2 - h^3\right),$$
$$h(0) = 0,\ h(R) = 1. \tag{3.11}$$

We set

$$\alpha(r) = \left(\frac{r}{R}\right)^2,\ \beta(r) = \frac{r^2}{r^2 + t\lambda_t^2}\left(1 + \frac{t\lambda_t^2}{R^2}\right),$$

where λ_t has been defined in (3.6). One can directly check that $N[\alpha] \geqslant 0$ and $\alpha(0) = 0$, $\alpha(R) = 1$. This establishes the lower bound in (3.7).

The upper bound argument needs more care. Firstly, we set $f(r) = \frac{r^2}{r^2+t\lambda_t^2}$ so that

$$\beta(r) = f(r)\left(1 + \frac{t\lambda_t^2}{R^2}\right).$$

From [10], it is known that

$$N[f] \leqslant 0. \tag{3.12}$$

A direct computation shows that

$$N[\beta] = \left(1 + \frac{t\lambda_t^2}{R^2}\right)\left(N[f] - f^3(r)\left(1 + \frac{3h_+}{t}\right)\left(2\frac{t\lambda_t^2}{R^2} + \left(\frac{t\lambda_t^2}{R^2}\right)^2\right) + \frac{3h_+}{t}\frac{t\lambda_t^2}{R^2}f^2(r)\right). \tag{3.13}$$

From the definition of λ_t in (3.6), we have for $t \geqslant 200$,

$$\frac{6}{17} \leqslant t\lambda_t^2 \leqslant 3. \tag{3.14}$$

We consider two cases: (i) $f(r) \geqslant \frac{1}{10}$ and (ii) $0 \leqslant f(r) \leqslant \frac{1}{10}$. In case (i), we simply note that for $t \geqslant 200$,

$$f^2(r)\frac{3h_+}{t} \leqslant 2f^3(r), \tag{3.15}$$

which combined with (3.12) yields $N[\beta] \leqslant 0$ for $f(r) \geqslant \frac{1}{10}$. In case (ii), we note that

$$f(r) = \frac{r^2}{r^2 + t\lambda_t^2} \leqslant \frac{1}{10}$$

necessarily implies $r^2 \leqslant \frac{t\lambda_t^2}{9} \leqslant \frac{1}{3}$. Straightforward but tedious computations show that

$$N[f] \leqslant -f \quad \text{for } r^2 \leqslant \frac{1}{3} \tag{3.16}$$

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so that

$$N[\beta] \leqslant \left(1+\frac{t\lambda_t^2}{R^2}\right)\left(-f-f^3(r)\left(1+\frac{3h_+}{t}\right)\left(2\frac{t\lambda_t^2}{R^2}+\left(\frac{t\lambda_t^2}{R^2}\right)^2\right)+\frac{3h_+}{t}\frac{t\lambda_t^2}{R^2}f^2(r)\right)$$
$$\text{for} \quad r^2 \leqslant \frac{1}{3}. \quad (3.17)$$

One can readily check that $\frac{3h_+}{t}\frac{t\lambda_t^2}{R^2}f^2 < f$ so that $N[\beta] < 0$ for case (ii) too. Hence, $N[\beta] \leqslant 0$, $\beta(r)$ satisfies the boundary conditions in (3.11) and the upper bound in (3.7) follows. □

Proposition 3.3 *Consider the radial-hedgehog solution*

$$\mathbf{Q}^*(\mathbf{r}) = \sqrt{\frac{3}{2}}h^*(r)\left(\frac{\mathbf{r}\otimes\mathbf{r}}{r^2}-\frac{1}{3}\mathbf{I}\right),$$

where h^* is a global minimiser of $I[h]$ in (2.15) in the admissible space $\mathscr{A}_h$. Then $\mathbf{Q}^*$ is not the global minimiser of $\tilde{\mathscr{I}}_{LG}$ in (2.10) in the admissible space $\mathscr{A}_{\mathbf{Q}}$ defined in (2.11) for $R \geqslant 200$ and $t \geqslant 200$. In particular, the biaxial state

$$\hat{\mathbf{Q}}(\mathbf{r}) = \begin{cases}\mathbf{Q}^*(\mathbf{r}) + \frac{1}{(r^2+12)^2}\left(1-\frac{r}{\sigma}\right)\left(\mathbf{z}\otimes\mathbf{z}-\frac{\mathbf{I}}{3}\right) & 0 \leqslant r \leqslant \sigma,\\ \mathbf{Q}^*(\mathbf{r}) & \sigma \leqslant r \leqslant R,\end{cases} \quad (3.18)$$

where $\mathbf{z} = (0,0,1)$ is the unit vector in the z-direction, has lower Landau–de Gennes free energy than $\mathbf{Q}^*$ for

$$\sigma = 10, \ R = 200, \ t = 200. \quad (3.19)$$

Proof Consider a general biaxial perturbation

$$\hat{\mathbf{Q}}(\mathbf{r}) = \begin{cases}\mathbf{Q}^*(\mathbf{r}) + p(r)\left(\mathbf{z}\otimes\mathbf{z}-\frac{\mathbf{I}}{3}\right) & 0 \leqslant r \leqslant \sigma,\\ \mathbf{Q}^*(\mathbf{r}) & \sigma \leqslant r \leqslant R,\end{cases}$$

where $p : [0,R] \to \mathbb{R}$ is non-zero for $0 \leqslant r < \sigma$ and $p(r) = 0$ for all $\sigma \leqslant r \leqslant R$, $\mathbf{Q}^*$ is the radial-hedgehog solution in (2.19), $\mathbf{r} = (x,y,z)$ is the position vector, $\mathbf{z} = (0,0,1)$ is the unit-vector in the z-direction and $\mathbf{I}$ is the 3×3 identity matrix. In particular, the perturbation $\hat{\mathbf{Q}}$ is localised in a ball of radius σ around the origin or equivalently, is localised around the isotropic core of the radial-hedgehog solution and the radius σ will be determined as part of the problem.

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Let (r, θ, ϕ) with $r \in [0, R], \theta \in [0, \pi], \phi \in [0, 2\pi)$ denote a spherical coordinate system centred at the origin. Straightforward computations show that

$$\begin{aligned}
|\nabla \hat{\mathbf{Q}}|^2 &= |\nabla \mathbf{Q}^*|^2 + \frac{2}{3}\left(\frac{dp}{dr}\right)^2 + \sqrt{6}\frac{dh^*}{dr}\frac{dp}{dr}\left(\cos^2\theta - \frac{1}{3}\right), \\
\mathrm{tr}\hat{\mathbf{Q}}^2 &= \mathrm{tr}\mathbf{Q}^{*2} + \frac{2}{3}p^2(r) + \sqrt{6}h^*(r)p(r)\left(\cos^2\theta - \frac{1}{3}\right), \\
\mathrm{tr}\hat{\mathbf{Q}}^3 &= \mathrm{tr}\mathbf{Q}^{*3} + \frac{2}{9}p^3(r) + \left(\sqrt{\frac{2}{3}} + \frac{1}{\sqrt{6}}\right)h^*(r)p^2(r)\left(\cos^2\theta - \frac{1}{3}\right) \\
&\quad + \frac{3}{2}h^{*2}(r)p(r)\left(\cos^2\theta - \frac{1}{3}\right), \\
(\mathrm{tr}\hat{\mathbf{Q}}^2)^2 &= \left(\mathrm{tr}\mathbf{Q}^{*2}\right)^2 + \frac{4}{9}p^4(r) + 6\left(h^*(r)\right)^2 p^2(r)\left(\cos^2\theta - \frac{1}{3}\right)^2 \\
&\quad + \frac{4}{3}\left(h^*(r)\right)^2 p^2(r) + 2\sqrt{6}h^*(r)p(r)\left(\cos^2\theta - \frac{1}{3}\right)\left[h^{*2} + \frac{2}{3}p^2(r)\right].
\end{aligned} \tag{3.20}$$

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:

$$\begin{aligned}
&\frac{1}{4\pi}[\tilde{\mathscr{I}}_{LG}[\hat{\mathbf{Q}}] - \tilde{\mathscr{I}}_{LG}[\mathbf{Q}^*]] \\
&= \int_0^\sigma \frac{r^2}{3}\left(\frac{dp}{dr}\right)^2 - \frac{r^2}{3}p^2(r) - 2\sqrt{6}\frac{h_+}{9t}r^2p^3(r) + \frac{r^2h_+^2}{2t}\left\{\frac{4}{9}p^4(r) + \frac{28}{15}h^{*2}(r)p^2(r)\right\} dr,
\end{aligned} \tag{3.21}$$

where h_+ has been defined in (2.8). Recalling the bounds (3.7), we have that

$$\begin{aligned}
&\frac{1}{4\pi}[\tilde{\mathscr{I}}_{LG}[\hat{\mathbf{Q}}] - \tilde{\mathscr{I}}_{LG}[\mathbf{Q}^*]] \\
&< \int_0^\sigma \frac{r^2}{3}\left(\frac{dp}{dr}\right)^2 - \frac{r^2}{3}p^2(r) - 2\sqrt{6}\frac{h_+}{9t}r^2p^3(r) + \frac{r^2h_+^2}{2t} \\
&\quad \times \left\{\frac{4}{9}p^4(r) + \frac{28}{15}\left(\frac{r^2}{r^2 + t\lambda_t^2}\right)^2\left(1 + \frac{t\lambda_t^2}{R^2}\right)^2 p^2(r)\right\} dr,
\end{aligned} \tag{3.22}$$

where $\lambda_t^2 = \frac{24}{9+8t+3\sqrt{9+8t}}$. Let

$$p(r) = \frac{1}{(r^2+12)^2}\left(1 - \frac{r}{\sigma}\right). \tag{3.23}$$

One can then directly substitute (3.23), $\sigma = 10$, $R = 200$ and $t = 200$ into (2.8) and (3.22)

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to find that the associated free energy difference

$$\frac{1}{4\pi}\left[\tilde{\mathscr{I}}_{LG}[\hat{\mathbf{Q}}]-\tilde{\mathscr{I}}_{LG}[\mathbf{Q}^*]\right]<0,$$

i.e. we have found a biaxial perturbation localised in a ball $B(0,\sigma)$ that has lower free energy than the radial-hedgehog solution for $R, t = 200$. Therefore, the radial-hedgehog solution cannot be a global Landau–de Gennes minimiser in this regime.

