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Calculus of Variations

On minimizers for the isotropic–nematic interface problem

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Abstract In this paper, we investigate the structure and stability of the isotropic-nematic interface in 1-D. In the absence of the anisotropic energy, the uniaxial solution is the only global minimizer. In the presence of the anisotropic energy, the uniaxial solution with the homeotropic anchoring is stable for $L_2 < 0$ and unstable for $L_2 > 0$. We also present many interesting open questions, some of which are related to De Giorgi conjecture.

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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. It has attracted many scientists due to its complex and fascinating structures for various applications. There are several phases in liquid crystals and phase transitions between different phases give rise to a variety of mathematical questions of great interest. In this article, we shall confine ourselves to the interface problem which appears

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ubiquitously in the physics literature. Interfacial behavior of liquid crystals differs from that of a normal fluid due to the anisotropic structure. For mixed fluids, there are many models for interface problems in the systems of coexistence of two phases including the Cahn–Hilliard and Allen–Cahn equations which have been extensively studied. In most cases with simple models, it is known that an interface tends to evolve proportionally to its mean curvature, and minimal surface appears to be a stationary interface. In systems of liquid crystals, molecular director field may play an important role in the shape of interface and interfacial stability.

Liquid crystals are characterized by aggregation of molecules, where a positional disorder of molecules may coexist with a marked degree of orientational order. Their anisotropic property gives a birth to various shapes of the molecules. Among many other phases, we are interested in nematic liquid crystals which can be described by the local average orientational order of the aggregation of the molecules at each position. Due to the head–tail symmetry, let $f : \Omega \times \mathbb{S}^2 \to \mathbb{R}$ be a nonnegative orientational probability density satisfying $f(x, \mathbf{m}) = f(x, -\mathbf{m})$ for any $\mathbf{m} \in \mathbb{S}^2$ and $\int_{\mathbb{S}^2} f(x, \mathbf{m})\, d\mathbf{m} = 1$ for each position x. Since the first moment of the density becomes zero, liquid crystals can be described by the order parameter $\mathbf{Q}$ defined by

$$\mathbf{Q}(x) = \int_{\mathbb{S}^2} \mathbf{m}\mathbf{m} f(x, \mathbf{m})\, \mathrm{d}\mathbf{m} - \frac{1}{3}\mathbf{I}. \tag{1.1}$$

For a vector $\mathbf{v} \in \mathbb{R}^3$, we denote by $\mathbf{v}\mathbf{v}$ the tensor product $\mathbf{v} \otimes \mathbf{v}$ whose (i, j)-entry is $v_i v_j$. 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. We 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.

Although there are many other questions regarding interfaces, we are primarily interested in the behavior of the molecular direction field near the phase transition and the shape of the interface that is closely related to De Giorgi conjecture. In [5], Doi and Kuzuu used the number density theory to study the structure of the interface between isotropic and nematic phases of rodlike molecules. They obtained the magnitude of the interface tension and their result indicates that near the phase transition, the parallel alignment which we refer to as *the planar anchoring* of molecules is energetically more favorable than the perpendicular alignment referred to as *the homeotropic anchoring*. For more general systems consisting of both uniaxial and biaxial liquid crystals, Wincure and Ray in [16] investigated interfacial moving fronts via nematodynamic equations based on the Landau-de Gennes theory. They studied the growth of 2D nematic droplet upon rapid cooling the isotropic phase to temperatures in the unstable and metastable states. With a certain fixed temperature, their numerical simulations exhibit the biaxial interface with plannar anchoring and uniaxial interface with the homeotropic anchoring at some times t. But the interfacial behavior for minimizers of the governing energy may or may not differ from those of dynamic problems.

Based on the framework of the Ginzburg–Landau, de Gennes studied the interface between the isotropic and nematic phases [3]. With a special ansatz that de Gennes made on the variation of the order tensor, the biaxility does not appear in the isotropic–nematic interface. Recently, numerical simulations done by Kamil et al. [9] agree with the de Gennes ansatz in the absence of anisotropic elastic energy corresponding to L_2-term (see Sect. 2). With the presence of the anisotropic elastic energy term in the governing energy functional, the interfacial profile can be very complex. Popa-Nita et al. [12,13] investigated the isotropic–nematic interface by numerical and asymptotic analysis. They showed that the de Gennes' ansatz is valid when the bend and splay elastic energies dominate over the twist energy. In the absence of the anisotropic energy, the de Gennes' ansatz predicts that both the homeotropic and planar anchorings on the interface are possibly stable. In fact, Kamil et al. in [9,10] obtained a positive answer by investigating numerical solutions of equations associated with the Landau-de Gennes theory. When the anisotropic energy(L_2 term) is present, de Gennes argued energetically that the homeotropic anchoring is stable when $L_2 < 0$ while the planar anchoring is stable when $L_2 > 0$. It turns out that uniaxiality may lose in the interfacial profile [9,13]. In fact, the ratio of the coefficients in the isotropic and anisotropic energies plays an important role in the structure of the interfaces [9,13]. Another interesting problem is to understand whether or not the orientation of molecules being neither homeotropic nor planar on the interfaces is stable. This problem remains open although some numerical and experimental results are found in [6,8,10,11,13].

To the best knowledge of the authors, there are no rigorous mathematical works regarding the questions discussed above. In this paper, we formulate rigorous variational problems and investigate the structure of the isotropic–nematic interface in 1-D. In the absence of the anisotropic energy, the uniaxial solution is the only global minimizer. In the presence of the anisotropic energy, the uniaxial solution with the homeotropic anchoring is stable for $L_2 < 0$ and unstable for $L_2 > 0$. Many interesting questions remain to be open, and we will provide some open questions in the last section.

