



Local minimizer and De Giorgi's type conjecture for the isotropic–nematic interface problem

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Abstract

In this paper, we investigate the structure of local minimizers for the isotropic–nematic interface based on the Landau-de Gennes energy. In the absence of the anisotropic energy, the uniaxial solution is the only local minimizer in 1-D. In 3-D, we propose a De Giorgi's type conjecture and give an affirmative answer under a mild assumption. In the presence of the anisotropic energy with $L_2 > -1$ and homeotropic anchoring, the uniaxial solution is also the only local minimizer in a class of diagonal form in 1-D.

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1 Introduction

Liquid crystal is a state of matter between liquid and solid, in which molecules tend to align a preferred direction. One of the most common phases is the nematic phase, in which the molecules tend to have the same alignment but their positions are not correlated. In physics, the different order parameters are used to describe the anisotropic behavior of liquid crystals.

The most simple one is the vector theory, which uses a unit vector field $\mathbf{n}(x)$ to describe the locally preferred alignment of liquid crystal molecules near the material point x . Onsager introduced the molecular theory, in which the orientational distribution function $f(x, \mathbf{m})$ is introduced to describe the number density of molecules whose orientation is parallel to \mathbf{m} at material point x . The Q -tensor theory uses a symmetric traceless 3×3 matrix \mathbf{Q} to describe the alignment behaviour of liquid crystals. Physically, \mathbf{Q} could be understood as the second momentum of f :

$$\mathbf{Q}(x) = \int_{\mathbb{S}^2} \left(\mathbf{m}\mathbf{m} - \frac{1}{3}\mathbf{I} \right) f(x, \mathbf{m}) d\mathbf{m}.$$

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We may classify a liquid crystal by the tensor \mathbf{Q} : *uniaxial* if \mathbf{Q} has only two distinct eigenvalues; *biaxial* if \mathbf{Q} has three distinct eigenvalues; *isotropic* if all eigenvalues are zero.

Since the order tensor \mathbf{Q} vanishes when f is the probability density $\frac{1}{4\pi}$ for the isotropic phase, the tensor \mathbf{Q} measures how the second moments of a given probability density deviates from the isotropic value. Thus, it is convenient to use the Q -tensor theory to model the isotropic–nematic phase transition problem, which is based on the so-called Landau-de Gennes energy:

$$\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\Omega} \left\{ \underbrace{\frac{a}{2}\text{Tr}\mathbf{Q}^2 - \frac{b}{3}\text{Tr}\mathbf{Q}^3 + \frac{c}{4}(\text{Tr}\mathbf{Q}^2)^2}_{F_b:\text{bulk energy}} + \underbrace{\frac{1}{2}(L_1|\nabla\mathbf{Q}|^2 + L_2Q_{ij,j}Q_{ik,k} + L_3Q_{ij,k}Q_{ik,j} + L_4Q_{ij}Q_{kl,i}Q_{kl,j})}_{F_e:\text{elastic energy}} \right\} dx.$$

Here a, b, c are material and temperature dependent nonnegative constants and L_i ($i = 1, 2, 3, 4$) are material dependent elastic constants. We refer the reader to [3] for more details. As in [2,10], we take $L_3 = L_4 = 0$ in the elastic energy F_e . Then the energy functional is reduced to

$$\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\Omega} \left\{ \frac{1}{2}(L_1|\nabla\mathbf{Q}|^2 + L_2Q_{ij,j}Q_{ik,k}) + F_b(\mathbf{Q}) \right\} dx. \tag{1.1}$$

The bulk energy F_b can characterize the isotropic–nematic phase transition for liquid crystals. The critical points of the bulk energy are

$$\mathbf{Q} = 0 \quad \text{or} \quad s^{\pm} \left(\mathbf{n}\mathbf{n} - \frac{1}{3}\mathbf{I} \right), \tag{1.2}$$

where s^{\pm} are the solutions of $3a - bs + 2cs^2 = 0$, and $\mathbf{n} \in \mathbb{S}^2$. In addition, if $0 < a < \frac{b^2}{24c}$, then $\mathbf{Q} = 0$ and $\mathbf{Q} = s^+(\mathbf{n}\mathbf{n} - \frac{1}{3}\mathbf{I})$ are stable critical points, which correspond to isotropic phase and nematic phase respectively, and $\mathbf{Q} = s^-(\mathbf{n}\mathbf{n} - \frac{1}{3}\mathbf{I})$ is unstable. See [14] for the details. Since we are interested in the stable interface between the two co-existence phases, we impose the condition $b^2 = 27ac$, which means that the bulk energy at each phase is equal.

In this paper, we are concerned with the structure of the molecular directional field near the phase transition and the shape of the interface. To this end, we assume that the transition between 0 and $s^+(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I})$ appears in a thin region of width $\sqrt{L_1}$. By a rescaling and limiting process as in [10], the energy functional (1.1) can be reduced to

$$\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}^3} \left\{ \frac{1}{6}|\nabla\mathbf{Q}|^2 + \frac{L}{4}Q_{ij,j}Q_{ik,k} + \frac{1}{3}F_b(\mathbf{Q}) \right\} dx. \tag{1.3}$$

Furthermore, after scaling if necessary, we may take

$$a = 1, \quad b = 9, \quad c = 3$$

so that $s^+ = 1$ and $s^- = 1/2$ and $F_b(\mathbf{Q}) = 0$ if $\mathbf{Q} = 0$ or $\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}$. The energy functional (1.3) becomes

$$\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}^3} \left\{ \frac{1}{6}|\nabla\mathbf{Q}|^2 + \frac{L}{4}Q_{ij,j}Q_{ik,k} + \frac{1}{6}\text{Tr}\mathbf{Q}^2 - \text{Tr}\mathbf{Q}^3 + \frac{1}{4}(\text{Tr}\mathbf{Q}^2)^2 \right\} dx. \tag{1.4}$$

Now the isotropic–nematic interface problem is reduced to study the minimizers of (1.4) in the class so that $\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q})$ is finite and satisfying

$$\mathbf{Q}(x_1, x_2, +\infty) = \mathbf{nn} - \frac{1}{3}\mathbf{I}, \quad \mathbf{Q}(x_1, x_2, -\infty) = 0. \tag{1.5}$$

Let us refer to [6,8,9,11] and references therein for some numerical results on the isotropic–nematic interface problem based on the Landau-de Gennes’s framework. Numerical results show that the ratio of the coefficients in the isotropic and anisotropic energies and different anchoring condition make an important effect on the structure and stability of minimizers. To our knowledge, there are few rigorous results on this problem. In [10], the authors made a first effort to 1-D problem, which will be introduced in next section.

Let us conclude the introduction by introducing the following notations. We define

$$\mathcal{A} = \left\{ \mathbf{Q} \in W^{1,2}(\mathbf{R}^N, S_0) : \mathbf{Q}(x_1, \dots, x_{N-1}, +\infty) = \mathbf{nn} - \frac{1}{3}\mathbf{I}, \mathbf{Q}(x_1, \dots, x_{N-1}, -\infty) = 0 \right\}$$

so that $\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q})$ is finite for $\mathbf{Q} \in \mathcal{A}$, where S_0 denotes the set of all symmetric traceless 3×3 matrices. We take $N = 3$ or 1 throughout this paper.

Definition 1.1 $\mathbf{Q}^* \in \mathcal{A}$ is called a global minimizer of $\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q})$ if it satisfies $\mathcal{F}(\mathbf{Q}^*, \nabla\mathbf{Q}^*) \leq \mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q})$ for all $\mathbf{Q} \in \mathcal{A}$; $\mathbf{Q}^* \in \mathcal{A}$ is called a local minimizer if it satisfies $\mathcal{F}(\mathbf{Q}^*, \nabla\mathbf{Q}^*) \leq \mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q})$ for $\mathbf{Q} \in \mathcal{A}$ in some open neighbourhood of \mathbf{Q}^* ; $\mathbf{Q}^* \in \mathcal{A}$ is called a stable solution of the Euler-Lagrange equation associated with \mathcal{F} , e.g. (2.1), if it admits a local minimizer of \mathcal{F} .

2 De Giorgi’s type conjecture

Let us first consider the case of $L = 0$. The associated Euler-Lagrange equation takes

$$-\Delta\mathbf{Q} + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2\mathbf{Q} + 3|\mathbf{Q}|^2\mathbf{I} = 0 \tag{2.1}$$

with boundary condition

$$\mathbf{Q}(x_1, x_2, +\infty) = \mathbf{nn} - \frac{1}{3}\mathbf{I}, \quad \mathbf{Q}(x_1, x_2, -\infty) = 0. \tag{2.2}$$

This system is similar to the Allen-Cahn equation

$$\Delta u - (1 - u^2)u = 0 \quad \text{in } \mathbf{R}^N, \tag{2.3}$$

which also arises from the phase transition problem. In 1978, De Giorgi made the following well-known conjecture:

Let u be a bounded solution of (2.3) such that $\partial_{x_N} u > 0$. Then the level sets of u are all hyperplanes, at least for dimension $N \leq 8$.