One can check that for fixed t, σ and $p(r)$ as in (3.23), the function

$$H(r,t,R)=\frac{r^2h_+^2}{2t}\left\{\frac{4}{9}p^4(r)+\frac{28}{15}\left(\frac{r^2}{r^2+t\lambda_t^2}\right)^2\left(1+\frac{t\lambda_t^2}{R^2}\right)^2p^2(r)\right\}$$

is a decreasing function of R and hence

$$\tilde{\mathscr{I}}_{LG}[\hat{\mathbf{Q}}]-\tilde{\mathscr{I}}_{LG}[\mathbf{Q}^*]<0$$

for the perturbation $\hat{\mathbf{Q}}$ defined above for all $R \geqslant 200$ and $t = 200$. As $t \to \infty$, the cubic term $\frac{h_+}{t} \sim \frac{1}{\sqrt{t}} \to 0$ and $\frac{h_+^2}{2t} \to \frac{1}{4}$ [10] and one can verify that

$$\int_0^\sigma \frac{r^2}{4}\left\{\frac{4}{9}p^4(r)+\frac{28}{15}\left(\frac{r^2}{r^2+t\lambda_t^2}\right)^2\left(1+\frac{t\lambda_t^2}{R^2}\right)^2p^2(r)\right\}-\frac{r^2}{3}p^2(r)\,dr<0$$

for the function p defined in (3.23). Combining the two observations above, we have

$$\left[\tilde{\mathscr{I}}_{LG}[\hat{\mathbf{Q}}]-\tilde{\mathscr{I}}_{LG}[\mathbf{Q}^*]\right]<0$$

for the perturbation $\hat{\mathbf{Q}}$ defined in (3.18) for all $t, R \geqslant 200$. Proposition 3.1 now follows. □

3.2 Local stability results

In this section, we demonstrate that the radial-hedgehog solution is locally stable with respect to small perturbations for R sufficiently small (of the order of the biaxial correlation length). We consider the one-constant elastic energy density and the effects of elastic anisotropy separately. We note that Propositions 3.4 and 3.5 are known from numerical investigations and we present rigorous proofs partly for completeness and partly because these proofs give insight into how the temperature and droplet radius collectively affect stability properties.

Proposition 3.4 *Let $B(0,R)$ denote a droplet of radius R centred at the origin in $\mathbb{R}^3$. The corresponding radial-hedgehog solution $\mathbf{Q}_R^*$ is stable against all small, smooth perturbations of the form*

$$\mathbf{Q}=\mathbf{Q}_R^*+\epsilon\mathbf{P}, \tag{3.24}$$

where $\epsilon \in \mathbb{R}$, $|\epsilon| \ll 1$, $\mathbf{P} \in \bar{S}$ and $\mathbf{P} = 0$ on $\partial B(0,R)$, provided that the radius R is sufficiently

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small, i.e.

$$R^2 < \frac{1}{4}\left(\frac{1}{1+\frac{4\sqrt{6}h_+}{t}}\right). \tag{3.25}$$

In terms of the original variables (see (2.7)), (3.25) is equivalent to

$$R_o^2 < \frac{\xi^2}{4t}\left(\frac{1}{1+\frac{4\sqrt{6}h_+}{t}}\right), \tag{3.26}$$

where $\xi = \sqrt{27c^2L/b^4}$ *as in (2.7).*

Proof The results in Proposition 2.1 are true for any $R > 0$, i.e. for every $R > 0$, we are guaranteed the existence of a radial-hedgehog solution $\mathbf{Q}_R^*$ of the form (2.19), which satisfies the energy bound (2.20) and the inequalities (2.21). Consider the dimensionless free energy in (2.10) and introduce the change of variable

$$\hat{r} = \frac{r}{R}$$

so that the free energy becomes

$$I[\mathbf{Q}] = \int_0^{2\pi}\int_0^{\pi}\int_0^1 \left\{\frac{1}{2}|\nabla\mathbf{Q}|^2 - \frac{R^2}{2}\mathrm{tr}\mathbf{Q}^2 - \frac{\sqrt{6}h_+}{t}R^2\mathrm{tr}\mathbf{Q}^3 + \frac{h_+^2}{2t}R^2\left(\mathrm{tr}\mathbf{Q}\right)^2\right\}\hat{r}^2\sin\theta\, d\hat{r}\, d\theta\, d\phi. \tag{3.27}$$

We consider small perturbations

$$\mathbf{Q}_\epsilon = \mathbf{Q}_R^* + \epsilon\mathbf{P} \quad 0 < \epsilon \ll 1 \tag{3.28}$$

such that $\mathbf{P} = 0$ on $\partial B(0, R)$. We compute the second variation of the Landau–de Gennes energy functional

$$\frac{d^2}{d\epsilon^2}I[\mathbf{Q}_\epsilon]|_{\epsilon=0} = \int_0^{2\pi}\int_0^{\pi}\int_0^1 \left\{|\nabla\mathbf{P}|^2 - R^2|\mathbf{P}|^2 - \frac{6\sqrt{6}h_+}{t}R^2\mathbf{P}_{ij}\mathbf{P}_{jp}\mathbf{Q}^*_{R_{pi}} + \frac{h_+^2R^2}{2t}\left[8\left(\mathbf{Q}_R^*\cdot\mathbf{P}\right)^2 + 4|\mathbf{P}|^2|\mathbf{Q}_R^*|^2\right]\right\} dV, \tag{3.29}$$

where $dV = \hat{r}^2\sin\theta\, d\hat{r}\, d\theta\, d\phi$.

We, next, make an elementary observation

$$\mathbf{P}_{ij}\mathbf{P}_{jp}\mathbf{Q}^*_{R_{pi}} = h^*(r)\left[\mathbf{r}_i\mathbf{P}_{ij}\mathbf{r}_p\mathbf{P}_{pj}/r^2 - |\mathbf{P}|^2/3\right] \leqslant \frac{2}{3}|\mathbf{P}|^2$$

so that

$$\frac{d^2}{d\epsilon^2}I[\mathbf{Q}_\epsilon]|_{\epsilon=0} \geqslant \int_0^{2\pi}\int_0^{\pi}\int_0^1 \left\{|\nabla\mathbf{P}|^2\hat{r}^2 - R^2\hat{r}^2|\mathbf{P}|^2 - \frac{4\sqrt{6}h_+}{t}R^2\hat{r}^2|\mathbf{P}|^2\right\}\sin\theta\; d\hat{r}\; d\theta\; d\phi. \tag{3.30}$$

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We note that

$$|\nabla \mathbf{P}|^2 \geqslant \left(\frac{\partial \mathbf{P}}{\partial \hat{r}}\right)^2$$

and use the following inequality from [5, 15]:

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

for a real-valued function α defined on the interval $[0,1]$. Substituting the above inequality in (3.30), we have that

$$\frac{d^2}{d\epsilon^2} I\left[\mathbf{Q}_\epsilon\right]|_{\epsilon=0} \geqslant \int_0^{2\pi} \int_0^{\pi} \int_0^1 \left\{ \frac{1}{4}|\mathbf{P}|^2 - |\mathbf{P}|^2 R^2 \left(1 + \frac{4\sqrt{6} h_+}{t}\right)\right\} \sin\theta \, d\hat{r} \, d\theta \, d\phi \tag{3.31}$$

since $\hat{r} \leqslant 1$. It follows that

$$\frac{d^2}{d\epsilon^2} I\left[\mathbf{Q}_\epsilon\right]|_{\epsilon=0} > 0$$

if

$$R^2 < \frac{1}{4} \frac{1}{1 + \frac{4\sqrt{6} h_+}{t}} \tag{3.32}$$

or equivalently if

$$R_o^2 < \frac{\xi^2}{4t} \left(\frac{1}{1 + \frac{4\sqrt{6} h_+}{t}}\right), \tag{3.33}$$

where $R_o = \frac{\xi}{\sqrt{t}} R$ from (2.7). Proposition 3.4 now follows. □

In Proposition 3.5, we generalise the above to include the effects of elastic anisotropy. We consider a Landau–de Gennes elastic energy density of the form

$$w(\nabla \mathbf{Q}) = \frac{1}{2}\left(L_1 |\nabla \mathbf{Q}|^2 + L_2 \mathbf{Q}_{ij,j} \mathbf{Q}_{ik,k} + L_3 \mathbf{Q}_{ij,k} \mathbf{Q}_{ik,j}\right), \tag{3.34}$$

where

$$L_1 > 0, \ -L_1 < L_3 < 2L_1, \ -\frac{3}{5} L_1 - \frac{1}{10} L_3 < L_2. \tag{3.35}$$

The inequalities (3.35) are established in [6] and as a consequence, there exists a positive constant Θ such that

$$w(\nabla \mathbf{Q}) \geqslant \Theta |\nabla \mathbf{Q}|^2. \tag{3.36}$$

We work in a dimensionless framework as before (see (2.7)), drop the *tildes* on the dimensionless variables and the corresponding dimensionless energy density is

$$e^*(\mathbf{Q}, \nabla \mathbf{Q}) = \frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{\eta_2}{2} \mathbf{Q}_{ij,j} \mathbf{Q}_{ik,k} + \frac{\eta_3}{2} \mathbf{Q}_{ij,k} \mathbf{Q}_{ik,j} - \frac{1}{2}|\mathbf{Q}|^2 - \sqrt{6} \frac{h_+}{t} \mathrm{tr} \mathbf{Q}^3 + \frac{h_+^2}{2t} |\mathbf{Q}|^4, \tag{3.37}$$

where $\eta_2 = \frac{L_2}{L_1}, \eta_3 = \frac{L_3}{L_1}$ and

$$-1 < \eta_3 < 2, \ 6 + 10\eta_2 + \eta_3 > 0. \tag{3.38}$$

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There exists another positive constant Θ' such that

$$\frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{\eta_2}{2}\mathbf{Q}_{ij,j}\mathbf{Q}_{ik,k} + \frac{\eta_3}{2}\mathbf{Q}_{ij,k}\mathbf{Q}_{ik,j} \geqslant \Theta'|\nabla \mathbf{Q}|^2 \quad \mathbf{Q} \in W^{1,2}\left(B(0,R);\bar{S}\right). \tag{3.39}$$

The inequalities (3.38) and (3.39) follow directly from (3.35) and (3.36).