2 Landau-de Gennes theory

In this section, we present the energy density written in terms of the tensor order parameter $\mathbf{Q}$ and its gradient $\nabla\mathbf{Q}$ following de Gennes (1974). Suppose that a bounded domain Ω in $\mathbb{R}^3$ is occupied by liquid crystals. As defined in (1.1), the traceless tensor $\mathbf{Q}$ is a function from Ω to $\mathcal{S}_0$, where $\mathcal{S}_0$ denotes the set of all symmetric traceless 3×3 matrices. For each point $x \in \mathbf{Q}$, eigenvalues and the corresponding eigenvectors of $\mathbf{Q}(x)$ determine the structure of molecules. For $\mathbf{Q} \in \mathcal{S}_0$, $\mathbf{Q}$ can be written as

$$\mathbf{Q} = S_1\mathbf{nn} + S_2\mathbf{mm} - \frac{1}{3}(S_1 + S_2)\mathbf{I},$$

where $\mathbf{n}$ and $\mathbf{m}$ are orthonormal eigenvectors of $\mathbf{Q}$.

Let $B_{\mathbf{Q}}$ be a symmetric traceless 3×3 matrix satisfying

$$\frac{1}{\int_{\mathbb{S}^2}\exp(B_{\mathbf{Q}}(\mathbf{x}) : \mathbf{mm})\,\mathrm{d}\mathbf{m}}\int_{\mathbb{S}^2}\left(\mathbf{mm} - \frac{1}{3}I\right)\exp(B_{\mathbf{Q}}(\mathbf{x}) : \mathbf{mm})\,\mathrm{d}\mathbf{m} = \mathbf{Q}(\mathbf{x}),$$

where $A : B$ denotes $\mathrm{tr}(B^t A)$ for 3×3 matrices A and B. Using the Bingham closure, the following generalized Landau-de Gennes energy was introduced in [7]

$$\tilde{\mathcal{F}}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\Omega}\{F_e(\mathbf{Q}, \nabla\mathbf{Q}) + \tilde{F}_b(\mathbf{Q})\}\,\mathrm{d}\mathbf{x}, \tag{2.1}$$

where

$$F_e = \frac{1}{2}\left(L_1|\nabla\mathbf{Q}|^2 + L_2 Q_{ij,j}Q_{ik,k} + L_3 Q_{ij,k}Q_{ik,j} + L_4 Q_{ij}Q_{kl,i}Q_{kl,j}\right),$$
$$\tilde{F}_b = k_B T c\left(\mathbf{Q} : B_{\mathbf{Q}} - \ln Z_{\mathbf{Q}} - \gamma|\mathbf{Q}|^2\right).$$

Here $\gamma > 0$, $c > 0$, and

$$Z_{\mathbf{Q}} = \int_{\mathbb{S}^2}\exp(B_{\mathbf{Q}} : \mathbf{m}\otimes\mathbf{m})\,\mathrm{d}\mathbf{m}.$$

In the case that $L_1 > 0$, $L_1 + L_2 + L_3 > 0$ and $L_4 = 0$, the direct method of the calculus of variations guarantees the existence of minimizers for $\tilde{\mathcal{F}}$ in the space

$$\mathcal{A} = \left\{ \mathbf{Q} \in W^{1,2}(\Omega, \mathcal{S}_0) : \mathbf{Q} = \mathbf{Q}_b \text{ on } \partial\Omega \right\},$$

where $\mathbf{Q}_b$ is a smooth boundary data on $\partial\Omega$.

The global minimizer for the bulk energy is uniaxial and near the isotropic–nematic transition the bulk energy $\tilde{F}_b$ is approximated by

$$\frac{a}{2}\mathrm{Tr}\mathbf{Q}^2 - \frac{b}{3}\mathrm{Tr}\mathbf{Q}^3 + \frac{c}{4}(\mathrm{Tr}\mathbf{Q}^2)^2 + \text{ higher order terms.}$$

In this paper, we focus on a special form of the energy, which is so-called the Landau-de Gennes energy, that is

$$\begin{aligned}\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_\Omega \Big\{ & \underbrace{\frac{a}{2}\mathrm{Tr}\mathbf{Q}^2 - \frac{b}{3}\mathrm{Tr}\mathbf{Q}^3 + \frac{c}{4}(\mathrm{Tr}\mathbf{Q}^2)^2}_{F_b:\text{bulk energy}} \\ & + \underbrace{\frac{1}{2}\Big(L_1|\nabla\mathbf{Q}|^2 + L_2 Q_{ij,j}Q_{ik,k} + L_3 Q_{ij,k}Q_{ik,j} + L_4 Q_{ij}Q_{kl,i}Q_{kl,j}\Big)}_{F_e:\text{elastic energy}} \Big\} d\mathbf{x}.\end{aligned} \tag{2.2}$$

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 [4] for more details. The bulk energy F_b is a potential function for uniaxial nematic liquid crystals, meaning that F_b favors molecules to be uniaxial nematic. We note that the total energy functional may not be bounded due to the term $L_4 Q_{ij}Q_{kl,i}Q_{kl,j}$ when $L_4 \neq 0$. The reader is referred to see [2] for detailed discussion. In order to avoid this situation, we restrict ourselves to the case $L_4 = 0$. It is also easy to check that the integration of the difference between L_2 and L_3 terms depends only on the boundary data for $\mathbf{Q}$. Without loss of generality, we may consider the energy functional given by

$$\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_\Omega \left\{ \frac{1}{2}\left(L_1 Q_{ij,k}Q_{ij,k} + L_2 Q_{ij,j}Q_{ik,k}\right) + F_b(\mathbf{Q}) \right\} d\mathbf{x}. \tag{2.3}$$