This conjecture has been solved by Ghoussoub-Gui [7] for $N = 2$, Ambrosio-Cabr e [1] for $N = 4$ and Savin [12] for $4 \leq N \leq 8$. The conjecture is not true for $N \geq 9$ [4].

Motivated by De Giorgi’s conjecture, we propose a similar conjecture:

(GDC): *Let \mathbf{Q} be symmetric, traceless and a bounded solution of (2.1)–(2.2). Let λ_3 be the largest eigenvalue of \mathbf{Q} . If $\partial_{x_3} \lambda_3 > 0$, then all level sets $\{x \in \mathbf{R}^3 : Q_{ij}(x) = s\}$ are hyperplanes.*

Compared with (2.3), this conjecture seems more difficult even in 1-D since (2.1) is a system with five independent components. In [5], Fazly and Ghoussoub also considered the

De Giorgi type conjecture for the elliptic system: $\Delta u = \nabla H(u)$ in \mathbf{R}^N , where $u : \mathbf{R}^N \rightarrow \mathbf{R}^m$ and $H \in C^2(\mathbf{R}^m)$, and proved that the solution $u = \{u_i\}_{i=1}^m$ is necessarily one-dimensional under various conditions on the nonlinearity H and some monotonicity assumption on u . The elliptic system we considered in this paper does not fall into this system due to the traceless constraint on \mathbf{Q} . Even for the results in 1-D to be presented, there are no additional assumptions on the solution. Let us mention [13], which may be the first paper on the vectorial Allen-Cahn system.

In [10], Park et al. consider the global minimizer of the 1-D total energy functional

$$\mathcal{F}(\mathbf{Q}, \mathbf{Q}') = \int_{\mathbb{R}} \left\{ \frac{1}{6} |\mathbf{Q}'|^2 + \frac{1}{6} \text{Tr} \mathbf{Q}^2 - \text{Tr} \mathbf{Q}^3 + \frac{1}{4} (\text{Tr} \mathbf{Q}^2)^2 \right\} ds, \tag{2.4}$$

where $'$ denotes $\frac{d}{ds} = \frac{d}{dz}$. The associated Euler-Lagrange equation becomes

$$-\mathbf{Q}'' + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2\mathbf{Q} + 3|\mathbf{Q}|^2\mathbf{I} = 0 \tag{2.5}$$

with the boundary condition

$$\mathbf{Q}(+\infty) = \mathbf{nn} - \frac{1}{3}\mathbf{I}, \quad \mathbf{Q}(-\infty) = 0. \tag{2.6}$$

Theorem 2.1 [10] *The global minimizer of (2.4) subject to (2.6) must take the form*

$$\mathbf{Q}(s) = \frac{1}{2} \left(1 + \tanh \frac{1}{2}(s - t) \right) \left(\mathbf{nn} - \frac{1}{3}\mathbf{I} \right), \tag{2.7}$$

where t is an arbitrary constant due to translation symmetry.

To solve (GDC), a key step is to study the structure of local minimizers in 1-D. Thanks to Theorem 2.1, it is natural to ask the following question:

Whether the local minimizers of (2.4) subject to (2.6) must take the form (2.7)?

In Sect. 3, we will give an affirmative answer to this question. For the global minimizer, one can reduce \mathbf{Q} to a diagonal form (2.8). For the local minimizer, we have to consider general \mathbf{Q} . To reduce the problem, we used many elegant structures hidden in the system. In Sect. 4, we will prove the conjecture (GDC) under the mild assumption that the eigenvector of \mathbf{Q} corresponding to the largest eigenvalue is a constant vector.

For the case of $L \neq 0$, the problem becomes more complex. In this case, the direction vector \mathbf{n} on the anchoring condition at $+\infty$ could make a significant effect on the behavior for the minimizers. There are three different types of the alignment director \mathbf{n} on the boundary as below:

- (1) Homeotropic anchoring: $\mathbf{n} \cdot (0, 0, 1) = 1$;
- (2) Planar anchoring: $\mathbf{n} \cdot (0, 0, 1) = 0$;
- (3) Tilt anchoring: $0 < \mathbf{n} \cdot (0, 0, 1) < 1$.

For simplicity, we will first seek minimizers of the diagonal form

$$\mathbf{Q} = \begin{pmatrix} -\frac{1}{3}(S + T) & 0 & 0 \\ 0 & -\frac{1}{3}(S - T) & 0 \\ 0 & 0 & \frac{2}{3}S \end{pmatrix}, \tag{2.8}$$

which is meaningful due to the rotation invariant of the bulk energy. Then in 1-D, the energy functional is reduced to

$$\mathcal{F}_L(S, T) = \frac{2}{9} \int_{\mathbb{R}} \left(\frac{1+L}{2} (S')^2 + \frac{1}{6} (T')^2 + \frac{1}{6} (3S^2 + T^2) - S(S^2 - T^2) + \frac{1}{18} (3S^2 + T^2)^2 \right) ds. \tag{2.9}$$

The associated Euler–Lagrange equation of (2.9) takes as follows

$$\begin{cases} -\frac{1+L}{2}S'' + \frac{S}{2} - \frac{3S^2}{2} + \frac{T^2}{2} + \frac{S(3S^2+T^2)}{3} = 0, \\ -\frac{1}{6}T'' + \frac{T}{6} + ST + \frac{T(3S^2+T^2)}{9} = 0. \end{cases} \tag{2.10}$$

Here we consider the homeotropic anchoring condition, which leads to the following boundary conditions for (S, T) :

$$S(+\infty) = 1, \quad T(+\infty) = S(-\infty) = T(-\infty) = 0. \tag{2.11}$$

It is obvious that (2.10)–(2.11) has a uniaxial solution with $T = 0$ and $S(s)$ solving

$$-(1 + L)S'' + S - 3S^2 + 2S^3 = 0.$$

That is, an uniaxial equilibrium state takes

$$\mathbf{Q}_0(s) = S(s)\text{diag} \left\{ -\frac{1}{3}, -\frac{1}{3}, \frac{2}{3} \right\}, \quad S(s) = S^*(s/\sqrt{1+L}), \tag{2.12}$$

where S^* solves

$$-S'' + S - 3S^2 + 2S^3 = 0, \quad S(-\infty) = 0, \quad S(+\infty) = 1. \tag{2.13}$$

In [10], the authors investigate the stability of this solution.

Theorem 2.2 *The uniaxial equilibrium state \mathbf{Q}_0 is stable for the energy functional (2.4) when $L \leq 0$ and unstable when $L > 0$.*

In Sect. 5, we will prove that all the solutions of (2.10)–(2.11) must take $\mathbf{Q}_0(s)$ when $L > -1$. This in particular implies that the stable equilibrium state for the energy functional (2.4) cannot be of diagonal form (2.8) when $L > 0$ and under the homeotropic anchoring condition.

For $L \neq 0$, the structure of equilibrium solutions with planar and tilt anchoring boundary conditions is still an open question. In this case, the anisotropic term should play a key role in the study of the behavior for minimizers near the isotropic–nematic phase transition. See [8,9] for numerical results and [10] for more discussions and open questions.

3 Local minimizer in 1-D for $L = 0$

In this section, we study the local minimizer of (2.4) with $L = 0$.

Theorem 3.1 *All the local minimizers of (2.4) subject to (2.6) must take the form*

$$\mathbf{Q}(s) = \frac{1}{2} \left(1 + \tanh \frac{1}{2}(s - t) \right) \left(\mathbf{nn} - \frac{1}{3}\mathbf{I} \right), \tag{3.1}$$

where t is an arbitrary parameter. In fact, (3.1) gives all solutions of (2.5)–(2.6).

For the global minimizer, the proof relies on the fact that we may assume that \mathbf{Q} is the diagonal form (2.8). Thus, it suffices to consider an ODE system with two components. For the local minimizer, we have to consider an ODE system with five components. To reduce the problem, we need the following key lemmas. In what follows, we always assume that \mathbf{Q} is a solution of (2.5)–(2.6). We will often use the following spectral decomposition of \mathbf{Q} :

$$\mathbf{Q} = \lambda_1 \mathbf{n}_1 \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \mathbf{n}_3. \tag{3.2}$$

Lemma 3.2 *It holds that*

$$\text{Tr}(\mathbf{Q}')^2 = \sum_{i=1}^3 |\lambda'_i|^2 + 2 \sum_{i < j} (\lambda_i - \lambda_j)^2 (\mathbf{n}'_i \cdot \mathbf{n}_j)^2 = \text{Tr}(\mathbf{Q}^2) - 6\text{Tr}(\mathbf{Q}^3) + \frac{3}{2}(|\mathbf{Q}|^2)^2.$$

Moreover, $\mathbf{Q}(x^*) \neq 0$ for all finite x^* .