In [10], the authors demonstrate the existence of a radial-hedgehog solution, $\mathbf{Q}_H^R \in \mathscr{A}_{\mathbf{Q}}$, of the form (2.13), for the Euler–Lagrange equations associated with the energy density in (3.37). The radial-hedgehog solution, $\mathbf{Q}_H^R$, is completely characterised by its order parameter, $h(r)$, which is a solution of the following ordinary differential equation [10]:

$$\left(1 + \frac{2}{3}(\eta_2 + \eta_3)\right)\left(\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2}\right) + h - h^3 + \frac{3h_+}{t}\left(h^2 - h^3\right) = 0, \tag{3.40}$$

with

$$h(0) = 0 \quad h(R) = 1.$$

Corollary *Let $h \in \mathscr{A}_h$ be an arbitrary solution of (3.40) subject to the boundary conditions, $h(0) = 0$ and $h(R) = 1$. Then*

$$|h(r)| \leqslant 1 \quad r \in [0, R]. \tag{3.41}$$

Proof The proof follows from a standard maximum principle argument (see Proposition 2.1 and [19]) and the details are omitted here for brevity. □

Proposition 3.5 *Consider the Landau–de Gennes energy functional*

$$\mathscr{I}_{\mathscr{L}\mathscr{G}}[\mathbf{Q}] = \int_{B(0,R)} e^*(\mathbf{Q}, \nabla \mathbf{Q})\, dV, \tag{3.42}$$

where $e^*(\mathbf{Q}, \nabla \mathbf{Q})$ is defined in (3.37) and $B(0,R)$ denotes a droplet of radius R centred at the origin in $\mathbb{R}^3$. The corresponding radial-hedgehog solution $\mathbf{Q}_H^R$ is locally stable if the radius R is sufficiently small, i.e. if

$$R^2 < \frac{\Theta'}{2}\left(\frac{1}{1 + \frac{4\sqrt{6}h_+}{t}}\right), \tag{3.43}$$

where Θ' has been defined in (3.39). In terms of the original variables (see (2.7)), (3.43) is equivalent to

$$R_o^2 < \frac{\xi^2}{2t}\left(\frac{\Theta'}{1 + \frac{4\sqrt{6}h_+}{t}}\right), \tag{3.44}$$

where $\xi = \sqrt{27c^2L/b^4}$ as in (2.7).

Proof As in Proposition 3.4, we consider small, smooth perturbations of the form

$$\mathbf{Q}_\epsilon = \mathbf{Q}_H^R + \epsilon \mathbf{P} \quad 0 < \epsilon \ll 1, \tag{3.45}$$

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where $|\epsilon| \ll 1$ and $\mathbf{P} = 0$ on $\partial B(0, R)$. We compute the second variation of the Landau–de Gennes energy functional in (3.42) as shown below

$$\frac{d^2}{d\epsilon^2}\mathscr{I}_{\mathscr{LG}}[\mathbf{Q}_\epsilon]|_{\epsilon=0} = \int_0^{2\pi}\int_0^{\pi}\int_0^1 |\nabla \mathbf{P}|^2 + \eta_2 \mathbf{P}_{ij,j}\mathbf{P}_{ik,k} + \eta_3 \mathbf{P}_{ij,k}\mathbf{P}_{ik,j}\, dV$$
$$+ \int_0^{2\pi}\int_0^{\pi}\int_0^1 -R^2|\mathbf{P}|^2 - \frac{6\sqrt{6}h_+}{t}R^2\mathbf{P}_{ij}\mathbf{P}_{jp}\mathbf{Q}^R_{H_{pi}} + \frac{h_+^2 R^2}{2t}\left[8\left(\mathbf{Q}^R_H\cdot\mathbf{P}\right)^2 + 4|\mathbf{P}|^2|\mathbf{Q}^R_H|^2\right] dV, \tag{3.46}$$

where $\hat{r} = \frac{r}{R}$ and $dV = \hat{r}^2 \sin\theta\, d\hat{r}\, d\theta\, d\phi$. Recalling (3.39), we have

$$\frac{d^2}{d\epsilon^2}\mathscr{I}_{\mathscr{LG}}[\mathbf{Q}_\epsilon]|_{\epsilon=0} \geqslant \int_0^{2\pi}\int_0^{\pi}\int_0^1 2\Theta^{'}|\nabla \mathbf{P}|^2\, dV +$$
$$\int_0^{2\pi}\int_0^{\pi}\int_0^1 -R^2|\mathbf{P}|^2 - \frac{6\sqrt{6}h_+}{t}R^2\mathbf{P}_{ij}\mathbf{P}_{jp}\mathbf{Q}^R_{H_{pi}} + \frac{h_+^2 R^2}{2t}\left[8\left(\mathbf{Q}^R_H\cdot\mathbf{P}\right)^2 + 4|\mathbf{P}|^2|\mathbf{Q}^R_H|^2\right] dV. \tag{3.47}$$

We repeat the same steps as in Proposition 3.4 and the details are omitted here for brevity. These computations show that

$$\frac{d^2}{d\epsilon^2}\mathscr{I}_{\mathscr{LG}}[\mathbf{Q}_\epsilon]|_{\epsilon=0} > 0 \text{ for } R^2 < \frac{\Theta^{'}}{2}\left(\frac{1}{1+\frac{4\sqrt{6}h_+}{t}}\right). \tag{3.48}$$

Proposition 3.5 follows. □

We conclude this section with a result on the multiplicity of radial-hedgehog solutions for R sufficiently small. Using the change of variable $\hat{r} = \frac{r}{R}$, the ordinary differential equation (3.40) transforms to

$$\left(1 + \frac{2}{3}(\eta_2+\eta_3)\right)\left(\frac{d^2h}{d\hat{r}^2} + \frac{2}{\hat{r}}\frac{dh}{d\hat{r}} - \frac{6h}{\hat{r}^2}\right) + R^2\left(h - h^3 + \frac{3h_+}{t}\left(h^2-h^3\right)\right) = 0, \tag{3.49}$$

with

$$h(0) = 0 \quad \text{and} \quad h(1) = 1. \tag{3.50}$$

Corollary *For R sufficiently small, the ordinary differential equation (3.49), subject to the boundary conditions (3.50), has a unique solution.*

Proof The proof follows a standard pattern. Let $h_1, h_2 \in \mathscr{A}_h$ be two distinct solutions of (3.49), subject to the boundary conditions (3.50). Define

$$g[h] := \left(h^3 - h + \frac{3h_+}{t}\left(h^3 - h^2\right)\right). \tag{3.51}$$

Then

$$g[h] \leqslant 0 \; for \; 0 \leqslant h \leqslant 1,$$
$$g[h] \geqslant -C(t), \tag{3.52}$$

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where the positive constant C only depends on the reduced temperature t. Define

$$h_3(\hat{r}) = (h_1 - h_2)(\hat{r}) \quad \hat{r} \in [0,1],$$

with

$$h_3(0) = h_3(1) = 0.$$

If $h_1 \neq h_2$ somewhere, then $h_3(\hat{r})$ has a positive maximum at the point $r_0 \in (0,1)$ (unless $h_2 \geqslant h_1$ for $\hat{r} \in [0,1]$, in which case we define $h_3 = h_2 - h_1$.)

From (3.49) and (3.52), we have that

$$\left(1 + \frac{2}{3}(\eta_2 + \eta_3)\right)\left(\frac{d^2 h_3}{d\hat{r}^2} + \frac{2}{\hat{r}}\frac{dh_3}{d\hat{r}} - \frac{6h_3}{\hat{r}^2}\right) = R^2 \left(g[h_1] - g[h_2]\right) \geqslant -C(t)R^2. \qquad (3.53)$$

At $r = r_0$, we obtain the following sequence of inequalities (since the first derivative vanishes):

$$\left(1 + \frac{2}{3}(\eta_2 + \eta_3)\right)\frac{d^2 h_3}{d\hat{r}^2}|_{\hat{r}=r_0} \geqslant \left(1 + \frac{2}{3}(\eta_2 + \eta_3)\right)\frac{6h_3(r_0)}{r_0^2} - C(t)R^2$$
$$\geqslant \left(1 + \frac{2}{3}(\eta_2 + \eta_3)\right) 6h_3(r_0) - C(t)R^2. \qquad (3.54)$$

We note that $\left(1 + \frac{2}{3}(\eta_2 + \eta_3)\right) > 0$, since $\eta_2 + \eta_3 > -\frac{3}{2}$, from the inequalities in (3.38). It is clear that the right-hand side of (3.54) is necessarily positive if $h_3(r_0)$ is independent of R and R is sufficiently small. However, the definition of a maximum requires that [8]

$$\left.\frac{d^2 h_3}{d\hat{r}^2}\right|_{\hat{r}=r_0} \leqslant 0$$

yielding a contradiction for R sufficiently small. The proof is now complete, i.e. we have uniqueness of the radial-hedgehog solution for R sufficiently small. □

4 The *Ginzburg–Landau* limit

In this section, we return to the one-constant elastic energy density

$$w(\nabla \mathbf{Q}) = L\,|\nabla \mathbf{Q}|^2$$

and investigate the analogies between Ginzburg–Landau vortices and the radial-hedgehog solution.