We assume that the following conditions for elastic constants are satisfied

$$L_1 > 0, \quad L_1 + L_2 > 0$$

so that

$$\int_\Omega \left\{ L_1 Q_{ij,k}Q_{ij,k} + L_2 Q_{ij,j}Q_{ik,k} \right\} d\mathbf{x} \geq C \int_\Omega |\nabla\mathbf{Q}|^2 d\mathbf{x} + \text{ boundary terms,}$$

for some $C > 0$ and thus $\mathcal{F}$ achieves its minimum in the space $\mathcal{A}$. Here we have used the fact that

$$\begin{aligned}\int_{\mathbb{R}^3} L_1|\nabla \mathbf{Q}|^2 + L_2 Q_{ij,j}Q_{ik,k}\mathrm{d}\mathbf{x} &= \sum_{i=1}^{3}\int_{\mathbb{R}^3} L_1|\nabla \mathbf{Q}_i|^2 + L_2|\nabla\cdot\mathbf{Q}_i|^2\mathrm{d}\mathbf{x}\\ &= \sum_{i=1}^{3}\int_{\mathbb{R}^3} L_1|\nabla\times\mathbf{Q}_i|^2 + (L_1+L_2)|\nabla\cdot\mathbf{Q}_i|^2\mathrm{d}\mathbf{x}\\ &\quad + \text{ boundary terms}\\ &\geq \min(L_1, L_1+L_2)\int_{\mathbb{R}^3}|\nabla\mathbf{Q}|^2\mathrm{d}\mathbf{x} + \text{ boundary terms,}\end{aligned}$$

where $\mathbf{Q}_i = (Q_{i1}, Q_{i2}, Q_{i3})$.

3 Isotropic–nematic phase transition

The polynomial form of the bulk energy in (2.2) can characterize the isotropic–nematic phase transition for liquid crystals. The critical points of the bulk energy are

$$\mathbf{Q} = 0 \quad \text{or} \quad s^{\pm}\left(\mathbf{nn} - \frac{1}{3}\mathbf{I}\right), \tag{3.1}$$

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 $\mathbf{Q} = s^+(\mathbf{nn} - \frac{1}{3}\mathbf{I})$ are stable critical points, which correspond to isotropic phase and nematic phase respectively, and $\mathbf{Q} = s^-(\mathbf{nn} - \frac{1}{3}\mathbf{I})$ is unstable. See [15] for more details.

Since we are interested in the stable interface between the two co-existence phases, we impose the condition $b^2 = 27ac$, meaning that the bulk energy at each phase are equal.

Let Ω be a bounded domain in $\mathbb{R}^3$ occupied by a liquid crystal. The stable two constant states 0 and $s^+\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\right)$ could coexist in the global minimizer, but the elastic energy prevents instantaneous jump from one stable state to another. The transition between two states appears in a thin region of width $\sqrt{L_1}$. Thus, we introduce new variables

$$\tilde{\mathbf{x}} = \frac{1}{\sqrt{L_1}}\mathbf{x}, \quad \tilde{\mathbf{Q}}(\tilde{\mathbf{x}}) = \mathbf{Q}(\sqrt{L_1}\tilde{\mathbf{x}})$$

and consider the scaled energy

$$\frac{1}{3L_1\sqrt{L_1}}\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\frac{1}{\sqrt{L_1}}\Omega}\left\{\frac{1}{6}(|\nabla\tilde{\mathbf{Q}}|^2 + \frac{L_2}{L_1}\tilde{Q}_{ij,j}\tilde{Q}_{ik,k}) + F_b(\tilde{\mathbf{Q}})\right\}\mathrm{d}\tilde{\mathbf{x}}.$$

For the rest of this paper, we assume that the following limits exist

$$\lim_{L_1\to 0}\frac{2L_2}{3L_1} = L, \quad \lim_{L_1\to 0}\frac{a}{L_1} = \tilde{a}, \quad \lim_{L_1\to 0}\frac{b}{L_1} = \tilde{b}, \quad \lim_{L_1\to 0}\frac{c}{L_1} = \tilde{c}.$$

Passing to the limit as $L_1 \to 0$, we obtain the following limiting energy functional (not relabelled) after removing the tilde

$$\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}^3}\left\{\frac{1}{6}|\nabla\mathbf{Q}|^2 + \frac{L}{4}Q_{ij,j}Q_{ik,k} + \frac{1}{3}F_b(\mathbf{Q})\right\}\mathrm{d}\mathbf{x}. \tag{3.2}$$

In what follows, we always assume that the constants, after scaling if necessary, satisfy

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

so that $s^+ = 1$ and $s^- = 1/2$ and $F_b(\mathbf{Q}) = 0$ if $\mathbf{Q} = 0$ or $\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}$. In this case, the energy functional takes as follows

$$\mathcal{F}(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}^3} \left\{ \frac{1}{6}|\nabla\mathbf{Q}|^2 + \frac{L}{4} Q_{ij,j} Q_{ik,k} + \frac{1}{6}\mathrm{Tr}\mathbf{Q}^2 - \mathrm{Tr}\mathbf{Q}^3 + \frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2 \right\} \mathrm{d}\mathbf{x}. \quad (3.3)$$

4 Isotropic–nematic interface in 1-D

In this section, we consider the global minimizer of the Landau-de Gennes energy in the class of functions $\mathbf{Q}$ which depends only on x_3. In this case, the total energy functional (3.3) becomes

$$\mathcal{F}_L(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}} \left\{ \frac{1}{6}|\mathbf{Q}'|^2 + \frac{L}{4} \sum_{i=1}^{3} (Q'_{i3})^2 + \frac{1}{6}\mathrm{Tr}\mathbf{Q}^2 - \mathrm{Tr}\mathbf{Q}^3 + \frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2 \right\} \mathrm{d}s, \quad (4.1)$$

where $'$ denotes $\frac{\mathrm{d}}{\mathrm{d}s} = \frac{\mathrm{d}}{\mathrm{d}x_3}$.