Proof Using (3.2) and the identities like $|\mathbf{n}'_1|^2 = |\mathbf{n}'_1 \cdot \mathbf{n}_2|^2 + |\mathbf{n}'_1 \cdot \mathbf{n}_3|^2$, we obtain

$$\begin{aligned} |\mathbf{Q}'|^2 &= \sum_{i=1}^3 |\lambda'_i|^2 + 2 \sum_{i=1}^3 \lambda_i^2 |\mathbf{n}'_i|^2 + 4 \sum_{i < j} \lambda_i \lambda_j (\mathbf{n}_i \cdot \mathbf{n}'_j) (\mathbf{n}_j \cdot \mathbf{n}'_i) \\ &= \sum_{i=1}^3 |\lambda'_i|^2 + 2 \sum_{i < j} \left(\lambda_i (\mathbf{n}_j \cdot \mathbf{n}'_i) + \lambda_j (\mathbf{n}_i \cdot \mathbf{n}'_j) \right)^2 \\ &= \sum_{i=1}^3 |\lambda'_i|^2 + 2 \sum_{i < j} (\lambda_i - \lambda_j)^2 (\mathbf{n}_j \cdot \mathbf{n}'_i)^2, \end{aligned}$$

which gives the first equality.

Using the Eq. (2.5), we have

$$\begin{aligned} 0 &= \langle -\mathbf{Q}'' + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2\mathbf{Q} + 3|\mathbf{Q}|^2I, 2\mathbf{Q}' \rangle \\ &= \left(\text{Tr}(-\mathbf{Q}^2 + \mathbf{Q}^2 - 6\mathbf{Q}^3) + \frac{3}{2}(|\mathbf{Q}|^2)^2 \right)', \end{aligned}$$

where $\langle A, B \rangle \triangleq \text{Tr}(A^T B)$ denote the matrix inner product. Therefore, there exists some constant C_0 so that

$$|\mathbf{Q}'|^2 = |\mathbf{Q}|^2 - 6\text{Tr}(\mathbf{Q}^3) + \frac{3}{2}(|\mathbf{Q}|^2)^2 + C_0, \tag{3.3}$$

which implies $C_0 \geq 0$ due to $\mathbf{Q}(-\infty) = 0$. Moreover, due to that \mathbf{Q} is a continuous function and the boundary condition (2.6), \mathbf{Q} is bounded, and thus there exists some constant $C_1 > 0$ so that

$$|\mathbf{Q}'|^2 \leq C_1. \tag{3.4}$$

Using (2.5) again, we get by integration by parts and (3.3) that

$$\begin{aligned} 0 &= \int_{x_1}^{x_2} \langle -\mathbf{Q}'' + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2\mathbf{Q} + 3|\mathbf{Q}|^2I, \mathbf{Q} \rangle dx \\ &= -\text{Tr}(\mathbf{Q}'\mathbf{Q}) \Big|_{x_1}^{x_2} + \int_{x_1}^{x_2} (|\mathbf{Q}'|^2 + |\mathbf{Q}|^2 - 9\text{Tr}(\mathbf{Q}^3) + 3(|\mathbf{Q}|^2)^2) dx \\ &= -\text{Tr}(\mathbf{Q}'\mathbf{Q}) \Big|_{x_1}^{x_2} + \int_{x_1}^{x_2} (C_0 + 2|\mathbf{Q}|^2 - 15\text{Tr}(\mathbf{Q}^3) + \frac{9}{2}(|\mathbf{Q}|^2)^2) dx. \end{aligned} \tag{3.5}$$

If $C_0 > 0$, due to $\mathbf{Q}(-\infty) = 0$, there exists $M < 0$ sufficiently small so that

$$C_0 + 2|\mathbf{Q}|^2 - 15\text{Tr}(\mathbf{Q}^3) + \frac{9}{2}(|\mathbf{Q}|^2)^2 \geq \frac{C_0}{2}, \quad |\mathbf{Q}|^2 \leq 1 \quad \forall x < M. \tag{3.6}$$

Choosing $x_1 < x_2 < M$, and combining (3.4), (3.5) and (3.6), we deduce that

$$\begin{aligned}
 2\sqrt{C_1} &\geq 2\sqrt{\text{Tr}(\mathbf{Q}^2)\text{Tr}(\mathbf{Q}^2)} \geq \text{Tr}(\mathbf{Q}'\mathbf{Q}) \Big|_{x_1}^{x_2} \\
 &= \int_{x_1}^{x_2} (C_0 + 2|\mathbf{Q}|^2 - 15\text{Tr}(\mathbf{Q}^3) + \frac{9}{2}(|\mathbf{Q}|^2)^2)dx \geq \frac{C_0}{2} (x_2 - x_1).
 \end{aligned}$$

Letting $x_1 \rightarrow -\infty$, we get a contradiction, and thus $C_0 = 0$. This proves the second equality.

If $\mathbf{Q}(x^*) = 0$ for some finite x^* , then we have

$$\text{Tr}(\mathbf{Q}'^2(x^*)) = 0 \implies \mathbf{Q}'(x^*) = 0.$$

Due to $\mathbf{Q}(x^*) = \mathbf{Q}'(x^*) = 0$, the uniqueness theorem of ODE gives $\mathbf{Q}(x) \equiv 0$, which contradicts the boundary condition $\mathbf{Q}(+\infty) \neq 0$ in (2.6). □

We introduce two important quantities

$$A(x) = |\mathbf{Q}(x)|^2, \quad B(x) = |\mathbf{Q}'(x)|^2.$$

By Lemma 3.2, we have

$$\text{Tr}(\mathbf{Q}^3) = \frac{A - B}{6} + \frac{A^2}{4}, \quad \mathbf{Q}'(\pm\infty) = 0.$$

By (2.5), we have

$$\begin{aligned}
 0 &= (-\mathbf{Q}'' + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2\mathbf{Q} + 3|\mathbf{Q}|^2I, \mathbf{Q}) \\
 &= -\frac{(\text{Tr}(\mathbf{Q}^2))'' - 2\text{Tr}(\mathbf{Q}^2)}{2} + |\mathbf{Q}|^2 - 9\text{Tr}(\mathbf{Q}^3) + 3(|\mathbf{Q}|^2)^2 \\
 &= -\frac{(\text{Tr}(\mathbf{Q}^2))'' - 2\text{Tr}(\mathbf{Q}^2)}{2} + |\mathbf{Q}|^2 - 9\left(\frac{A - B}{6} + \frac{A^2}{4}\right) + 3(|\mathbf{Q}|^2)^2 \\
 &= -\frac{A'' - 2B}{2} + A - 9\left(\frac{A - B}{6} + \frac{A^2}{4}\right) + 3A^2.
 \end{aligned}$$

This gives the following useful differential equation

$$A'' = -A + 5B + \frac{3}{2}A^2. \tag{3.7}$$

Moreover,

$$B(\pm\infty) = 0, \quad A(-\infty) = 0, \quad A(+\infty) = \frac{2}{3}, \quad A'(\pm\infty) = 0. \tag{3.8}$$

Lemma 3.3 *It holds that*

$$B \geq A - \sqrt{6}A^{3/2} + \frac{3}{2}A^2.$$

The equality holds if and only if $\lambda_i = 2a > 0$, $\lambda_j = -a$, $j \neq i$ for some i and $a > 0$.

Proof By Lemma 3.2, it suffices to prove

$$\text{Tr}(\mathbf{Q}^3) \leq \frac{1}{\sqrt{6}}A^{3/2}. \tag{3.9}$$

Thanks to $\sum_{i=1}^3 \lambda_i = 0$, $\text{Tr}(\mathbf{Q}^3) = \sum_{i=1}^3 \lambda_i^3 = 3\lambda_1\lambda_2\lambda_3$. If $\lambda_1\lambda_2\lambda_3 \leq 0$, then we have $\text{Tr}(\mathbf{Q}^3) \leq 0 < A^{3/2}/\sqrt{6}$. Otherwise, we assume $\lambda_1, \lambda_2 < 0$ without loss of generality. Obviously,

$$\begin{aligned} (\text{Tr}(\mathbf{Q}^3))^2 &= 9\lambda_1^2\lambda_2^2\lambda_3^2 = 9(\lambda_1\lambda_2)(\lambda_1\lambda_2)(\lambda_1 + \lambda_2)^2 \\ &= 36(\lambda_1\lambda_2)(\lambda_1\lambda_2)\frac{(\lambda_1 + \lambda_2)^2}{4} \leq 36\left(\frac{\lambda_1\lambda_2 + \lambda_1\lambda_2 + (\lambda_1 + \lambda_2)^2/4}{3}\right)^3, \end{aligned}$$

from which and the following fact

$$\frac{\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2}{3} - \frac{\lambda_1\lambda_2 + \lambda_1\lambda_2 + (\lambda_1 + \lambda_2)^2/4}{3} = \frac{1}{4}(\lambda_1 - \lambda_2)^2 \geq 0,$$

we infer that

$$(\text{Tr}(\mathbf{Q}^3))^2 \leq 36\left(\frac{\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2}{3}\right)^3 = 36\left(\frac{A}{6}\right)^3 = \frac{A^3}{6},$$

which gives (3.9). The above arguments also show that the equality holds if and only if $\lambda_1 = \lambda_2 = -a, \lambda_3 = 2a$ for some $a > 0$. □

Lemma 3.4 For any $x \in \mathbf{R}$, $0 < A(x) < \frac{2}{3}$ and $A'(x) > 0$.