Consider the ordinary differential equation in (2.17) and the boundary conditions (2.18)

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

in the limit $t \to \infty$. For t sufficiently large,

$$\frac{h_+}{t} \leqslant \frac{\beta}{\sqrt{t}}$$

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for some $\beta > 0$ independent of t and hence for any non-negative solution h, we have

$$\left|\frac{3h_+}{t}\left(h^2 - h^3\right)\right| = o\left(h - h^3\right) \quad t \to \infty$$

since $0 \leqslant h(r) \leqslant 1$. In the limit $t \to \infty$, the ordinary differential equation (2.17) approximately reduces to

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} \approx -h + h^3 \tag{4.1}$$

although the influence of the perturbation term $\frac{3h_+}{t}\left(h^3 - h^2\right)$ needs to be carefully quantified. The limiting problem (4.1) has a very similar structure to the governing ordinary differential equation for vortex solutions in the Ginzburg–Landau theory of superconductivity [1]. Vortex solutions have been widely studied within the Ginzburg–Landau framework [9, 14]. They have the special structure

$$w(\mathbf{x}) = u(|\mathbf{x}|)g\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right) \quad \mathbf{x} \in \mathbb{R}^N,$$

where u is a solution of the following ordinary differential equation in $\mathbb{R}^N$:

$$\begin{aligned} &\frac{d^2u}{d|\mathbf{x}|^2} + \frac{N-1}{|\mathbf{x}|} - \frac{\lambda_K}{|\mathbf{x}|^2}u = -u + u^3, \\ &u(0) = 0 \end{aligned} \tag{4.2}$$

and λ_K is a characteristic constant. In what follows, we adapt Ginzburg–Landau techniques for (4.2) to the ordinary differential equation (2.17) in the limit $t \to \infty$ to establish uniqueness and global monotonicity of h^* in (2.19). In this sense, one could also refer to the $t \to \infty$ limit as the *Ginzburg–Landau limit.*

Lemma 4.1 *[2] For all $t > 1$ and any solution $\mathbf{Q}$ of the Euler–Lagrange equations (2.12), we have the following global upper bound for the gradient:*

$$\|\nabla\mathbf{Q}\|_{L^\infty(B(0,R))} \leqslant C, \tag{4.3}$$

where $C > 0$ is independent of t. For the radial-hedgehog solution $\mathbf{Q}^*(\mathbf{r}) = \sqrt{\frac{3}{2}}h^*(r)\left(\hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{1}{3}\mathbf{I}\right)$, this implies that for $t > 1$, we have the following inequality:

$$|\nabla\mathbf{Q}^*|^2 = \left(\frac{dh^*}{dr}\right)^2 + \frac{3h^{*2}}{r^2} \leqslant C^2 \quad \forall r \in [0, R], \tag{4.4}$$

where C is again independent of t.

Proof The proof of Lemma 4.1 can be found in [2] where the authors show that a solution u of the elliptic system

$$-\Delta u = f \quad on\ \Omega \subset \mathbb{R}^n$$

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satisfies

$$|\nabla u(\mathbf{r})|^2 \leqslant C\|f\|_{L^\infty(\Omega)}\|u\|_{L^\infty(\Omega)} \quad \forall \mathbf{r} \in \Omega.$$

In our case, we apply this result to the system (2.12), noting that $\mathbf{Q}^*$ is a solution of (2.12),

$$f = -\mathbf{Q}_{ij} - \frac{3\sqrt{6}h_+}{t}\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \frac{\delta_{ij}}{3}\mathrm{tr}(\mathbf{Q}^2)\right) + \frac{2h_+^2}{t}\mathbf{Q}_{ij}\left(\mathrm{tr}\mathbf{Q}^2\right)$$

for each $i, j = 1\dots 3$, $\|\mathbf{Q}^*\|_{L^\infty(\Omega)} \leqslant 1$ from the bounds in (2.21) and $\frac{h_+}{t} \leqslant \frac{9}{4}$ and $\frac{h_+^2}{t} \leqslant \frac{33}{4}$ for $t > 1$. □

Proposition 4.1 *Let $\{t^k\}$ be a sequence such that $t^k \to \infty$ as $k \to \infty$, with corresponding radius $R_k \to \infty$ as $k \to \infty$(since $R_k = R_o\sqrt{t_k}/\xi$, where R_o is the original droplet radius that is independent of the model parameters). For each t_k, let $h_k \in \mathscr{A}_h$ be a global minimiser of $I[h]$ in (2.15), as in Proposition 2.1. Then for all k sufficiently large, there exists $r_k > 0$ such that h_k is monotonically increasing for all $r \geqslant r_k$.*

Proof From Proposition 3.2, we have that there exists $R_0 > 0$ such that $h_k(r) > \frac{1}{2}$ for $R_0 \leqslant r \leqslant R_k$, for R_k and t_k sufficiently large (see the lower bound in (3.7)). Consider the right-hand side of (2.17) and define

$$F(h) = h^2 - 1 + \frac{3h_+}{t}(h^2 - h). \tag{4.5}$$

Then $F(1) = 0$ and $F'(h) > 0$ for $h > \frac{1}{2}$.

We prove Proposition 4.1 by contradiction. We assume that there exists $r_0 > R_0$ such that

$$\left.\frac{dh_k}{dr}\right|_{r=r_0} = 0.$$

There are three possibilities for $\frac{d^2h_k}{dr^2}|_{r=r_0}$, i.e. (a)$\frac{d^2h_k}{dr^2}|_{r=r_0} = 0$, (b) $\frac{d^2h_k}{dr^2}|_{r=r_0} < 0$ and (c) $\frac{d^2h_k}{dr^2}|_{r=r_0} > 0$.

Consider case (a). Then we have from (2.17) that

$$\frac{d^2h_k}{dr^2} + \frac{2}{r}\frac{dh_k}{dr} = h_k\left[F(h_k) + \frac{6}{r^2}\right] = 0 \quad \textit{at } r = r_0. \tag{4.6}$$

Secondly,

$$\frac{d}{dr}\left[F(h_k) + \frac{6}{r^2}\right] < 0 \quad \textit{at } r = r_0,$$

from which we deduce that

$$F(h_k) + \frac{6}{r^2} > 0 \quad r \in (r_0 - \delta, r_0) \tag{4.7}$$

for some $\delta > 0$. We deduce from (2.17) that

$$\frac{d}{dr}\left(r^2\frac{dh_k}{dr}\right) > 0 \quad r \in (r_0 - \delta, r_0)$$

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so that

$$r_0^2 \frac{dh_k}{dr}\bigg|_{r=r_0} > (r_0-\delta)^2 \frac{dh_k}{dr}\bigg|_{r_0-\delta}.$$

Since $\frac{dh_k}{dr}|_{r=r_0} = 0$, we deduce that $\frac{dh_k}{dr}|_{r_0-\delta} < 0$. This necessarily means that there exists a local minimum at $r = r_1 > r_0$, since $0 \leqslant h_k(r) \leqslant 1$ and $h_k \to 1$ as $r \to R_k$. We, therefore, have

$$\frac{d^2 h_k}{dr^2}|_{r=r_1} > 0$$

or equivalently

$$F(h_k(r_1)) + \frac{6}{r_1^2} > 0.$$

But

$$F(h_k(r_1)) + \frac{6}{r_1^2} < F(h_k(r_0)) + \frac{6}{r_0^2} = 0$$

since $F'(h) > 0$ for $h > \frac{1}{2}$ and $h_k(r_1) < h_k(r_0)$. This gives a contradiction and we deduce that $\frac{d^2h_k}{dr^2}|_{r=r_0} \neq 0$.

Case (b). We assume that $\frac{d^2h_k}{dr^2}|_{r=r_0} < 0$ ($h_k(r_0) > \frac{1}{2}$ because of our choice of r_0) i.e. we have a local maximum at $r = r_0$. The local maximum must be followed by a local minimum at $r = r_1 > r_0$, since $0 \leqslant h_k(r) \leqslant 1 \quad \forall r > 0$ and $h_k \to 1$ as $r \to R_k$. Thus,

$$F(h_k(r_1)) + \frac{6}{r_1^2} > 0$$

by definition of a local minimum from (4.6). However $h_k(r_1) < h_k(r_0)$ and

$$F(h_k(r_1)) + \frac{6}{r_1^2} < F(h_k(r_0)) + \frac{6}{r_0^2} < 0$$

yielding a contradiction.

Case (c). We assume that $\frac{d^2h_k}{dr^2}|_{r=r_0} > 0$. Then $\frac{dh_k}{dr} > 0$ for all $r > r_0 > R_0$, since the previous arguments show that we cannot have a point of inflection or a local maximum for $r \geqslant R_0$. Then we set r_k in Proposition 4.1 to be $r_k = r_0$. Proposition 4.1 now follows. □

Lemma 4.2 *Let $\{t^k\}$ be a sequence such that $t^k \to \infty$ as $k \to \infty$, with corresponding radius $R_k \to \infty$ as $k \to \infty$ (since $R_k = R_o\sqrt{t_k}/\xi$ is the re-scaled droplet radius in (2.7), where R_o is the original droplet radius that is independent of the model parameters). Let $h_k \in \mathscr{A}_h$ be a global minimiser of $I[h]$ in (2.15), as in Proposition 2.1. Then*

$$\lim_{r\to R_k} r^2 \frac{dh_k}{dr} = 0 \qquad \text{as } k \to \infty. \tag{4.8}$$

Proof From the bounds (3.7), we deduce that for k sufficiently large and $(R_k - r)$ sufficiently small

$$h_k(r) = 1 + \sigma(r), \qquad \text{where } -\frac{\alpha}{r^2} \leqslant \sigma(r) \leqslant -\frac{\beta}{r^2} \tag{4.9}$$

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for positive constants α, β independent of t_k. These bounds imply that $h_k(r) \to 1$ uniformly as $r \to R_k$, $\frac{dh_k}{dr} \to 0$ uniformly as $r \to R_k$ and from Proposition 4.1

$$\frac{dh_k}{dr} = \frac{d\sigma}{dr} > 0,$$

for $(R_k - r)$ sufficiently small and k sufficiently large.

We use (2.17) to obtain an ordinary differential equation for $\delta = \frac{dh_k}{dr}$ as shown below

$$\frac{d^2\delta}{dr^2} + \frac{2}{r}\frac{d\delta}{dr} - \frac{8}{r^2}\delta = -12\frac{h}{r^3} + \left[-1 + 3h^2 + \frac{3h_+}{t}\left(3h^2 - 2h\right)\right]\delta, \tag{4.10}$$

where $\delta \to 0$ as $r \to R_k$, for k sufficiently large. We can then use differential inequalities as in [10] to deduce that

$$\delta(r) = \frac{dh_k}{dr} \leqslant \frac{\gamma_1}{r^3} \quad r \to R_k, \tag{4.11}$$

where $\gamma > 2\beta > 0$ is a positive constant and β has been in defined in (4.9). Since β is independent of t_k and r, γ can be chosen to be a positive constant independent of t_k and (4.11) implies that

$$\lim_{r \to R_k} r^2 \frac{dh_k}{dr} = 0 \quad k \to \infty, \tag{4.12}$$

and the limit is uniform in k. Lemma 4.2 now follows. □

Proposition 4.2 *Let $\{t^k\}$ be a sequence such that $t^k \to \infty$ as $k \to \infty$, with corresponding radius $R_k \to \infty$ as $k \to \infty$ (since $R_k = R_o\sqrt{t_k}/\xi$ where R_k is the re-scaled droplet radius in (2.7) and R_o is the original droplet radius independent of the model parameters). Consider the ordinary differential equation*

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = -h + h^3 + \frac{3h_+^k}{t_k}\left(h^3 - h^2\right), \tag{4.13}$$

where $h_+^k = \frac{3+\sqrt{9+8t_k}}{4}$, subject to the boundary conditions

$$h(0) = 0 \quad h(R_k) = 1. \tag{4.14}$$

Then (4.13) has a unique non-negative solution in the limit $k \to \infty$.