4.1 The global minimizer for the case $L = 0$

We first investigate the global minimizer of the energy functional

$$\mathcal{F}_0(\mathbf{Q}, \mathbf{Q}') = \int_{\mathbb{R}} \left\{ \frac{1}{6}|\mathbf{Q}'|^2 + \frac{1}{6}\mathrm{Tr}\mathbf{Q}^2 - \mathrm{Tr}\mathbf{Q}^3 + \frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2 \right\} \mathrm{d}s \quad (4.2)$$

with the boundary condition

$$\mathbf{Q}(+\infty) = \mathbf{nn} - \frac{1}{3}\mathbf{I}, \quad \mathbf{Q}(-\infty) = 0. \quad (4.3)$$

We obtain the following theorem.

Theorem 4.1 *The global minimizer of $\mathcal{F}_0(\mathbf{Q}, \nabla\mathbf{Q})$ must take the form*

$$\mathbf{Q}(s) = \frac{1}{2}\left(1 + \tanh(s - t)\right)\left(\mathbf{nn} - \frac{1}{3}\mathbf{I}\right), \quad (4.4)$$

where t is an arbitrary constant due to the translation symmetry

Proof Let

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

Then for 3-D case we see that

$$\begin{aligned} |\nabla\mathbf{Q}|^2 &= |\nabla\lambda_1|^2 + |\nabla\lambda_2|^2 + |\nabla\lambda_3|^2 + 2\sum \lambda_i^2 |\nabla_k \mathbf{n}_i|^2 \\ &\quad + \sum_{k=1}^{3} \sum_{1 \le i < j \le 3} 4\lambda_i \lambda_j (\mathbf{n}_i \cdot \nabla_k \mathbf{n}_j)(\mathbf{n}_j \cdot \nabla_k \mathbf{n}_i) \\ &= |\nabla\lambda_1|^2 + |\nabla\lambda_2|^2 + |\nabla\lambda_3|^2 + \sum_{k=1}^{3} \sum_{1 \le i < j \le 3} 2\Big(\lambda_i(\mathbf{n}_j \cdot \nabla_k \mathbf{n}_i) + \lambda_j(\mathbf{n}_i \cdot \nabla_k \mathbf{n}_j)\Big)^2 \\ &\ge |\nabla\lambda_1|^2 + |\nabla\lambda_2|^2 + |\nabla\lambda_3|^2. \end{aligned}$$

Here we use the following property

$$\lambda_i^2|\nabla_k \mathbf{n}_i|^2 = \lambda_i^2 \sum_{j=1}^{3}(\mathbf{n}_j \cdot \nabla_k \mathbf{n}_i)^2 = \lambda_i^2 \sum_{j\neq i}(\mathbf{n}_j \cdot \nabla_k \mathbf{n}_i)^2.$$

Therefore, we obtain

$$\mathcal{F}(\mathbf{Q}) \geq \mathcal{F}(\mathrm{diag}\{\lambda_1, \lambda_2, \lambda_3\}).$$

We also have that the global minimizers $\mathbf{Q}$ satisfy that for all $1 \leq i < j \leq 3$, $1 \leq k \leq 3$,

$$\lambda_i(\mathbf{n}_j \cdot \nabla_k \mathbf{n}_i) + \lambda_j(\mathbf{n}_i \cdot \nabla_k \mathbf{n}_j) = 0,$$

which is equivalent to

$$(\lambda_i - \lambda_j)(\mathbf{n}_j \cdot \nabla_k \mathbf{n}_i) = 0.$$

If there is an eigenvalue which is different from the other two eigenvalues, (say $\lambda_1 \neq \lambda_2, \lambda_3$), then we have $\mathbf{n}_1 \cdot \nabla_k \mathbf{n}_1 = \mathbf{n}_2 \cdot \nabla_k \mathbf{n}_1 = \mathbf{n}_3 \cdot \nabla_k \mathbf{n}_1 = 0$, which means $\nabla \mathbf{n}_1 = 0$, i.e, $\mathbf{n}_1$ is a constant vector. In particular, for 1-D problem, we also have $\mathbf{n}_1$ being a constant vector.