Proof First of all, $A(x) > 0$ follows from Lemma 3.2. Next we show that $A(x) \leq \frac{2}{3}$. Otherwise, thanks to $A(-\infty) = -\infty$ and $A(+\infty) = \frac{2}{3}$, $A(x)$ achieves its global maximum at a finite point x^* and $A(x^*) > 2/3$. Then we infer that

$$A''(x^*) = -A(x^*) + 5B(x^*) + \frac{3}{2}A^2(x^*) > 0,$$

which contradicts with the fact that $A(x^*)$ is the global maximum. Hence, we have $A(x) \leq 2/3$.

To rule out $A(x) = 2/3$ for some x , we assume $A(x^*) = 2/3$. Again, $A(x^*)$ is the global maximum due to $A(x) \leq 2/3$ and it leads to $A'' \leq 0$. Then we have

$$0 \geq A''(x^*) = -A(x^*) + 5B(x^*) + \frac{3}{2}A^2(x^*) = 5B(x^*).$$

As $B(x^*)$ is non-negative, we deduce that $B(x^*) = \text{Tr}(\mathbf{Q}^2(x^*)) = 0$, hence, $\mathbf{Q}'(x^*) = 0$. Then it follows from Lemma 3.3 that

$$0 = B(x^*) \geq \left(A - \sqrt{6}A^{3/2} + \frac{3}{2}A^2\right)(x^*) = \frac{2}{3} - \frac{4}{3} + \frac{2}{3} = 0.$$

The equality implies that

$$\lambda_i(x^*) = 2a > 0, \quad \lambda_j(x^*) = -a < 0 \text{ for } j \neq i$$

for some i and $a > 0$. Hence, $2/3 = A(x^*) = \text{Tr}(\mathbf{Q}^2)(x^*) = 6a^2$, then $a = \frac{1}{3}$. Therefore,

$$\begin{aligned} Q(x^*) &= \sum_{k=1}^3 \lambda_k \mathbf{n}_k \mathbf{n}_k \Big|_{x=x^*} = -\frac{1}{3} \sum_{j \neq i} \mathbf{n}_j \mathbf{n}_j + \frac{2}{3} \mathbf{n}_i \mathbf{n}_i \Big|_{x=x^*} \\ &= -\frac{1}{3}(\mathbf{I} - \mathbf{n}_i \mathbf{n}_i) + \frac{2}{3} \mathbf{n}_i \mathbf{n}_i \Big|_{x=x^*} = \mathbf{n}_i \mathbf{n}_i - \frac{1}{3} \mathbf{I} \Big|_{x=x^*}. \end{aligned}$$

Let $\tilde{\mathbf{Q}}(x) \equiv \mathbf{n}_i(\mathbf{x}^*)\mathbf{n}_i(\mathbf{x}^*) - \frac{1}{3}\mathbf{I}$. Then $\tilde{\mathbf{Q}}(x)$ is a solution of (2.5) with

$$\tilde{\mathbf{Q}}(x^*) = \mathbf{n}_i(\mathbf{x}^*)\mathbf{n}_i(\mathbf{x}^*) - \frac{1}{3}\mathbf{I} = \mathbf{Q}(x^*), \quad \tilde{\mathbf{Q}}'(x^*) = 0 = \mathbf{Q}'(x^*).$$

The uniqueness theorem of ODE implies that $\tilde{\mathbf{Q}}(x) \equiv \mathbf{Q}(x)$. However, $\tilde{\mathbf{Q}}(-\infty) \neq 0 = \mathbf{Q}(-\infty)$ and it leads to a contradiction. This shows that

$$0 < A(x) < \frac{2}{3} \quad \forall x \in \mathbf{R}.$$

Finally, we show that $A(x)$ is strictly monotonic. Using (3.7) and Lemma 3.3, we get

$$A''(x) = -A + B + \frac{3}{2}A^2 \geq -A + \frac{3}{2}A^2 + 5 \left(A - \sqrt{6}A^{3/2} + \frac{3}{2}A^2 \right) = 4A - 5\sqrt{6}A^{3/2} + 9A^2. \tag{3.10}$$

Thanks to $A(-\infty) = A'(-\infty) = 0$, we have

$$A''(x) \geq 4A - 5\sqrt{6}A^{3/2} + 9A^2 = A(4 - 5\sqrt{6} + 9A) > 0 \quad \forall x < -M$$

for some large $M > 0$. Consequently, $A(x)$ is strictly convex and monotonic for $x < -M$. We define

$$x_1 = \sup \{x : A'(t) > 0, \forall t \in (-\infty, x)\}, \quad J = (-\infty, x_1).$$

We aim to prove $x_1 = +\infty$. Otherwise, we have $A'(x_1) = 0$. Multiplying $2A'(y)$ on both side of (3.10) and then integrating from $-\infty$ to some $x \in J$, we obtain

$$\begin{aligned} 0 &\leq \int_{-\infty}^x \left(A''(y) - \left(4A - 5\sqrt{6}A^{3/2} + 9A^2 \right) (y) \right) \cdot 2A'(y)dy \\ &= \left(A'^2 - (4A^2 - 4\sqrt{6}A^{3/2} + 6A^3) \right) \Big|_{-\infty}^x = A'^2(x) - (4A^2 - 4\sqrt{6}A^{3/2} + 6A^3)(x), \end{aligned}$$

which gives

$$A'(x)^2 \geq (4A^2 - 4\sqrt{6}A^{3/2} + 6A^3)(x) = A^2(2 - \sqrt{6A})(x).$$

Recall that $0 < A(x) < 2/3$ and $A'(x) > 0$ ($x \in J$). Thus,

$$A'(x) \geq A(2 - \sqrt{6A})(x).$$

Letting $x \rightarrow x_1$ gives

$$0 = A'(x_1) \geq A(2 - \sqrt{6A})(x_1) > 0.$$

This is a contradiction. Therefore, $x_1 = +\infty$ and $A'(x) > 0$ for $x \in \mathbf{R}$. □

Now we are in a position to prove Theorem 3.1.

Proof of Theorem 3.1 We infer from Lemma 3.4 and (3.10) that

$$\begin{aligned} 0 &\leq \int_{-\infty}^x \left(A''(y) - \left(4A - 5\sqrt{6}A^{3/2} + 9A^2 \right) (y) \right) \cdot 2A'(y)dy \\ &= A'(x)^2 - A^2(2 - \sqrt{6A})(x). \end{aligned}$$

Due to $A(+\infty) = A'(+\infty) = 0$, letting $x \rightarrow +\infty$ gives

$$0 \leq \int_{-\infty}^{+\infty} \left(A''(y) - \left(4A - 5\sqrt{6}A^{3/2} + 9A^2 \right) (y) \right) \cdot 2A'(y)dy = 0,$$

which implies that for $x \in \mathbf{R}$,

$$A''(x) - (4A - 5\sqrt{6}A^{3/2} + 9A^2)(x) = 0. \tag{3.11}$$

Consequently,

$$A'(x)^2 - A^2(2 - \sqrt{6A})^2(x) = 0, \quad \text{i.e. } A'(x) = A(2 - \sqrt{6A})(x). \tag{3.12}$$

Using (3.7) and (3.11), we find

$$-A + 5B + \frac{3}{2}A^2 = A'' = 4A - 5\sqrt{6}A^{3/2} + 9A^2 \implies B = A - \sqrt{6}A^{3/2} + \frac{3}{2}A^2. \tag{3.13}$$

While, by Lemma 3.3, the equality on B holds if and only if two eigenvalues of $\mathbf{Q}(x)$ are equal and negative for any $x \in \mathbf{R}$. As $\mathbf{Q}(x) \neq 0$ due to Lemma 3.2, it must hold that

$$\lambda_i(x) = \lambda_j(x) < 0 \quad \forall x \in \mathbf{R},$$

and $i \neq j$ are fixed for any x . Therefore, without loss of generality, we assume $\lambda_1(x) = \lambda_2(x) < 0$ and denote

$$\lambda_1(x) = \lambda_2(x) = -\frac{S(x)}{3}, \quad \lambda_3(x) = \frac{2S(x)}{3}, \quad S(x) > 0.$$

The boundary condition (2.6) implies that $S(-\infty) = 0, S(+\infty) = 1$. Consequently, we get $A = \text{Tr}(\mathbf{Q}^2) = \frac{2S^2}{3}$, and then we see from (3.12) that

$$\left(\frac{2S^2}{3}\right)' = \frac{2S^2}{3}(2 - 2S) \iff S' = S(S - 1). \tag{3.14}$$

With the boundary condition of S , we derive the explicit formula of S, A, λ_i as follows

$$S(x) = \frac{\exp(x - x_0)}{1 + \exp(x - x_0)}, \quad (\lambda_1, \lambda_2, \lambda_3) = \left(-\frac{S}{3}, -\frac{S}{3}, \frac{2S}{3}\right), \quad A = \frac{2S^2}{3}, \tag{3.15}$$

where x_0 is a parameter due to translation.