Proof Let h_1 and h_2 be two distinct non-negative solutions of (4.13) subject to the boundary conditions (4.14), i.e.

$$\begin{aligned} &\frac{h_1''}{h_1} + \frac{2}{r}\frac{h_1'}{h_1} - \frac{6}{r^2} + \left(1 - h_1^2\right) + \frac{3h_+^k}{t_k}\left(h_1 - h_1^2\right) = 0, \\ &\frac{h_2''}{h_2} + \frac{2}{r}\frac{h_2'}{h_2} - \frac{6}{r^2} + \left(1 - h_2^2\right) + \frac{3h_+^k}{t_k}\left(h_2 - h_2^2\right) = 0, \end{aligned} \tag{4.15}$$

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where $h_1^{'} = \frac{dh_1}{dr}$, $h_1^{''} = \frac{d^2 h_1}{dr^2}$ etc. We subtract the two equations to get

$$-\frac{h_1^{''}}{h_1} + \frac{h_2^{''}}{h_2} - \frac{2}{r}\left(\frac{h_1^{'}}{h_1} - \frac{h_2^{'}}{h_2}\right) = \left(1 + \frac{3h_+^k}{t_k}\right)\left(h_2^2 - h_1^2\right) + \frac{3h_+^k}{t_k}\left(h_1 - h_2\right). \tag{4.16}$$

Following the methods in [1], we multiply both sides of (4.16) by $r^2\left(h_1^2 - h_2^2\right)$ and integrate from $r = 0$ to $r = R_k$ to find

$$\begin{aligned}&\int_0^{R_k} r^2\left(\frac{h_1}{h_2}h_2^{'} - h_1^{'}\right)^2 dr + \int_0^{R_k} r^2\left(\frac{h_2}{h_1}h_1^{'} - h_2^{'}\right)^2 dr \\ &\quad + \int_0^{R_k}\left(1 + \frac{3h_+^k}{t_k}\right) r^2\left(h_1^2 - h_2^2\right)^2 dr - \frac{3h_+^k}{t_k}\int_0^{R_k}\left(h_1 - h_2\right)^2 r^2\left(h_1 + h_2\right) dr \\ &\quad = -r^2 h_2^{'}\left(\frac{h_1^2}{h_2} - h_2\right)\Big|_0^{R_k} - r^2 h_1^{'}\left(\frac{h_2^2}{h_1} - h_1\right)\Big|_0^{R_k}.\end{aligned} \tag{4.17}$$

Taking the limit $k \to \infty$, using (4.8) and Proposition 3.1, we have that

$$\begin{aligned}&\lim_{k\to\infty}\int_0^{R_k} r^2\left(\frac{h_1}{h_2}h_2^{'} - h_1^{'}\right)^2 dr + \int_0^{R_k} r^2\left(\frac{h_2}{h_1}h_1^{'} - h_2^{'}\right)^2 dr \\ &\quad + \int_0^{R_k}\left(1 + \frac{3h_+^k}{t_k}\right) r^2\left(h_1^2 - h_2^2\right)^2 dr - \frac{3h_+^k}{t_k}\int_0^{R_k}\left(h_1 - h_2\right)^2 r^2\left(h_1 + h_2\right) dr = 0.\end{aligned} \tag{4.18}$$

From (4.18), we deduce that

$$\int_0^{R_k}\left(1 + \frac{3h_+^k}{t_k}\right) r^2\left(h_1^2 - h_2^2\right)^2 dr - \frac{3h_+^k}{t_k}\int_0^{R_k}\left(h_1 - h_2\right)^2 r^2\left(h_1 + h_2\right) dr \to 0 \quad k \to \infty \tag{4.19}$$

(and the limit is uniform in k).

We first make the elementary observation that $\exists R_1 \in [0, R_k]$ such that

$$h_1(r) + h_2(r) > 1 \quad \forall r > R_1. \tag{4.20}$$

Recalling the inequalities (3.7), we have that R_1 can be bounded independently of t_k for k sufficiently large.

We partition the integral contribution in (4.18) into two sub-intervals $[0, R_1]$ and $[R_1, R_k]$, respectively.

$$\begin{aligned}&\int_0^{R_k}\left(1 + \frac{3h_+^k}{t_k}\right) r^2\left(h_1^2 - h_2^2\right)^2 dr - \frac{3h_+^k}{t_k}\int_0^{R_k}\left(h_1 - h_2\right)^2 r^2\left(h_1 + h_2\right) dr \\ &\quad = \int_0^{R_1}\left(1 + \frac{3h_+^k}{t_k}\right) r^2\left(h_1^2 - h_2^2\right)^2 - \frac{3h_+^k}{t_k} r^2\left(h_1 - h_2\right)^2\left(h_1 + h_2\right) dr \\ &\quad\quad + \int_{R_1}^{R_k} r^2\left(h_1^2 - h_2^2\right)^2 + r^2\frac{3h_+^k}{t_k}\left(h_1 - h_2\right)^2\left(h_1 + h_2\right)\left[h_1 + h_2 - 1\right] dr\end{aligned} \tag{4.21}$$

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and note from (4.20) that

$$\int_{R_1}^{R_k} r^2\left(h_1^2-h_2^2\right)^2+r^2\frac{3h_+^k}{t_k}(h_1-h_2)^2(h_1+h_2)\left[h_1+h_2-1\right]\,dr \geqslant \int_{R_1}^{R_k} r^2\left(h_1^2-h_2^2\right)^2\,dr.$$

Claim For k sufficiently large,

$$\int_0^{R_1}\left(1+\frac{3h_+^k}{t_k}\right)r^2\left(h_1^2-h_2^2\right)^2-\frac{3h_+^k}{t_k}r^2(h_1-h_2)^2(h_1+h_2)\,dr > \frac{1}{2}\int_0^{R_1} r^2\left(h_1^2-h_2^2\right)^2\,dr. \tag{4.22}$$

Recalling that R_1 can be bounded independently of t_k, we note that

$$\frac{3h_+^k}{t_k}\int_0^{R_1} r^2(h_1-h_2)^2(h_1+h_2)\,dr \leqslant \gamma_1\frac{h_+^k}{t_k}R_1^3 \leqslant \frac{\gamma_2}{\sqrt{t_k}},$$

where γ_1 and γ_2 are positive constants independent of t_k. Therefore, the claim in (4.22) is equivalent to

$$\sqrt{t_k} \geqslant \frac{\gamma_3}{\int_0^{R_1} r^2\left(h_1^2-h_2^2\right)^2\,dr}, \tag{4.23}$$

for a positive constant γ_3 independent of t_k.

We note that

$$\int_0^{R_1} r^2\left(h_1^2-h_2^2\right)^2\,dr \leqslant \frac{R_1^3}{3}$$

so that as $k\to\infty$, we have two possibilities: (a) $\int_0^{R_1} r^2\left(h_1^2-h_2^2\right)^2\,dr = O(1)$ as $k\to\infty$ and (b) $\int_0^{R_1} r^2\left(h_1^2-h_2^2\right)^2\,dr = o(1)$ as $k\to\infty$. In case (a), the condition (4.23) is clearly satisfied for k sufficiently large and the claim (4.22) follows.

For case (b), we have

$$\int_0^{R_1} r^2\left(h_1^2-h_2^2\right)^2\,dr \to 0 \quad \text{as } k\to\infty. \tag{4.24}$$

From Lemma 4.1 and the global bound (2.21), we obtain

$$\left|\nabla\left(h_1^2-h_2^2\right)\right| \leqslant D, \tag{4.25}$$

where D is a positive constant independent of t_k for k sufficiently large. Consider $r_0\in[0,R_1]$ and let

$$\left|\left(h_1^2-h_2^2\right)(r_0)\right| = \alpha_0 > 0.$$

Then from (4.25), we have that

$$\left|\left(h_1^2-h_2^2\right)(r)\right| \geqslant \frac{\alpha_0}{2} \quad r\in\left[r_0-\frac{\alpha_0}{2D}, r_0+\frac{\alpha_0}{2D}\right]$$

and therefore

$$\int_0^{R_1} r^2\left(h_1^2-h_2^2\right)^2\,dr \geqslant \int_{r_0-\frac{\alpha_0}{2D}}^{r_0+\frac{\alpha_0}{2D}} \frac{\alpha_0^2}{4}r^2\,dr \geqslant \gamma_4\alpha_0^5,$$

where γ_4 is a positive constant independent of t_k. Combining the above with (4.24), we have that $\alpha_0 \to 0$ uniformly as $k \to \infty$ and hence

$$(h_1 - h_2)(r) \to 0 \quad r \in [0, R_1] \tag{4.26}$$

uniformly as $k \to \infty$, since the choice of r_0 is arbitrary and we are interested in non-negative solutions.