We assume that $\mathbf{n} = (0, 0, 1)$, and $\mathbf{Q}(\infty) = \mathrm{diag}\{-\frac{1}{3}, -\frac{1}{3}, \frac{2}{3}\}$. This enables us to assume that global minimizers are of the form

$$\mathbf{Q} = \mathrm{diag}\left\{-\frac{S+T}{3}, -\frac{S-T}{3}, \frac{2S}{3}\right\}.$$

Then the energy functional reduces to

$$\mathcal{F}_0(S,T) = \frac{2}{9}\int_{\mathbb{R}} \Big(\frac{1}{2}(S')^2 + \frac{1}{6}(T')^2 + \frac{1}{6}(3S^2+T^2) - S(S^2-T^2) + \frac{1}{18}(3S^2+T^2)^2\Big)\mathrm{d}s, \tag{4.5}$$

and the boundary condition becomes

$$S(-\infty) = T(\pm\infty) = 0, \quad S(+\infty) = 1. \tag{4.6}$$

The Euler–Lagrange equations are

$$-S'' + S - 3S^2 + T^2 + \frac{2S(3S^2+T^2)}{3} = 0, -\infty < s < \infty, \tag{4.7}$$

$$-T'' + T + 6ST + \frac{2T(3S^2+T^2)}{3} = 0, -\infty < s < \infty. \tag{4.8}$$

The above system has an explicit solution

$$S(\tau) = S^*(\tau) \triangleq \frac{\exp(\tau - t)}{1+\exp(\tau - t)}, \quad T(\tau) = 0. \tag{4.9}$$

From now on, we shall prove that this solution is the only global minimizer for (4.5) and (4.6).

Let $z = S + Ti/\sqrt{3}$. It follows from (4.7) and (4.8) that

$$-z'' + z - 3\bar{z}^2 + 2|z|^2 z = 0.$$

We also express the energy functional in terms of z as

$$\mathcal{F}_0(z) = \frac{1}{9}\int_{\mathbb{R}} \Big((z')^2 + |z|^2 - (z^3 + \bar{z}^3) + |z|^4\Big)\mathrm{d}s.$$

With $z = re^{i\theta}$, the energy can be written as

$$\mathcal{F}_0(r,\theta) = \frac{1}{9}\int_{\mathbb{R}} \Big((r')^2 + r^2(\theta')^2 + r^2 - 2r^3\cos 3\theta + r^4\Big)\mathrm{d}s.$$

The boundary conditions (4.6) becomes

$$r(-\infty) = 0, \quad r(+\infty) = 1, \quad \theta(+\infty) = 0.$$

Then we have

$$\begin{aligned}\mathcal{F}_0(r,\theta) &= \frac{1}{9}\int_{\mathbb{R}} \Big((r')^2 + r^2(\theta')^2 + r^2 - 2r^3\cos 3\theta + r^4\Big)\mathrm{d}s \\ &\geq \frac{1}{9}\int_{\mathbb{R}} \Big((r')^2 + r^2 - 2r^3 + r^4\Big)\mathrm{d}s = \mathcal{F}(r,0).\end{aligned}$$

It is easy to see that the equality holds only if $\theta \equiv 0$. The minimizer for the energy functional

$$\int_{\mathbb{R}} \Big((r')^2 + r^2 - 2r^3 + r^4\Big)\mathrm{d}s, \quad r(-\infty) = 0,\ r(+\infty) = 1,$$

must solve

$$-r'' + r - 3r^2 + 2r^3 = 0.$$

This ODE has only one solution $r(s) = \frac{\exp(s-t)}{1+\exp(s-t)}$, where $t \in \mathbb{R}$.

Therefore, we can conclude that (4.9) is the only global minimizer for (4.5) and (4.6). The analysis at the beginning implies that the eigenvector corresponding to the third eigenvalue is a constant vector. We can finally see that the global minimizer must take the form (4.4). □

4.2 The global minimizer for the case $L \neq 0$

In the case of $L \neq 0$, the one-dimensional Landau-de Gennes energy functional reads

$$\mathcal{F}_L(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}} \left\{\frac{1}{6}|\mathbf{Q}'|^2 + \frac{L}{4}\sum_{i=1}^{3}(Q'_{i3})^2 + \frac{1}{6}\mathrm{Tr}\mathbf{Q}^2 - \mathrm{Tr}\mathbf{Q}^3 + \frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2\right\}\mathrm{d}s \tag{4.10}$$

with the boundary condition

$$\mathbf{Q}(+\infty) = \mathbf{nn} - \frac{1}{3}\mathbf{I}, \quad \mathbf{Q}(-\infty) = 0. \tag{4.11}$$

Unlike in the case of $L = 0$ the direction vector $\mathbf{n}$ on the anchoring condition at $+\infty$ makes a significant effect on the behavior for the global 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 the remaining part of this section, we consider the homeotropic anchoring condition on which the direction field $\mathbf{n}$ is perpendicular to the interface.

We look for minimizers of the diagonal form

$$\mathbf{Q} = \begin{pmatrix} -\frac{1}{3}(S+T) & 0 & 0 \\ 0 & -\frac{1}{3}(S-T) & 0 \\ 0 & 0 & \frac{2}{3}S \end{pmatrix} \tag{4.12}$$

with $S(+\infty)=1$, $T(+\infty)=S(-\infty)=T(-\infty)=0$. Then the energy functional becomes

$$\mathcal{F}_L(S,T)=\frac{2}{9}\int_{\mathbb{R}}\Big(\frac{1+L}{2}(S')^2+\frac{1}{6}(T')^2+\frac{1}{6}(3S^2+T^2)-S(S^2-T^2)+\frac{1}{18}(3S^2+T^2)^2\Big)\mathrm{d}s. \tag{4.13}$$

The corrresponding Euler–Lagrange equations are

$$-\frac{1+L}{2}S''+\frac{S}{2}-\frac{3S^2}{2}+\frac{T^2}{2}+\frac{S(3S^2+T^2)}{3}=0,\ -\infty<s<\infty, \tag{4.14}$$

$$-\frac{1}{6}T''+\frac{T}{6}+ST+\frac{T(3S^2+T^2)}{9}=0,\ -\infty<s<\infty. \tag{4.15}$$