By Lemma 3.3, we have

$$B = \sum_{i=1}^3 |\lambda'_i|^2 + 2 \sum_{i < j} (\lambda_i - \lambda_j)^2 (\mathbf{n}'_i \cdot \mathbf{n}_j)^2 = \text{Tr}(\mathbf{Q}^2) - 6\text{Tr}(\mathbf{Q}^3) + \frac{3}{2}(|\mathbf{Q}|^2)^2. \tag{3.16}$$

We infer from (3.14) and (3.15) that

$$B = \frac{2}{3}(S^2 - 2S^3 + S^4), \tag{3.17}$$

and

$$\sum_{i=1}^3 |\lambda'_i|^2 = \left(\frac{1}{9} + \frac{1}{9} + \frac{4}{9}\right)S'^2 = \frac{2}{3}S'^2 = \frac{2}{3}S^2(S - 1)^2. \tag{3.18}$$

Combining (3.16), (3.17) and (3.18), we obtain

$$2 \sum_{i < j} (\lambda_i - \lambda_j)^2 (\mathbf{n}'_i \cdot \mathbf{n}_j)^2 = B - \sum_{i=1}^3 |\lambda'_i|^2 = \frac{2}{3}(S^2 - 2S^3 + S^4) - \frac{2}{3}S^2(S - 1)^2 = 0.$$

As $\lambda_1, \lambda_2 \neq \lambda_3$, we deduce

$$(\mathbf{n}'_1 \cdot \mathbf{n}_3)^2 = (\mathbf{n}'_2 \cdot \mathbf{n}_3)^2 = 0 \implies |\mathbf{n}'_3|^2 = (\mathbf{n}'_1 \cdot \mathbf{n}_3)^2 + (\mathbf{n}'_2 \cdot \mathbf{n}_3)^2 = 0 \implies \mathbf{n}'_3 = 0.$$

Hence, $\mathbf{n}_3(x)$ is a constant vector \mathbf{n} . Finally, we obtain

$$\begin{aligned} \mathbf{Q}(x) &= \sum_{i=1}^3 \lambda_i \mathbf{n}_i \mathbf{n}_i = -\frac{S}{3} (\mathbf{n}_1 \mathbf{n}_1 + \mathbf{n}_2 \mathbf{n}_2) + \frac{2S}{3} \mathbf{n}_3 \mathbf{n}_3 = -\frac{S}{3} (\mathbf{I} - \mathbf{n}_3 \mathbf{n}_3) + \frac{2S}{3} \mathbf{n}_3 \mathbf{n}_3 \\ &= S \left(\mathbf{n}_3 \mathbf{n}_3 - \frac{\mathbf{I}}{3} \right) = S \left(\mathbf{nn} - \frac{\mathbf{I}}{3} \right) = \frac{\exp(x - x_0)}{1 + \exp(x - x_0)} \left(\mathbf{nn} - \frac{\mathbf{I}}{3} \right). \end{aligned}$$

This proves Theorem 3.1. □

4 Local minimizer in 3-D for $L = 0$

The Landau-de Gennes energy (1.4) without anisotropic term in 3-D takes

$$\mathcal{F}(\mathbf{Q}, \nabla \mathbf{Q}) = \int_{\mathbf{R}^3} \left\{ \frac{1}{6} |\nabla \mathbf{Q}|^2 + \frac{1}{6} \text{Tr} \mathbf{Q}^2 - \text{Tr} \mathbf{Q}^3 + \frac{1}{4} (\text{Tr} \mathbf{Q}^2)^2 \right\} dx,$$

and the associated Euler–Lagrange equation takes

$$-\Delta \mathbf{Q} + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2 \mathbf{Q} + 3|\mathbf{Q}|^2 \mathbf{I} = 0 \tag{4.1}$$

with boundary condition

$$\mathbf{Q}(x_1, x_2, +\infty) = \mathbf{nn} - \frac{1}{3} \mathbf{I}, \quad \mathbf{Q}(x_1, x_2, -\infty) = 0. \tag{4.2}$$

Considering the spectral decomposition of \mathbf{Q} :

$$\mathbf{Q} = \mathbf{N} \mathbf{3} \mathbf{N}^T = \lambda_1 \mathbf{n}_1 \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \mathbf{n}_3, \quad \mathbf{N} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3), \quad \mathbf{3} = \text{diag}(\lambda_1, \lambda_2, \lambda_3).$$

Then we can reformulate (4.1) as follows

$$-\mathbf{N}^T (\Delta \mathbf{Q}) \mathbf{N} + \mathbf{3} - 9\mathbf{3}^2 + 3|\mathbf{Q}|^2 \mathbf{3} + 3|\mathbf{Q}|^2 \mathbf{I} = 0,$$

which gives that for the diagonal elements,

$$\begin{aligned} -\Delta \lambda_1 - 2\Delta \mathbf{n}_1 \cdot \mathbf{n}_1 \lambda_1 - 2\lambda_2 |\mathbf{n}_2 \cdot \nabla \mathbf{n}_1|^2 - 2\lambda_3 |\mathbf{n}_3 \cdot \nabla \mathbf{n}_1|^2 + \lambda_1 - 9\lambda_1^2 + 3|\mathbf{Q}|^2 \lambda_1 + 3|\mathbf{Q}|^2 &= 0, \\ -\Delta \lambda_2 - 2\Delta \mathbf{n}_2 \cdot \mathbf{n}_2 \lambda_2 - 2\lambda_1 |\mathbf{n}_1 \cdot \nabla \mathbf{n}_2|^2 - 2\lambda_3 |\mathbf{n}_3 \cdot \nabla \mathbf{n}_2|^2 + \lambda_2 - 9\lambda_2^2 + 3|\mathbf{Q}|^2 \lambda_2 + 3|\mathbf{Q}|^2 &= 0, \\ -\Delta \lambda_3 - 2\Delta \mathbf{n}_3 \cdot \mathbf{n}_3 \lambda_3 - 2\lambda_1 |\mathbf{n}_1 \cdot \nabla \mathbf{n}_3|^2 - 2\lambda_2 |\mathbf{n}_2 \cdot \nabla \mathbf{n}_3|^2 + \lambda_3 - 9\lambda_3^2 + 3|\mathbf{Q}|^2 \lambda_3 + 3|\mathbf{Q}|^2 &= 0, \end{aligned} \tag{4.3}$$

and for the off-diagonal elements,

$$\begin{aligned} &\lambda_1 \Delta \mathbf{n}_1 \cdot \mathbf{n}_2 + \lambda_2 \Delta \mathbf{n}_2 \cdot \mathbf{n}_1 + 2 \sum_{k=1}^3 \partial_k (\lambda_1 - \lambda_2) \cdot (\partial_k \mathbf{n}_1 \cdot \mathbf{n}_2) \\ &+ 2\lambda_3 \sum_{k=1}^3 (\partial_k \mathbf{n}_3 \cdot \mathbf{n}_1) (\partial_k \mathbf{n}_3 \cdot \mathbf{n}_2) = 0, \\ &\lambda_2 \Delta \mathbf{n}_2 \cdot \mathbf{n}_3 + \lambda_3 \Delta \mathbf{n}_3 \cdot \mathbf{n}_2 + 2 \sum_{k=1}^3 \partial_k (\lambda_2 - \lambda_3) \cdot (\partial_k \mathbf{n}_2 \cdot \mathbf{n}_3) \\ &+ 2\lambda_1 \sum_{k=1}^3 (\partial_k \mathbf{n}_1 \cdot \mathbf{n}_2) (\partial_k \mathbf{n}_1 \cdot \mathbf{n}_3) = 0, \end{aligned}$$

$$\begin{aligned} &\lambda_3 \Delta \mathbf{n}_3 \cdot \mathbf{n}_1 + \lambda_1 \Delta \mathbf{n}_1 \cdot \mathbf{n}_3 + 2 \sum_{k=1}^3 \partial_k (\lambda_3 - \lambda_1) \cdot (\partial_k \mathbf{n}_3 \cdot \mathbf{n}_1) \\ &+ 2\lambda_2 \sum_{k=1}^3 (\partial_k \mathbf{n}_2 \cdot \mathbf{n}_3) (\partial_k \mathbf{n}_2 \cdot \mathbf{n}_1) = 0. \end{aligned} \tag{4.4}$$

It follows from (4.2) that

$$\begin{cases} \lambda_i(x_1, x_2, +\infty) = \frac{2}{3}, \mathbf{n}_i(x_1, x_2, +\infty) = \mathbf{n}, \lambda_j(x_1, x_2, +\infty) = -\frac{1}{3} \forall j \neq i; \\ \lambda_k(x_1, x_2, -\infty) = 0, k = 1, 2, 3 \end{cases} \tag{4.5}$$

for some $i \in \{1, 2, 3\}$. Without loss of generality, we assume $i = 3$.