From (4.19) and (4.20), we have that

$$\begin{aligned}
&\int_0^{R_k} \left(1 + \frac{3h_+^k}{t_k}\right) r^2 \left(h_1^2 - h_2^2\right)^2 \, dr - \frac{3h_+^k}{t_k} \int_0^{R_k} (h_1 - h_2)^2 \, r^2 \, (h_1 + h_2) \, dr \\
&\quad \geqslant \int_0^{R_1} \left(1 + \frac{3h_+^k}{t_k}\right) r^2 \left(h_1^2 - h_2^2\right)^2 \, dr - \frac{3h_+^k}{t_k} \int_0^{R_1} (h_1 - h_2)^2 \, r^2 \, (h_1 + h_2) \, dr \\
&\qquad + \int_{R_1}^{R_k} r^2 \left(h_1^2 - h_2^2\right)^2 \, dr.
\end{aligned} \tag{4.27}$$

For case (a),(4.22) holds and (4.27) can be written as

$$\begin{aligned}
&\frac{1}{2} \int_0^{R_1} r^2 \left(h_1^2 - h_2^2\right)^2 \, dr + \int_{R_1}^{R_k} r^2 \left(h_1^2 - h_2^2\right)^2 \, dr \\
&\leqslant \int_0^{R_k} \left(1 + \frac{3h_+^k}{t_k}\right) r^2 \left(h_1^2 - h_2^2\right)^2 \, dr - \frac{3h_+^k}{t_k} \int_0^{R_k} (h_1 - h_2)^2 \, r^2 \, (h_1 + h_2) \, dr \to 0 \quad k \to \infty,
\end{aligned} \tag{4.28}$$

from which we deduce that

$$\left(h_1^2 - h_2^2\right)^2 \to 0 \quad \text{as } k \to \infty \tag{4.29}$$

or equivalently

$$|h_1 - h_2| \, (r) \to 0 \quad \text{for } r \in [0, R] \tag{4.30}$$

uniformly, as $k \to \infty$.

For case (b), we have established in (4.26) that $(h_1 - h_2)(r) \to 0$ uniformly as $k \to \infty$ for $r \in [0, R_1]$ and hence

$$\int_0^{R_1} \left(1 + \frac{3h_+^k}{t_k}\right) r^2 \left(h_1^2 - h_2^2\right)^2 \, dr - \frac{3h_+^k}{t_k} \int_0^{R_1} (h_1 - h_2)^2 \, r^2 \, (h_1 + h_2) \, dr \to 0 \quad k \to \infty.$$

From (4.19), we deduce that

$$\int_{R_1}^{R_k} r^2 \left(h_1^2 - h_2^2\right)^2 \, dr \to 0 \quad k \to \infty,$$

and hence,

$$(h_1 - h_2)(r) \to 0 \quad r \in [R_1, R_k]$$

uniformly as $k \to \infty$. Combining the above with (4.26), we have that

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$$(h_1 - h_2)(r) \to 0 \quad r \in [0, R] \tag{4.31}$$

uniformly as $k \to \infty$, in case (b) too. Proposition 4.2 now follows. □

We, next, illustrate the applications of shooting arguments to the ordinary differential equation (4.13) in the limit $k \to \infty$. The methods are similar to those for the Ginzburg–Landau system for superconductivity [4, 9] and we reproduce all necessary details for completeness. From Proposition 3.1, we have that for any solution h_k of (4.13) subject to the boundary condition

$$h_k(0) = 0,$$

$\exists$ a constant a_2 such that

$$h_k(r) \sim a_2 r^2 \quad r \to 0. \tag{4.32}$$

Given a_2, we denote the corresponding solution by $h_k(a_2, r)$. We are interested in non-negative solutions, and hence, we take $a_2 > 0$. By analogy with [4, 9], we call a_2 the *shooting parameter*. We consider three different classes of solutions

- $\mathscr{P} = \left\{a_2 > 0;\ \exists z \in (0, R_a)\ \textit{such that}\ \frac{dh_k(a_2,z)}{dr} = 0\right\}$,
- $\mathscr{Q} = \left\{a_2 > 0;\ \frac{dh_k(a_2,z)}{dr} > 0\ \textit{and}\ h_k(a_2, r) \leqslant 1\ \textit{for all}\ r > 0\right\}$,
- $\mathscr{R} = \left\{a_2 > 0;\ \frac{dh_k(a_2,z)}{dr} > 0 \forall r \in (0, R_a)\ \textit{and}\ \max_{r \in (0,R_a)} h_k(a_2, r) > 1\right\}$,

where R_a is the maximal interval of existence of the solution $h_k(a_2, r)$ (in our case, $R_a = R_k$, where $R_k = R_o\sqrt{t_k}/\xi$ is the re-scaled droplet radius in (2.7) and R_o is the original droplet radius independent of model parameters). Clearly

$$\mathscr{P} \cap \mathscr{Q} = \mathscr{P} \cap \mathscr{R} = \mathscr{Q} \cap \mathscr{R} = \phi$$

and

$$\mathscr{P} \cup \mathscr{Q} \cup \mathscr{R} = (0, \infty).$$

Our aim is to show that $\mathscr{P}$ and $\mathscr{R}$ are non-empty and open. Then $\mathscr{Q}$ is also non-empty. We have a unique solution of the ordinary differential equation (4.13) subject to the boundary conditions (4.14) in the limit $k \to \infty$. Therefore, if we can show that $a_2 \in \mathscr{Q}$ implies that the corresponding $h_k(a_2, r)$ is a solution of (4.13) and (4.14), then we have that $h_k \in \mathscr{Q}$ in the limit $k \to \infty$ and hence $\frac{dh_k}{dr} > 0$ for all $r > 0$, i.e. we have global monotonicity in the limit $k \to \infty$. We note that in Proposition 4.1, we prove monotonicity close to the boundary whereas the proposed shooting methods will yield global monotonicity for all $r > 0$.

It is evident that a solution of (4.13) subject to the boundary conditions (4.14) cannot belong to $\mathscr{R}$ owing to the global bounds (2.21). It remains to rule out the possibility $a_2 \in \mathscr{P}$. We start with an elementary lemma.

Lemma 4.3 *If $a_2 \in \mathscr{Q}$, then $h_k(a_2, r)$ is a solution of (4.13) subject to the boundary conditions (4.14), in the limit $k \to \infty$.*

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Proof Since $h_k(a_2, r)$ is monotonically increasing (from the definition of $\mathscr{Q}$) and is bounded above by 1, $b = \lim_{r\to R_k} h_k(a_2, r)$ exists and $b \in (0, 1]$. Hence, to finish the proof, we need to show that $b = 1$. In fact, if $b < 1$, then as $r \to R_k$ for k sufficiently large, (2.17) can be written as

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

so that

$$\frac{dh}{dr} \sim \frac{6b}{r} + \frac{r}{3}\left(b^3 - b + \frac{3h_+}{t}\left(b^3 - b^2\right)\right)$$

contradicting the hypothesis that $\frac{dh}{dr} > 0$ for all $r > 0$. Therefore, $b = 1$ and Lemma 4.3 follows. □

Next we need to show that $\mathscr{Q}$ is non-empty. For this, we need

Lemma 4.4 *The set $\mathscr{P}$ is not empty; more precisely, there exists a positive constant m such that $(0, m) \subset \mathscr{P}$.*

Proof We set for any $a_2 > 0$,

$$w(a_2, r) = \frac{h_k(a_2, r)}{a_2}; \tag{4.33}$$

then w satisfies the following ordinary differential equation from (4.13)

$$\begin{aligned}&\frac{d^2w}{dr^2} + \frac{2}{r}\frac{dw}{dr} - 6\frac{w}{r^2} + w = a_2^2w^3 + \frac{3h_+^k}{t_k}\left(a_2^2w^3 - a_2w^2\right),\\ &w\left(a_2, r\right) \sim r^2 \quad r \to 0.\end{aligned} \tag{4.34}$$

Then as $a_2 \to 0$, $w(a_2, r) \to w(0, r)$ where $w(0, r)$ is the solution of

$$\begin{aligned}&\frac{d^2w}{dr^2} + \frac{2}{r}\frac{dw}{dr} - 6\frac{w}{r^2} + w = 0,\\ &w(0, r) \sim r^2 \quad r \to 0,\end{aligned} \tag{4.35}$$

and the general solution of this ordinary differential equation exhibits oscillatory behaviour. From (4.33), we deduce that $w(a_2, r)$ has oscillatory behaviour as $a_2 \to 0$ and hence so does $h_k(a_2, r) = a_2w(a_2, r)$. This completes the proof of the lemma. □

Lemma 4.5 *The set $\mathscr{P}$ is open.*

Proof For $a_2 \in \mathscr{P}$, define

$$z_0(a_2) = \inf\left\{r \in (0, R_k)\,;\ \frac{dh_k(a_2, r)}{dr} = 0\right\}, \tag{4.36}$$

i.e. $z_0(a_2)$ is the smallest stationary point of $h_k(a_2, r)$. We can show that

$$\frac{d^2h_k\left(a_2, z_0(a_2)\right)}{dr^2} < 0. \tag{4.37}$$

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The definition of $z_0(a_2)$ implies that

$$\frac{dh_k(a_2, z_0(a_2))}{dr} = 0 \ \textit{and} \ \frac{d^2 h_k\,(a_2, z_0(a_2))}{dr^2} \leqslant 0$$

since we are interested in non-negative solutions.

From the governing ordinary differential equation (4.13), we have that

$$\frac{d^2 h_k}{dr^2} + \frac{2}{r}\frac{dh_k}{dr} = h_k\left(\frac{6}{r^2} + h_k^2 - 1 + \frac{3h_+^k}{t_k}\left(h_k^2 - h_k\right)\right) \leqslant 0 \ \textit{at} \ r = z_0(a_2) \tag{4.38}$$

and note that

$$\frac{d}{dr}\left[\frac{6}{r^2} + h_k^2 - 1 + \frac{3h_+^k}{t_k}\left(h_k^2 - h_k\right)\right] < 0 \ \textit{at} \ r = z_0(a_2).$$

If

$$\frac{d^2 h_k\,(a_2, z_0(a_2))}{dr^2} = 0$$

then

$$\frac{6}{r^2} + h_k^2 - 1 + \frac{3h_+^k}{t_k}\left(h_k^2 - h_k\right) = 0 \ \textit{at} \ r = z_0(a_2).$$

This implies that

$$\frac{6}{r^2} + h_k^2 - 1 + \frac{3h_+^k}{t_k}\left(h_k^2 - h_k\right) > 0 \ \textit{on} \ r \in [z_0(a_2) - \delta, z_0(a_2))$$

for some $\delta > 0$. On the other hand,

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{dh_k}{dr}\right] = h_k\left[\frac{6}{r^2} + h_k^2 - 1 + \frac{3h_+^k}{t_k}\left(h_k^2 - h_k\right)\right]$$

from (2.17) so that

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{dh_k}{dr}\right] > 0 \ \textit{on} \ r \in [z_0(a_2) - \delta, z_0(a_2)).$$

This, in turn, implies that

$$z_0^2(a_2)\frac{dh_k(a_2, z_0(a_2))}{dr} > (z_0(a_2) - \delta)^2\,\frac{dh_k(a_2, z_0(a_2) - \delta)}{dr} > 0 \tag{4.39}$$

(since $\frac{dh_k}{dr} > 0$ for $r \in (0, z_0(a_2))$ from the definition (4.36)), contradicting the definition of $z_0(a_2)$. Hence, (4.37) holds.