It follows from direct calculations that (4.12) is a solution to the Euler–Lagrange equation corresponding to (4.10) if (S,T) satisfies (4.14)–(4.15). It is also clear that a uniaxial state with $T=0$ and $S(s)=S^*(s/\sqrt{1+L})$ [see (4.9)] solves

$$-(1+L)S''+S-3S^2+2S^3=0. \tag{4.16}$$

Thus, we obtain a uniaxial solution

$$\mathbf{Q}_0(s)=S(s)\mathrm{diag}\left\{-\frac{1}{3},-\frac{1}{3},\frac{2}{3}\right\},\qquad S(s)=S^*(s/\sqrt{1+L}), \tag{4.17}$$

to the Euler–Lagrange equation corresponding to (4.10). Therefore, $\mathbf{Q}_0$ is an equilibrium state for (4.10) with boundary condition (4.11).

Next, we investigate the stability of this solution.

Theorem 4.2 *The uniaxial equilibrium state $\mathbf{Q}_0$ for (4.2) is stable for the energy functional (4.10) when $L\le 0$ and unstable when $L>0$.*

Proof For any $\mathbf{P}=(P_{ij})\in C_c^\infty(\mathbb{R},\mathcal{S}_0)$, we calculate

$$\begin{aligned}
&\lim_{\xi\to 0}\frac{1}{\xi^2}\big(\mathcal{F}_L(\mathbf{Q}_0+\xi\mathbf{P})-\mathcal{F}_L(\mathbf{Q}_0)\big)\\
&=\int_{\mathbb{R}}\Big(\frac{1}{6}|\mathbf{P}'|^2+\frac{L}{4}\big((P_{13}')^2+(P_{23}')^2+(P_{33}')^2\big)\\
&\quad+\frac{1}{6}|\mathbf{P}|^2-3\,\mathrm{tr}(\mathbf{Q}_0\mathbf{P}^2)+(\frac{1}{2}|\mathbf{Q}_0|^2|\mathbf{P}|^2+(\mathbf{Q}_0:\mathbf{P})^2)\Big)\mathrm{d}s\\
&=\int_{\mathbb{R}}\Big\{\frac{1}{6}|\mathbf{P}'|^2+\frac{L}{4}\big((P_{13}')^2+(P_{23}')^2+(P_{33}')^2\big)+\frac{1}{6}|\mathbf{P}|^2\\
&\quad-3\Big(-\frac{S+T}{3}(P_{11}^2+P_{12}^2+P_{13}^2)-\frac{S-T}{3}(P_{21}^2+P_{22}^2+P_{23}^2)+\frac{2S}{3}(P_{31}^2+P_{32}^2+P_{33}^2)\Big)\\
&\quad+(\frac{3S^2+T^2}{9}|Q|^2+(\frac{S+T}{3}P_{11}+\frac{S-T}{3}P_{22}-\frac{2S}{3}P_{33})^2)\Big\}\mathrm{d}s\\
&=\int_{\mathbb{R}}\Big\{\frac{1}{6}|\mathbf{P}'|^2+\frac{L}{4}\big((P_{13}')^2+(P_{23}')^2+(P_{33}')^2\big)+\frac{1}{6}|\mathbf{P}|^2\\
&\quad+S\Big(P_{11}^2+2P_{12}^2+P_{22}^2-(P_{31}^2+P_{32}^2+2P_{33}^2)\Big)+\frac{S^2}{9}\big(3|\mathbf{P}|^2+(P_{11}+P_{22}-2P_{33})^2\big)\Big\}\mathrm{d}s.
\end{aligned}$$

For the terms of P_{12}, we see that

$$\frac{1}{3}(P_{12}')^2+\left(\frac{1}{3}+2S+\frac{2S^2}{3}\right)P_{12}^2\geq 0,$$

by using the fact that $S(s)=S^*(s/\sqrt{1+L})>0$.

Next, we take a look at the terms of P_{11}, P_{22}, P_{33}. Since $\mathbf{P}$ is trace free, we have $P_{11}+P_{22}=-P_{33}$ so that

$$P_{11}^2+P_{22}^2\geq\frac{1}{2}(P_{11}+P_{22})^2=\frac{1}{2}P_{33}^2,\quad (P_{11}')^2+(P_{22}')^2\geq\frac{1}{2}(P_{11}'+P_{22}')^2=\frac{1}{2}(P_{33}')^2.$$

Then we have

$$\begin{aligned}&\int_{\mathbb{R}}\Big\{\frac{1}{6}\big((P_{11}')^2+(P_{22}')^2+(P_{33}')^2\big)+\frac{L}{4}(P_{33}')^2+\frac{1}{6}\big(P_{11}^2+P_{22}^2+P_{33}^2\big)\\&\quad+S\Big(P_{11}^2+P_{22}^2-2P_{33}^2\Big)+\frac{S^2}{3}\big(P_{11}^2+P_{22}^2+P_{33}^2+3P_{33}^2\big)\Big\}\mathrm{d}s\\&\geq\int_{\mathbb{R}}\Big\{\frac{1+L}{4}(P_{33}')^2+\frac{1}{4}P_{33}^2-\frac{3S}{2}P_{33}^2+\frac{3S^2}{2}P_{33}^2\Big\}\mathrm{d}s.\end{aligned}$$