The system (4.3)–(4.5) are difficult to solve since it is a system with degree of freedom 5. For this, we assume that the eigenvector of \mathbf{Q} corresponding to the largest eigenvalue is a constant vector, and then we can reduce (4.3)–(4.5) to a PDE system with degree of freedom 3. In this case, we give an affirmative answer to (GDC) proposed in Sect. 2.

Theorem 4.1 *The level set of global solutions of (4.1)–(4.2) [or (4.3)–(4.5)] satisfying $\mathbf{n}_3(x_1, x_2, x_3) \equiv \mathbf{n}$ and $\partial_{x_3} \lambda_3 > 0$ are hyperplanes in \mathbf{R}^3 . Moreover, $\mathbf{Q}(x_1, x_2, x_3) = S^*(x_3)(\mathbf{nn} - \frac{1}{3}\mathbf{I})$, where $S^*(x_3)$ solves (2.13).*

Using identities like $-\Delta \mathbf{n}_i \cdot \mathbf{n}_i = |\nabla \mathbf{n}_i|^2 = |\mathbf{n}_2 \cdot \nabla \mathbf{n}_1|^2 + |\mathbf{n}_3 \cdot \nabla \mathbf{n}_1|^2$, we have

$$\begin{aligned} -2\Delta \mathbf{n}_i \cdot \mathbf{n}_i \lambda_i - \sum_{j \neq i} 2\lambda_j |\mathbf{n}_j \cdot \nabla \mathbf{n}_i|^2 &= 2|\nabla \mathbf{n}_i|^2 \lambda_i - \sum_{j \neq i} 2\lambda_j |\mathbf{n}_j \cdot \nabla \mathbf{n}_i|^2 \\ &= 2 \sum_{j \neq i} (\lambda_i - \lambda_j) |\mathbf{n}_j \cdot \nabla \mathbf{n}_i|^2. \end{aligned}$$

Thus, under the assumption that \mathbf{n}_3 is a constant vector, we can reduce (4.3) to

$$\Delta \lambda_1 = 2(\lambda_1 - \lambda_2) |\mathbf{n}_2 \cdot \nabla \mathbf{n}_1|^2 + \lambda_1 - 9\lambda_1^2 + 3|\mathbf{Q}|^2 \lambda_1 + 3|\mathbf{Q}|^2, \tag{4.6}$$

$$\Delta \lambda_2 = 2(\lambda_2 - \lambda_1) |\mathbf{n}_1 \cdot \nabla \mathbf{n}_2|^2 + \lambda_2 - 9\lambda_2^2 + 3|\mathbf{Q}|^2 \lambda_2 + 3|\mathbf{Q}|^2, \tag{4.7}$$

$$\Delta \lambda_3 = \lambda_3 - 9\lambda_3^2 + 3|\mathbf{Q}|^2 \lambda_3 + 3|\mathbf{Q}|^2. \tag{4.8}$$

Yet, the above equations are not independent due to $\sum_{i=1}^3 \lambda_i = 0$. Denote

$$(\lambda_1, \lambda_2, \lambda_3) = \left(-\frac{S+T}{3}, -\frac{S-T}{3}, \frac{2S}{3} \right).$$

Then $|\mathbf{Q}|^2 = 2(3S^2 + T^2)/9$, and (4.6)–(4.8) are equivalent to

$$\Delta S = S - 3S^2 + T^2 + \frac{2S(3S^2 + T^2)}{3}, \tag{4.9}$$

$$\Delta T = 4|\mathbf{n}_1 \cdot \nabla \mathbf{n}_2|^2 \cdot T + T + 6ST + \frac{2T(3S^2 + T^2)}{3}, \tag{4.10}$$

where (4.9) comes from (4.8), and (4.10) comes from subtracting (4.7) by (4.6). Due to (4.5), the boundary conditions of (S, T) take

$$\lim_{x_3 \rightarrow \pm\infty} T(x_1, x_2, x_3) = \lim_{x_3 \rightarrow -\infty} S(x_1, x_2, x_3) = 0, \quad \lim_{x_3 \rightarrow +\infty} S(x_1, x_2, x_3) = 1. \tag{4.11}$$

To prove Theorem 4.1, we need the following lemmas.

Lemma 4.2 *If $S \geq 0$ and T is bounded, then $T \equiv 0$.*

Proof Firstly, we apply $S \geq 0$ and (4.10) to yield

$$\Delta T^2 = 2|\nabla T|^2 + 2T^2 \left(4|\mathbf{n}_1 \cdot \nabla \mathbf{n}_2|^2 + 1 + 6S + 2S^2 + \frac{2T^2}{3} \right) \geq 0.$$

That is, T^2 is subharmonic. Define

$$\varphi(x, r) = \int_{\partial B(x,r)} T(y)^2 dy \text{ for } x \in \mathbf{R}^3, r > 0 \text{ and } \varphi(x, 0) = T(x)^2.$$

Taking r derivatives on φ gives

$$\frac{\partial \varphi}{\partial r} = \frac{2}{4\pi r^2} \int_{B(x,r)} |\nabla T|^2 + \Delta T \cdot T dy \geq \frac{2}{4\pi r^2} \int_{B(x,r)} \Delta T \cdot T dy,$$

which along with (4.10) gives

$$\frac{\partial \varphi}{\partial r} \geq \frac{2}{4\pi r^2} \int_{B(x,r)} T^2 \left(4|\mathbf{n}_1 \cdot \nabla \mathbf{n}_2|^2 + 1 + 6S + 2S^2 + \frac{2T^2}{3} \right) dy \geq \frac{2}{4\pi r^2} \int_{B(x,r)} T^2 dy.$$

As T^2 is subharmonic, we infer

$$\frac{\partial \varphi}{\partial r} \geq \frac{2}{4\pi r^2} \cdot \frac{4\pi r^3}{3} T(x)^2 = \frac{2r}{3} T(x)^2.$$

Since T is bounded and $|\varphi(x, r)| \leq \|T\|_\infty^2$, it must hold that $T(x) = 0$. □

Lemma 4.3 *If $0 \leq S \leq M$ for some $M > 0$, then $T \equiv 0$.*

Proof By Lemma 4.2, we only need to prove that T is bounded. Define

$$\psi(x, r) = \int_{\partial B(x,r)} S(y) dy \text{ for } x \in \mathbf{R}^3, r > 0; \quad \psi(x, 0) = S(x).$$

We claim that $T^2(x) \leq 2$. Otherwise, there exists $x^* \in \mathbf{R}^3$ so that $T(x^*)^2 > 2$. Taking r derivatives on ψ gives

$$\frac{\partial \psi}{\partial r} = \frac{1}{4\pi r^2} \int_{B(x^*,r)} \Delta S(y) dy.$$

Applying (4.9) and the fact that T^2 is subharmonic, we obtain

$$\begin{aligned} \frac{\partial \psi}{\partial r} &= \frac{1}{4\pi r^2} \int_{B(x^*,r)} \left(S - 3S^2 + T^2 + \frac{2S(3S^2 + T^2)}{3} \right) dy \\ &\geq \frac{1}{4\pi r^2} \int_{B(x^*,r)} (T^2 - 1) dy \geq \frac{1}{4\pi r^2} \cdot \frac{4\pi r^3}{3} (T(x^*)^2 - 1) \geq \frac{r}{3}. \end{aligned}$$

Here we used $S - 3S^2 + 2S^3 \geq -1$ and $S \geq 0$. As $0 \leq S \leq M$ and $|\psi(x, r)| \leq M$, we get

$$2M \geq |\psi(x^*, 6M + 2) - \psi(x^*, 2)| = 6M |\psi_r(x^*, \xi)| \geq 6M \cdot \frac{\xi}{3} > 2M$$

for some $\xi \in [2, 6M + 2]$. This is a contradiction. Hence, T is bounded. □

Proof of Theorem 4.1 The monotonic assumption on $\lambda_3 = 2S/3$ implies $\partial_{x_3} S > 0$, which along with the boundary condition

$$\lim_{x_3 \rightarrow -\infty} S(x_1, x_2, x_3) = 0, \quad \lim_{x_3 \rightarrow +\infty} S(x_1, x_2, x_3) = 1.$$

gives $0 \leq S \leq 1$. Lemma 4.3 yields $T \equiv 0$. Consequently, we can reduce (4.9)–(4.11) to

$$\Delta S = S - 3S^2 + 2S^3 \tag{4.12}$$

with the boundary conditions

$$\lim_{x_3 \rightarrow -\infty} S(x_1, x_2, x_3) = 0, \quad \lim_{x_3 \rightarrow +\infty} S(x_1, x_2, x_3) = 1,$$

and yield

$$\mathbf{Q} = \sum_{i=1}^3 \lambda_i \mathbf{n}_i \mathbf{n}_i = -\frac{S}{3} \mathbf{n}_1 \mathbf{n}_1 - \frac{S}{3} \mathbf{n}_2 \mathbf{n}_2 + \frac{2S}{3} \mathbf{n}_3 \mathbf{n}_3 = S \left(\mathbf{n}_3 \mathbf{n}_3 - \frac{1}{3} \mathbf{I} \right) = S \left(\mathbf{nn} - \frac{1}{3} \mathbf{I} \right).$$