Finally, we note that for any $a_0 \in \mathscr{P}$, by the Implicit Function Theorem and (4.37), there exists a smooth function $y(a_2)$ defined in a neighbourhood of a_0 such that $y(a_0) = z_0(a_0)$ and $\frac{dh_k(a_2, y(a_2))}{dr} = 0$. Hence, $\mathscr{P}$ is open as required. □

Lemma 4.6 *The set $\mathscr{R}$ is non-empty and open.*

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Proof We introduce the function

$$v(r) = bh_k(a_2, br) \text{ where } b = a_2^{-1/3}. \tag{4.40}$$

Then one can check that v satisfies the following ordinary differential equation:

$$\frac{d^2v}{dr^2} + \frac{2}{r}\frac{dv}{dr} - \frac{6v}{r^2} - \left(1 + \frac{3h_+^k}{t_k}\right)v^3 + b^2 v + \frac{3h_+^k}{t_k}bv^2 = 0 \tag{4.41}$$

with

$$v(r) \sim r^2 \quad r \to 0. \tag{4.42}$$

If we let $b \to 0$, then the limiting problem is

$$\begin{aligned} &\frac{d^2v}{dr^2} + \frac{2}{r}\frac{dv}{dr} - \frac{6v}{r^2} - \left(1 + \frac{3h_+^k}{t_k}\right)v^3 = 0, \\ &v(r) \sim r^2 \quad r \to 0. \end{aligned} \tag{4.43}$$

From the hypothesis, we have that $v, \frac{dv}{dr} > 0$ for $r > 0$. We claim that there does not exist $l > 0$ such that $\lim_{k\to\infty} v(R_k) = l$. We prove the claim by contradiction. Assume $\exists l > 0$ such that $\lim_{k\to\infty} v(R_k) = l$. Then (4.43) implies that

$$\frac{d}{dr}\left(r^2\frac{dv}{dr}\right) \sim 6l + r^2\left(1 + \frac{3h_+^k}{t_k}\right)l^3 \quad r \to R_k$$

so that

$$\frac{dv}{dr} \sim \frac{6l}{r} + \frac{r}{3}\left(1 + \frac{3h_+^k}{t_k}\right)l^3 \quad r \to R_k$$

as $k \to \infty$. Therefore, $v(r) \gg l$ for r sufficiently large, which contradicts the hypothesis. The other possibility is $l = 0$ but this contradicts the definition of $\mathscr{R}$, which requires that $\frac{dv}{dr} > 0$ for all $r > 0$. Therefore,

$$v(R_k) \to \infty \qquad \text{as } k \to \infty. \tag{4.44}$$

Consequently, $h_k(a_2, r)$ is large when a_2 is large enough and the set $\mathscr{R}$ is non-empty. By the continuous dependence of h_k on a_2 and the definition of $\mathscr{R}$, we deduce that $\mathscr{R}$ is open. □

Lemma 4.7 *The set $\mathscr{Q}$ is non-empty.*

Proof This is immediate from Lemmas 4.4 and 4.6. We omit the proof for brevity. □

Proposition 4.3 *Let $\{t^k\}$ be a sequence such that $t^k \to \infty$ as $k \to \infty$, with corresponding radius $R_k \to \infty$ as $k \to \infty$ (since $R_k = R_o\sqrt{t_k}/\xi$, where R_k is the re-scaled droplet radius in (2.7) and R_o is the original droplet radius independent of the model parameters). For each $t_k > 0$, let $h_k \in \mathscr{A}_h$ be a global minimiser of $I[h]$ in (2.15), as in Proposition 2.1. The function h_k is monotonically increasing in the limit $k \to \infty$.*

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Proof From Lemmas 4.3, 4.4, 4.6 and 4.7, we have that there exists a $a_2 \in \mathcal{Q}$ such that $h_k(a_2, r)$ is a solution of (4.13) subject to the boundary conditions (4.14), in the limit $k \to \infty$. From Proposition 4.2, we have that (4.13) and (4.14) admit a unique solution h_k in the limit $k \to \infty$. Hence, we deduce that the corresponding shooting parameter $a_2 \in \mathcal{Q}$, i.e. h_k is monotonically increasing everywhere away from the origin. An immediate consequence of this global monotonicity is $0 < h_k(r) < 1$ for $r \in (0, R_k)$ as $k \to \infty$. □

We conclude this section with an explicit far-field expansion for h_k in the limit $k \to \infty$.

Proposition 4.4 *Let $\{t^k\}$ be a sequence such that $t^k \to \infty$ as $k \to \infty$, with corresponding radius $R_k \to \infty$ as $k \to \infty$ (since $R_k = R_o\sqrt{t_k}/\xi$, where R_k is the re-scaled droplet radius in (2.7) and R_o is the original droplet radius independent of the model parameters). Let $h_k \in \mathcal{A}_h$ be a global minimiser of $I[h]$ in (2.15), as in Proposition 2.1. Then h_k is a non-negative solution of the following ordinary differential equation:*

$$\frac{d^2h}{dr^2} + \frac{2}{r}\frac{dh}{dr} - \frac{6h}{r^2} = h\left(h^2 - 1 + \frac{3h_+^k}{t_k}\left(h^2 - h\right)\right) \tag{4.45}$$

subject to the boundary conditions

$$h(0) = 0 \quad \text{and } h(R_k) = 1. \tag{4.46}$$

We have the following far-field estimates as $k \to \infty$:

$$r^2\left|\frac{d^2h_k}{dr^2}\right| + r\left|\frac{dh_k}{dr}\right| + \left|6 - r^2h_k(1-h_k)\left(1 + \left(1 + \frac{3h_+^k}{t_k}\right)h_k\right)\right| = o(1) \quad r \to R_k. \tag{4.47}$$

Proof The proof of Proposition 4.4 follows some of the methods described in a recent paper [21] on Ginzburg–Landau theory for three-dimensional domains. All necessary details are reproduced below for completeness.

The bounds (3.7) imply that for R_k and t_k sufficiently large,

$$1 - \frac{\alpha}{r^2} \leqslant h_k(r) \leqslant 1 - \frac{\beta}{r^2}$$

as $r \to R_k$, for positive constants α, β independent of k. As demonstrated in (4.8), this implies

$$\lim_{r\to R_k} r^2\frac{dh_k}{dr} = 0 \quad \text{as } k \to \infty, \tag{4.48}$$

and hence,

$$\lim_{r\to R_k} r\frac{dh_k}{dr} = 0 \quad \text{as } k \to \infty. \tag{4.49}$$

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For any $m \in (0,1)$ fixed, we multiply (4.45) by r^2, average over (mR_k, R_k), take the limit $k \to \infty$ and obtain

$$\frac{1}{(1-m)R_k}\int_{mR_k}^{R_k} \frac{d}{dr}\left(r^2\frac{dh_k}{dr}\right)dr + \frac{1}{(1-m)R_k}\int_{mR_k}^{R_k} r^2 h_k(r)\,(1-h_k(r))\left(1+\left(1+\frac{3h_+^k}{t_k}\right)h_k\right)dr$$
$$= \frac{6}{(1-m)R_k}\int_{mR_k}^{R_k} h_k(r)\,dr. \tag{4.50}$$

As $k \to \infty$, $h_k \to 1$ uniformly (see (3.7)), $\frac{dh_k}{dr} > 0$ as $r \to R_k$ (from Proposition 4.1) and using (4.48), we obtain the following sequence of inequalities:

$$\limsup_{k\to\infty} m^2 R_k^2\,(1-h_k(R_k))\left(1+\left(1+\frac{3h_+^k}{t_k}\right)h_k(R_k)\right) \leqslant 6$$
$$\leqslant \liminf_{k\to\infty} R_k^2(1-h_k(mR_k))\left(1+\left(1+\frac{3h_+^k}{t_k}\right)h_k(mR_k)\right). \tag{4.51}$$

It immediately follows that

$$r^2\,(1-h_k(r))\left(1+\left(1+\frac{3h_+^k}{t_k}\right)h_k(r)\right) \to 6 \tag{4.52}$$

uniformly as $r \to R_k$ in the limit $k \to \infty$.

Finally, using the estimates (4.49) and (4.52) in (4.45), we deduce that

$$r^2\left|\frac{d^2h_k}{dr^2}\right| \to 0 \tag{4.53}$$

uniformly in the limit $r \to R_k$ as $k \to \infty$. Proposition 4.4 now follows. □

One immediate consequence of (4.47) is that

$$h_k(r) = 1 - \frac{6}{r^2\left(2+\frac{3h_+^k}{t_k}\right)} + o\left(\frac{1}{r^2}\right) \qquad r \to R_k \tag{4.54}$$

as $k \to \infty$. Although this information is qualitatively contained in (4.9), (4.54) is a stronger result since it is an exact expression that captures the effects of geometry and the temperature on the far-field structure. Further, (4.54) yields estimates for the higher order derivatives of h_k as $r \to R_k$ for k large, and this information cannot be immediately inferred from (4.9).

5 Conclusion

This paper aims to build a self-contained and rigorous mathematical framework for the study of the radial-hedgehog solution within the Landau–de Gennes theory for nematic liquid crystals and to elucidate the analogies between the mathematical formulation of defects in the Landau–de Gennes framework and defects in the Ginzburg–Landau theory of superconductivity. These analogies need to be highlighted in the applied mathematics literature so that mathematical techniques from other branches of materials science can be effectively used in the context of liquid crystals. We study radial-hedgehog solutions on spherical droplets subject to *homeotropic* anchoring or *strong radial* anchoring conditions and define a radial-hedgehog solution to be an energy minimiser within the class of spherically symmetric uniaxial solutions as demonstrated in Proposition 2.1. We consider two different regimes in this paper: (a) large droplet radius R and (b) small droplet radius R. In Proposition 3.3, we demonstrate that the radial-hedgehog solution cannot be globally energy minimising for large (but finite) values of R and t, i.e. for $R, t \geqslant 200$. In Propositions 3.4 and 3.5, we prove that the radial-hedgehog solution is locally stable for droplets of sufficiently small radius, i.e. when R is of the order of the biaxial correlation length. These stability results take elastic anisotropy into account, show that elastic anisotropy does not change the qualitative trend (compare equations (3.32) and (3.43)) and identify relationships between the elastic constants, the reduced temperature t and the droplet radius R that guarantee local stability of the radial-hedgehog solution against small perturbations.