Since $S'(z)>0$, we can let $P_{33}=S'u$ with $u\in C_c^\infty(\mathbb{R})$. Then it follows that

$$\begin{aligned}&\int_{\mathbb{R}}\Big\{\frac{1+L}{4}((S'u)')^2+\frac{1}{4}(S'u)^2-\frac{3S}{2}(S'u)^2+\frac{3S^2}{2}(S'u)^2\Big\}\mathrm{d}s\\&=\int_{\mathbb{R}}\Big\{\frac{1+L}{4}((S''u)^2+2S''uS'u'+(S'u')^2)+\frac{1}{4}(S'u)^2-\frac{3S}{2}(S'u)^2+\frac{3S^2}{2}(S'u)^2\Big\}\mathrm{d}s\\&=\int_{\mathbb{R}}\Big\{\frac{1+L}{4}(S'u')^2+u^2\Big(\frac{1+L}{4}[(S'')^2-(S''S')']+\frac{1}{4}(S')^2-\frac{3S}{2}(S')^2+\frac{3S^2}{2}(S')^2\Big)\Big\}\mathrm{d}s\\&=\int_{\mathbb{R}}\frac{1+L}{4}(S'u')^2\mathrm{d}s\geq 0.\end{aligned}$$

Here the last equality is obtained by $(1+L)S'''=S'-6SS'+6S^2S'$, which is a consequence of (4.16).

Now, let us look at the terms of P_{13}, P_{23}. Taking P_{13} or $P_{23}=Sv$ with $v\in C_c^\infty(\mathbb{R})$, we have

$$\begin{aligned}&\int_{\mathbb{R}}\Big\{\frac{1}{3}\big((P_{13}')^2+(P_{23}')^2\big)+\frac{L}{4}\big((P_{13}')^2+(P_{23}')^2\big)+\frac{1}{3}\big(P_{13}^2+P_{23}^2\big)\\&\quad-S\big(P_{13}^2+P_{23}^2\big)+\frac{2S^2}{3}\big(P_{13}^2+P_{23}^2\big)\Big\}\mathrm{d}s\\&=\int_{\mathbb{R}}\Big\{\frac{4+3L}{12}\big((P_{13}')^2+(P_{23}')^2\big)+\left(\frac{1}{3}-S+\frac{2S^2}{3}\right)\big(P_{13}^2+P_{23}^2\big)\Big\}\mathrm{d}s.\end{aligned}$$

When $L\leq 0$, the above integral is not less than

$$\int_{\mathbb{R}}\Big\{\frac{1+L}{3}\big((P_{13}')^2+(P_{23}')^2\big)+\left(\frac{1}{3}-S+\frac{2S^2}{3}\right)\big(P_{13}^2+P_{23}^2\big)\Big\}\mathrm{d}s,$$

which is nonnegative because

$$\begin{aligned}
&\int_{\mathbb{R}}\left\{\frac{1+L}{3}\big((Sv)'\big)^2+\left(\frac{1}{3}-S+\frac{2S^2}{3}\right)(Sv)^2\right\}\mathrm{d}s\\
&=\int_{\mathbb{R}}\left\{\frac{1+L}{3}\big((S'v)^2+2S'vSv'+(Sv')^2\big)+\left(\frac{1}{3}-S+\frac{2S^2}{3}\right)(Sv)^2\right\}\mathrm{d}s\\
&=\int_{\mathbb{R}}\left\{\frac{1+L}{3}(Sv')^2+v^2\Big(\frac{1+L}{3}\big(-(S'S)'+(S')^2\big)+\left(\frac{1}{3}-S+\frac{2S^2}{3}\right)S^2\Big)\right\}\mathrm{d}s\\
&=\int_{\mathbb{R}}\frac{1+L}{3}(Sv')^2\mathrm{d}s\geq 0.
\end{aligned}$$

Here we use (4.16).

From the above estimates, we conclude that

$$\lim_{\xi\to 0}\frac{1}{\xi^2}\big(\mathcal{F}_L(\mathbf{Q}_0+\xi\mathbf{P})-\mathcal{F}_L(\mathbf{Q}_0)\big)\geq 0$$

and thus the uniaxial solution $\mathbf{Q}_0$ is stable.

Next, we shall show that the uniaxial solution is unstable when $L>0$. Let $P_{23}=0$ and $P_{13}=S(s)u(s)$. Then we have

$$\begin{aligned}
&\int_{\mathbb{R}}\left\{\frac{4+3L}{12}(P_{13}')^2+\left(\frac{1}{3}-S+\frac{2S^2}{3}\right)P_{13}^2\right\}\mathrm{d}s\\
&=\int_{\mathbb{R}}\left\{\frac{1+L}{3}(P_{13}')^2+\left(\frac{1}{3}-S+\frac{2S^2}{3}\right)P_{13}^2-\frac{L}{12}(P_{13}')^2\right\}\mathrm{d}s\\
&=\int_{\mathbb{R}}\left\{\frac{1+L}{3}(S(s)u'(s))^2-\frac{L}{12}\big[(S(s)u(s))'\big]^2\right\}\mathrm{d}s.
\end{aligned}$$

Now we verify that for any $L>0$, there exists $u(x)$ satisfies $u(+\infty)=0, u(-\infty)$ being bounded, such that

$$\sup_{u(+\infty)=0,|u(-\infty)|<\infty}\frac{\int_{\mathbb{R}}\big((Su)'\big)^2\mathrm{d}s}{\int_{\mathbb{R}}(Su')^2\mathrm{d}s}=\infty,$$

or equivalently

$$\sup_{u(+\infty)=0,|u(-\infty)|<\infty}\frac{\int_{\mathbb{R}}(S'u)^2\mathrm{d}s}{\int_{\mathbb{R}}(Su')^2\mathrm{d}s}=\infty.$$