Replacing S by $(u + 1)/2$ and x by $x/\sqrt{2}$, we can reformulate (4.12) as

$$\Delta u = u^3 - u \tag{4.13}$$

with

$$\partial_3 u > 0, \quad \lim_{x_3 \rightarrow \pm\infty} u(x_1, x_2, x_3) = \pm 1.$$

By De Giorgi’s conjecture for (4.13), the level set of u are hyperplanes. As $S = (u + 1)/2$, we deduce that the level set of S are hyperplanes. It further implies

$$S(x, y, z) = S^*(z), \quad \mathbf{Q}(x, y, z) = S^*(z) \left(\mathbf{nn} - \frac{1}{3} \mathbf{I} \right),$$

where S^* solves (2.13), and the level set of each component of \mathbf{Q} are hyperplanes. □

Finally, under the assumption that \mathbf{n}_3 is a constant vector \mathbf{n} as Theorem 4.1, we give a criterion that \mathbf{Q} is uniaxial, i.e. $\mathbf{Q} = S(\mathbf{nn} - \frac{1}{3}\mathbf{I})$, which may be independent of interest.

Theorem 4.4 *Let*

$$\mathbf{Q} = -\frac{S+T}{3} \mathbf{n}_1 \mathbf{n}_1 - \frac{S-T}{3} \mathbf{n}_2 \mathbf{n}_2 + \frac{2S}{3} \mathbf{nn}$$

be the solution of (4.1)–(4.2) [or equivalently (4.4), (4.9)–(4.11)], where \mathbf{n} is a constant vector. Assume that $S \geq 0$ and there exist $0 < \alpha \cdot \ln 4 < 1$, a constant C and $x^ \in \mathbf{R}^3$ so that*

$$|A(r)| \leq C e^{\alpha \cdot \ln^2(r)} \quad \text{for } r \gg 1, \tag{4.14}$$

where $A(r) = \int_{B(x^,r)} S(y) dy$. Then $T \equiv 0$ and $\mathbf{Q} = S(\mathbf{nn} - \frac{1}{3}\mathbf{I})$, where S solves (4.12) with boundary condition (4.11).*

- Remark 4.1**
- (a) The non-negative assumption on $\lambda_3 = 2S/3$ is natural since $\lambda_3(x, y, z)$ is always the largest eigenvalue of $\mathbf{Q}(x, y, z)$.
 - (b) If S is monotonic in x_3 , then we have $0 \leq S \leq 1$. The boundedness of S leads to that $A(r)$ is bounded. Hence, we can apply Theorem 4.1 to yield $T \equiv 0$.
 - (c) The condition (4.14) states that T is trivial unless the growth rate of the average of S in some ball $B(x, r)$ is faster than any polynomial growth.

Proof By Lemma 4.2, it suffices to prove that T is bounded. Without loss of generality, we take $x^* = 0$. For $A > 0$ to be determined later, there exists a constant $B > 0$ so that

$$S - 3S^2 + 2S^3 \geq A \cdot S - B. \tag{4.15}$$

If T is unbounded, then there exists x_0 depending on A such that $T(x_0)^2 > B > 0$. As S is non-negative, T^2 is subharmonic from the proof of Lemma 4.2.

Let $\psi(x, r)$ be as in Lemma 4.3 and $D = B(x_0, r)$. Then we get by (4.15) that

$$\begin{aligned} \frac{\partial \psi}{\partial r} \Big|_{x=x_0} &\geq \frac{1}{4\pi r^2} \int_D \left(S - 3S^2 + T^2 + \frac{2S(3S^2 + T^2)}{3} \right) dy \\ &\geq \frac{1}{4\pi r^2} \int_D \left(AS - B + T^2 \left(1 + \frac{2S}{3} \right) \right) dy \\ &\geq \frac{1}{4\pi r^2} \left(\int_D AS \, dy + \int_{B(x_0, r)} (T^2 - B) dy \right) \\ &\geq \frac{A}{4\pi r^2} \int_D S dy + \frac{1}{4\pi r^2} \frac{4\pi r^3}{3} (T(x_0)^2 - B) \\ &> \frac{A}{4\pi r^2} \int_D S dy \geq 0. \end{aligned} \tag{4.16}$$

Hence, $\psi(x_0, r)$ is strictly monotonic. We drop the notation x_0 in ψ for convenience. Note that

$$\int_{B(x_0, r)} S(y) \, dy = \int_0^r 4\pi s^2 \psi(s) \, ds,$$

which along with (4.16) gives

$$\frac{\partial \psi}{\partial r} \geq \frac{A}{r^2} \int_0^r s^2 \psi(s) \, ds \quad \text{for any } r > 0. \tag{4.17}$$

For any $r > 0$, there exists $\xi \in [2r, 4r]$ so that $\psi(4r) - \psi(2r) = 2r \cdot \psi_r(\xi)$. As ψ is monotonic, we infer from (4.17) that

$$\begin{aligned} \psi(4r) &\geq \psi(4r) - \psi(2r) = 2r \cdot \psi_r(\xi) \geq 2r \frac{A}{\xi^2} \int_0^\xi s^2 \psi(s) \, ds \\ &\geq 2r \frac{A}{\xi^2} \frac{\xi}{2} \left(\frac{\xi}{2} \right)^2 \psi \left(\frac{\xi}{2} \right) \geq \frac{Ar^2}{2} \psi(r), \end{aligned} \tag{4.18}$$

which implies

$$\psi(4^n) \geq \left(\frac{A}{2} \right)^n 4^{n(n-1)} \psi(1) = \left(\frac{A}{8} \right)^n 4^{n^2} \psi(1).$$

Define $M(x, r) := \int_{B(x, r)} S(y) \, dy$. Then

$$M(x_0, 2 \cdot 4^n) = \int_0^{2 \cdot 4^n} 4\pi s^2 \psi(s) \, ds > 4\pi (4^n)^3 \psi(4^n) \geq 4\pi (8A)^n 4^{n^2} \psi(1).$$

For sufficiently large n so that $|x_0| \leq 2 \cdot 4^n$, we have

$$M(0, 4^{n+1}) \geq M(x_0, 2 \cdot 4^n) \geq 4\pi (8A)^n 4^{n^2} \psi(1).$$

Now we choose $A > 1$ (therefore, x_0 can be determined) and combine (4.14) to obtain

$$e^{\ln 4 \cdot n^2} \psi(1) = 4^{n^2} \psi(1) < M(0, 4^{n+1}) \leq C4^{3n} e^{\alpha \ln^2(4^{n+1})} = C4^{3n} e^{(\alpha \cdot \ln^2 4)(n+1)^2}.$$

Since $\alpha \cdot \ln 4 < 1$, we reach a contradiction as $n \rightarrow +\infty$. Hence, T is bounded. □

5 Local minimizer in 1-D for $L \neq 0$

In this section, we study the local minimizer of (2.4) with $L \neq 0$. However, we consider \mathbf{Q} in the diagonal form (2.8) with the homeotropic anchoring. In this case, (S, T) satisfies the following Euler–Lagrange equation

$$\begin{cases} (1 + L)S'' = S - 3S^2 + T^2 + \frac{2S(3S^2 + T^2)}{3}, \\ T'' = T + 6ST + \frac{2T(3S^2 + T^2)}{3}, \end{cases} \tag{5.1}$$

with the boundary condition

$$S(-\infty) = T(\pm\infty) = 0, \quad S(+\infty) = 1. \tag{5.2}$$

Theorem 5.1 *For all $L > -1$, the ODE system (5.1) and (5.2) has only one solution $T(x) \equiv 0$, $S(x) = S^*(\frac{x}{\sqrt{1+L}})$, where S^* is the solution of the following equation*

$$-S'' + S - 3S^2 + 2S^3 = 0, \quad S(-\infty) = 0, \quad S(+\infty) = 1. \tag{5.3}$$

Remark 5.1 For $L > 0$, the solution $(0, S)$ is unstable by Theorem 2.2. Thus, the stable equilibrium \mathbf{Q} of (2.4) subject to the homeotropic anchoring can not be of the diagonal form (2.8) when $L > 0$.