In [3], 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

$$\Delta \mathbf{u} + \mathbf{u}\left(1 - |\mathbf{u}|^2\right) = 0 \tag{5.1}$$

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

$$\mathbf{U}(\mathbf{r}) = \frac{\mathbf{r}}{r} f(r) \tag{5.2}$$

for a unique function f vanishing at zero and increasing to one at infinity. In [21], the authors show that every non-constant local minimiser of the Ginzburg–Landau energy functional associated with (5.1),

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

is of the form (5.2), 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 (2.12) necessarily of the form (2.19), i.e. are radial-hedgehog solutions the only possible uniaxial solutions of the system (2.12) in $\mathbb{R}^3$? If so, then we will have a complete characterisation of all admissible uniaxial solutions and the interplay between uniaxiality and biaxiality can be partially understood in terms of the comparatively tractable radial-hedgehog problem. We expect that the methods in [21] will not readily transfer to the Landau–de Gennes framework and there will be analogies only in certain parameter regimes, such as the $t \to \infty$ limit studied in this paper [13].

Finally, we compare our results with previous work in this area. As stated in Section 1, the instability of the radial-hedgehog solution has been demonstrated in the limit $R, t \to \infty$ in [10]. In [10], the authors consider the second variation of the Landau–de Gennes energy functional and treat the instability condition as a Schrodinger eigenvalue problem, which has to be solved numerically. We have demonstrated instability of the radial-hedgehog solution for all values $R, t \geqslant 200$. This result is an improvement over the instability result in [10]. A pivotal ingredient in the instability analysis is the construction of explicit bounds for the scalar order parameter of the radial-hedgehog solution for finite values of R and t. We have constructed explicit lower and upper bounds for the scalar order parameter in Proposition 3.2 for $R, t \geqslant 200$. In Proposition 3.3, we construct an explicit biaxial perturbation, localised near the isotropic core of the radial-hedgehog solution and use the bounds in Proposition 3.2 to show that this biaxial perturbation has lower Landau–de Gennes energy than the radial-hedgehog solution for $R, t \geqslant 200$. The biaxial perturbation is energetically preferable only when localised in a ball $B(0,\sigma)$ centred at the origin and one can check that $[\tilde{\mathscr{I}}_{LG}[\hat{\mathbf{Q}}] - \tilde{\mathscr{I}}_{LG}[\mathbf{Q}^*]] > 0$ if σ is too small or too large, i.e. σ needs to be large enough for the biaxiality to manifest itself and yet be small enough so as not to perturb the far-field properties. We expect that our methods can be further refined to demonstrate instability for modest values of R and t, as suggested by numerical simulations. There are two possible routes for achieving this: (i) obtain better upper bounds for the scalar order parameter near the isotropic core following the methods in Proposition 3.2 and (ii) use partial differential equations-based techniques to obtain refined bounds for the gradient of the radial-hedgehog solution as in Lemma 4.1 and these bounds will yield global upper bounds for the corresponding scalar order parameter. In [11], the authors numerically study the stability of the radial-hedgehog solution as a function of the droplet radius, reduced temperature and elastic constants. From Propositions 3.4 and 3.5, we are guaranteed local stability of the radial-hedgehog solution if

$$\frac{R^2}{\xi^2} \leqslant \frac{\alpha}{t + \beta(3 + \sqrt{9 + 8t})},$$

where α, β are positive constants independent of t. This prescribes a curve in the (R, t)-plane that is in qualitative agreement with the numerical simulations reported in [11]. It is noteworthy that elastic anisotropy does not change the qualitative features of the stability curve in the (R, t)-plane.

Further, in [27], the authors find that the radial-hedgehog solution only occurs either in very small droplets or very close to the nematic-isotropic transition temperature; the symmetry-breaking biaxial torus solution is energetically preferable everywhere else. This is consistent with Propositions 3.4 and 3.5 and with Proposition 3.3. In [25], the authors work within the Lyuksyutov constraint, which requires that $\mathrm{tr}\mathbf{Q}^2 = \frac{2}{3}s_+^2$, where s_+ has been defined in (2.5), everywhere inside the droplet. They demonstrate that the radial-hedgehog solution is always locally *unstable* within the one-constant approximation for the elastic energy density, i.e. when the elastic energy density is simply taken to $|\nabla \mathbf{Q}|^2$, as has been done in Propositions 3.3 and 3.4. This is evidently in agreement with Proposition 3.3 and does *not* contradict Proposition 3.4 where we demonstrate local stability in droplets of sufficiently small radius. The Lyuksyutov constraint is valid in the $R \to \infty$ limit or for droplets of sufficiently large radius, and hence, Proposition 3.4 is outside the remit of this instability result.

While careful attention is paid to the effect of elastic constants in some of the previous work, we focus on the one-constant case in this paper. We point out that the mathematical results in Sections 2 and 3 will readily extend to an anisotropic elastic energy density as considered in Proposition 3.5. However, the results in Section 4 are restricted to the one-constant elastic energy density since there are no *anisotropic* versions of the Ginzburg–Landau theory for superconductors. Hence, the one-constant case is the best paradigm for illustrating the generalisations of Ginzburg–Landau techniques to the Landau–de Gennes framework.

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References

[1] Bethuel, F., Brezis, H. & Helein, F. (1994) *Ginzburg–Landau Vortices, Progress in Nonlinear Differential Equations and their Applications*, Vol. 13, Birkhauser, Boston.

[2] Bethuel, F., Brezis, H. & Orlandi, G. (2001) Asymptotics for the Ginzburg–Landau Equation in Arbitrary Dimensions. *J. Funct. Anal.* **186**, 432–520.

[3] Brezis, H. (1999) Symmetry in nonlinear PDEs, Differential equations: La Pietra 1996 (Florence). In: *Proceedings of Symposia in Pure Mathematics*, Florence, vol. 65, pp. 1–12.

[4] Chen, X., Elliott, C. & Tang, Q. (1994) Shooting method for vortex solutions of a complex valued Ginzburg–Landau equation. *Proc. Roy. Soc. Edinburgh, Sec. A* **124**(6), 1075–1088.

[5] Chi, D. P. & Park, G. H. (1992) Weak-stability of $x/|x|$ and symmetries of liquid crystals. *J. Korean Math. Soc.* **29**(2), 251–260.

[6] Davis, T. & Gartland, E. C., Jr (1998) Finite element analysis of the Landau–de Gennes minimization problem for liquid crystals. *SIAM J. Numer. Anal.* **35**, 336–362.

[7] De Gennes, P. G. (1974) *The Physics of Liquid Crystals*, Clarendon Press, Oxford.

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

[9] Farina, A. & Guedda, M. (2000) Qualitative study of radial solutions of the Ginzburg–Landau system in $\mathbb{R}^N$ $(N \geqslant 3)$. *Appl. Math. Lett.* **13**, 59–64.

[10] Gartland, E. C., Jr & Mkaddem, S. (1999) Instability of radial hedgehog configurations in nematic liquid crystals under Landaude–Gennes free-energy models. *Phys. Rev. E* **59**, 563–567.

[11] Mkaddem, S. & Gartland, E. C., Jr (2000) Fine structure of defects in radial nematic droplets. *Phys. Rev. E* **62**, 6694–6705.

[12] Gustafson, S. (1997) Symmetric solutions of the Ginzburg–Landau equation in all dimensions. *Int. Math. Res. Not.* **16**, 807–816.

[13] Henao, D. & Majumdar, A. Radial symmetry of uniaxial minimizers in Landau–de Gennes theory. In preparation.

[14] Herve, R-M. & Herve, M. (1994) Etude qualitative des solutions reelles d'une equation differentielle liee e lequation de Ginzburg–Landau. *Ann. Inst. H. Poincar Anal. Non Lineaire* **11**, 427–440.

[15] Kinderlehrer, D. & Ou, B. (1992) Second variation of liquid crystal energy at $x/|x|$. *Proc. R. Soc. A: Math., Phys. Eng. Sci.* **437**, 475–487.

[16] Kralj, S. & Virga, E. (2001) Universal fine structure of nematic hedgehogs. *J. Phys. A: Math. Gen.* **24**, 829–838.

[17] Kralj, S., Rosso, R. & Virga, E. G. (2010) Finite-size effects on order reconstruction around nematic defects. *Phys. Rev. E* **81**, 021702.

[18] Majumdar, A. & Zarnescu, A. (2010) The Landau–de Gennes theory of nematic liquid crystals: The Oseen–Frank limit and beyond. *Arch. Ration. Mech. Anal.* **196**(1), 227–280.

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

[20] Majumdar, A. The Landau–de Gennes theory for nematic liquid crystals: Uniaxiality versus Biaxiality [online]. Under review in Communications in Pure and Applied Analysis.

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

[22] Mottram, N. J. & Newton, C. (2004) *Introduction to **Q**-tensor Theory*, University of Strathclyde Mathematics, Research Report no. 10.

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

[24] Priestley, E. B., Wojtowicz, P. J. & Sheng, P. (1975) *Introduction to Liquid Crystals*, Plenum, New York.

[25] Rosso, R. & Virga, E. (1996) Metastable nematic hedgehogs. *J. Phys. A: Math. Gen.* **29**, 4247–4264.

[26] Schopohl, N. & Sluckin, T. J. (1988) Hedgehog structures in nematic and magnetic systems. *J. Phys.* (France) **49**, 1097.

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

[28] Sun, D. & Sun, J. (2002) Strong semismoothness of eigenvalues of symmetric matrices and its application to inverse eigenvalue problems. *SIAM J. Numer. Anal.* **40**, 2352–2367.