Lemma 5.2 *Let (S, T) be the solution of (5.1)–(5.2). Then $S \leq 1$ and $S'(+\infty) = 0$.*

Proof We first prove that $S \leq 1$. Otherwise, the boundary condition $|S(\pm\infty)| \leq 1$ and the fact that $S \in C^2$ implies that there exists a global maximum point x^* of S . Consequently, $S(x^*) > 1$ and $S''(x^*) \leq 0$. Using (5.1), we find

$$(1 + L)S''(x^*) = \left(S - 3S^2 + 2S^3 + T^2 \left(1 + \frac{2S}{3} \right) \right) (x^*) > 0$$

due to $S(x^*) > 1$ and $S - 3S^2 + 2S^3 = S(S - 1)(2S - 1)$. This contradicts with $S''(x^*) \leq 0$. Hence, $S \leq 1$.

Next, we show that $S'(+\infty) = 0$. From the boundary condition $T(+\infty) = 0$ and $S(+\infty) = 1$, there exists $M > 0$ such that for $x > M$, $S(x) > 2/3$, $|T(x)| < 1/10$, and $1 + 6S + 2(S^2 + T^2/3) > 1$.

We claim that there does not exist $x_1, x_2 \in [M, +\infty)$ so that $\text{sign}(T(x_1)) \neq \text{sign}(T(x_2))$, i.e $\text{sign}(T)$ is preserved in $[M, +\infty)$. Otherwise, assume that $\text{sign}(T(x_1)) \neq \text{sign}(T(x_2))$ for $M \leq x_1 < x_2$. Obviously, there exists $x_0 \in (x_1, x_2)$ such that $T(x_0) = 0$. As $T(x_0) = T(+\infty) = 0$ and $T(x_2) \neq 0$, there exists a critical point x_3 of T in the interval $(x_0, +\infty)$ with nonzero value. Using (5.1), we have

$$T''(x_3) = T(x_3) \left(1 + 6S(x_3) + \frac{2(3S(x_3)^2 + T(x_3)^2)}{3} \right),$$

which along with the fact $1 + 6S(x_3) + 2(S(x_3)^2 + T(x_3)^2)/3 > 0$ gives

$$\text{sign}(T''(x_3)) = \text{sign}(T(x_3)). \tag{5.4}$$

However, if x_3 is a maximum point, then $T(x_3) > 0$ and $T''(x_3) \leq 0$, which contradicts with (5.4). Similarly, if x_3 is a minimum point, then $T(x_3) < 0$ and $T''(x_3) \geq 0$, which also contradicts with (5.4). Hence, $\text{sign}(T)$ is preserved in $[M, +\infty)$.

Without loss of generality, assume $T(x) \geq 0$ for $x \in [M, +\infty)$. Accordingly, T is a convex function in this interval, and thus $T(+\infty) = 0$ gives $T'(+\infty) = 0$. Subtracting the first equation of (5.1) by $\frac{1}{3}$ the second equation of (5.1), we obtain

$$\left((1 + L)S - \frac{T}{3} \right)'' = \left(S - \frac{T}{3} \right) \left(1 - 3S - 3T + 2 \left(S^2 + \frac{T^2}{3} \right) \right) \leq 0$$

due to $1/10 > T(x) \geq 0$, $S(x) \geq 2/3$ for $x > M$. That is, $(1 + L)S - \frac{T}{3}$ is concave on $[M, +\infty)$. Consequently, the boundary condition $((1 + L)S - \frac{T}{3})(+\infty) = 1 + L$ shows that $((1 + L)S - \frac{T}{3})'(+\infty) = 0$. Combining it with $T'(+\infty) = 0$ yields $S'(+\infty) = 0$. \square

Lemma 5.3 *If $T(x_0) = 0$, $S(x_0) = 0$ for some $-\infty \leq x_0 < +\infty$ and $S(x) \geq 0$ for $x > x_0$, then $x_0 = -\infty$, $T \equiv 0$ and $S(x) = S^*(x/\sqrt{1 + L})$. Here S^* is a solution of (5.3).*

Proof Firstly, we reformulate the second equation of (5.1) as follows

$$T'' = T \left(1 + 6S + \frac{2}{3}(3S^2 + T^2) \right).$$

Due to $1 + 6S + 2/3(3S^2 + T^2) > 0$, we have

$$\text{sign}(T'') = \text{sign}(T) \quad \text{for } x > x_0.$$

We claim that $T(x) = 0$ for $x \geq x_0$. Otherwise, there exists a local critical point of T with nonzero value. A similar argument as in (5.4) yields a contradiction. Hence, $T(x) = 0$ for $x \geq x_0$.

Next, we show that $x_0 = -\infty$. Actually, if x_0 is finite, we have $T'(x_0) = 0$, and (5.1) can be reduced to

$$(1 + L)S'' = S - 3S^2 + 2S^3 \quad \text{for } x \geq x_0 \tag{5.5}$$

with $S(x_0) = 0$, $S(+\infty) = 1$. Multiplying $2S'$ on both side of (5.5) and then integrating them on $[x_0, a]$ for some finite $a > x_0$, we obtain

$$\begin{aligned} (1 + L)[(S'(a))^2 - (S'(x_0)^2)] &= (S^2 - 2S^3 + S^4)(a) - (S^2 - 2S^3 + S^4)(x_0) \\ &= (S^2 - 2S^3 + S^4)(a). \end{aligned}$$

Recall that $S'(+\infty) = 0$ due to Lemma 5.2 and $S(+\infty) = 1$. Letting $a \rightarrow +\infty$ gives $-S'(x_0)^2 = 0$. Thus, we have

$$S(x_0) = T(x_0) = S'(x_0) = T'(x_0) = 0,$$

which implies that $S, T \equiv 0$, which contradicts with (5.2). Hence, $x_0 = -\infty$.

Thus, $T \equiv 0$ and S is a solution of (5.5). By a scaling, we conclude $S(x) = S^*(x/\sqrt{1 + L})$. \square

Proof of Theorem 5.1 We only need to prove that $T \equiv 0$. If $S(x) \geq 0$ for $x \in \mathbf{R}$, we may take $x_0 = -\infty$ and apply Lemma 5.3 to yield that $T \equiv 0$.

Otherwise, there exists some x_0 such that $S(x_0) < 0$. We aim to derive a contradiction. Due to $S(+\infty) = 1$, we can find some $x > x_0$ so that $S(x) = 0$. Consequently, we can define $x_1 := \sup\{x : x > x_0, S(x) = 0\}$. Obviously, $x_0 < x_1 < +\infty$ and

$$S(x_1) = 0, \quad S'(x_1) \geq 0, \quad S(x) \geq 0 \quad \forall x \geq x_0.$$

We claim $T(x_1) \neq 0$. Otherwise, Lemma 5.3 shows that $T \equiv 0$ and $x_1 = -\infty$, which contradicts that x_1 is finite.

On the other hand, from (5.1), we have

$$(1 + L)S''(x_1) = T^2(x_1) > 0 \implies S''(x_1) > 0,$$

where we used $1 + L > 0$. As a result, there exists $\delta > 0$ so that for $x \in (x_1, x_1 + \delta)$, we have $S'(x) > S'(x_1) \geq 0$.

Let $A \triangleq \{x > x_1 : S'(x) = 0\}$. We then define x_2 as follows

$$x_2 \triangleq \begin{cases} +\infty & \text{if } A = \emptyset; \\ \inf\{x \in A\} & \text{otherwise.} \end{cases}$$

Then we have $S'(x_2) = 0$. By definition of δ and x_2 , we know that $x_2 \geq x_1 + \delta > x_1$. Next, we reformulate the first equation of (5.1) as follows

$$(1 + L)S'' = S - 3S^2 + 2S^3 + T^2 \left(1 + \frac{2S}{3}\right).$$

Multiplying $2S'$ on both sides and then integrating them from x_1 to x_2 (if $x_2 = +\infty$, we first integrate both side from x_1 to a and then let $a \rightarrow +\infty$), we obtain

$$\int_{x_1}^{x_2} 2(1 + L)S'S'' dx = \int_{x_1}^{x_2} 2S'(S - 3S^2 + 2S^3) dx + \int_{x_1}^{x_2} 2S'T^2 \left(1 + \frac{2S}{3}\right) dx.$$

Using $S'(x_2) = 0$ and $S(x_1) = 0$, we obtain

$$-(1 + L)S'^2(x_1) = S^2(S - 1)^2(x_2) + \int_{x_1}^{x_2} 2S'T^2 \left(1 + \frac{2S}{3}\right) dx. \tag{5.6}$$

By definition of x_2 , $S(x)' > 0 \quad \forall x \in (x_1, x_2)$, which further implies that $S(x) > S(x_1) = 0 \quad \forall x \in (x_1, x_2]$. Now, the left hand side of (5.6) is non-positive, the first and second term on the right hand side are non-negative. Hence, we conclude

$$S'(x_1) = 0, \quad S(x_2) = 1, \quad T(x) = 0 \quad \forall x \in (x_1, x_2).$$

Hence $T'(x) = 0$ for $x \in (x_1, x_2)$. The continuity of T, T' implies that $T'(x_1) = T(x_1) = 0$. Therefore

$$S'(x_1) = S(x_1) = T'(x_1) = T(x_1) = 0.$$

Thus, $S \equiv T \equiv 0$, which contradicts with (5.2). □

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