For this, we prove that

$$\sup_{u(+\infty)=0,|u(-\infty)|<\infty}\frac{\int_0^\infty(S'u)^2\mathrm{d}s}{\int_0^\infty(Su')^2\mathrm{d}s}=\infty. \tag{4.18}$$

After translation with respect to s, we may assume that $S'\geq Ce^{-\alpha s}$, for some $C,\alpha>0$. Let $u(s)=e^{-\lambda s}$, then

$$\frac{\int_0^\infty(S'u)^2\mathrm{d}s}{\int_0^\infty(Su')^2\mathrm{d}s}\geq\frac{\int_0^\infty(Ce^{-\alpha x}u)^2\mathrm{d}s}{\int_0^\infty(u')^2\mathrm{d}s}=\frac{C^2}{\lambda(\lambda+\alpha)}.$$

Taking $\lambda\to 0$, we obtain (4.18). □

For non-zero L, we do not fully understand the behavior of equilibrium solutions for the Landau-de Gennes energy with plannar and tilt anchoring boundary conditions. In fact, the term $L\int_\Omega Q_{ij,j}Q_{ik,k}\mathrm{d}\mathbf{x}$ is $L\int_\Omega |\operatorname{div}\mathbf{Q}|^2\mathrm{d}\mathbf{x}$ and can also be written as $-L\int_\Omega |\operatorname{curl}\mathbf{Q}|^2\mathrm{d}\mathbf{x}+\int_{\partial\Omega} g\,\mathrm{d}\mathcal{H}^2$ for some function g depending only on the boundary data. This term plays a key role in the study of the behavior for minimizers near the isotropic–nematic phase transition.

5 Open questions

In this section, we formulate some of interesting mathematical problems arising from phase transitions in liquid crystals. Some of problems bear a striking resemblance to the famous De Giorgi's conjecture which we address later in this section.

Consider the local minimizers of the following Landau-de Gennes energy

$$\mathcal{F}(\mathbf{Q},\nabla\mathbf{Q})=\int_{\mathbb{R}^3}\left\{\frac{1}{6}|\nabla\mathbf{Q}|^2+\frac{L}{4}Q_{ij,j}Q_{ik,k}+\frac{1}{6}\mathrm{Tr}\mathbf{Q}^2-\mathrm{Tr}\mathbf{Q}^3+\frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2\right\}\mathrm{d}\mathbf{x}, \tag{5.1}$$

or more generally, the solution to the Euler–Lagrange equation

$$-\Delta\mathbf{Q}+\mathbf{Q}-9\mathbf{Q}^2+3|\mathbf{Q}|^2\mathbf{Q}+3|\mathbf{Q}|^2\mathbf{I}=0, \tag{5.2}$$

with boundary condition

$$\lim_{x_3\to+\infty}\mathbf{Q}(x_1,x_2,x_3)=\left(\mathbf{nn}-\frac{1}{3}\mathbf{I}\right),\quad \lim_{x_3\to-\infty}\mathbf{Q}(x_1,x_2,x_3)=0. \tag{5.3}$$

Here $\mathbf{n}\in\mathbb{S}^2$ is fixed. We remark that for a function $\mathbf{Q}$ with the boundary condition (5.3), the energy may not be bounded. For this reason, we say that $\mathbf{Q}$ is a local minimizer of (5.1) if $\mathbf{Q}$ is a solution to the Euler–Lagrange equation (5.2) and is energetically stable with compact perturbation, that is for all $\mathbf{P}\in C_c^\infty(\mathbb{R}^3,\mathcal{S}_0)$ it holds

$$\begin{aligned}\lim_{\varepsilon\to 0}\int_{\mathbb{R}^3}&\left\{\frac{1}{6}|\nabla(\mathbf{Q}+\varepsilon\mathbf{P})|^2+\frac{L}{4}(Q+\varepsilon P)_{ij,j}(Q+\varepsilon P)_{ik,k}+\frac{1}{6}\mathrm{Tr}(\mathbf{Q}+\varepsilon\mathbf{P})^2-\mathrm{Tr}(\mathbf{Q}+\varepsilon\mathbf{P})^3\right.\\&\left.+\frac{1}{4}(\mathrm{Tr}(\mathbf{Q}+\varepsilon\mathbf{P})^2)^2-\left(\frac{1}{6}|\nabla\mathbf{Q}|^2+\frac{L}{4}Q_{ij,j}Q_{ik,k}+\frac{1}{6}\mathrm{Tr}\mathbf{Q}^2-\mathrm{Tr}\mathbf{Q}^3+\frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2\right)\right\}\mathrm{d}\mathbf{x}\geq 0.\end{aligned}$$

We begin with the case of $L=0$. Assume

$$\mathbf{Q}(\mathbf{x})=s(\mathbf{x})\left(\mathbf{nn}-\frac{1}{3}\mathbf{I}\right)\text{ and let }u(\mathbf{x})=2s(\mathbf{x})-1.$$

By replacing $\mathbf{x}$ by $\frac{3}{2}\mathbf{x}$ in (5.2) and (5.3), we obtain

$$\Delta u+u-u^3=0,\qquad \lim_{x_3\to\pm\infty}u(x_1,x_2,x_3)=\pm 1.$$

Assuming that $|u|\leq 1$ and $\partial_{x_3}u>0$, Savin [14] proved that De Giorgi's conjecture holds true for local minimizers of the Ginzburg–Landau energy

$$\int_{\mathbb{R}^n}\left(\frac{1}{2}|\nabla u|^2+\frac{1}{4}(1-u^2)^2\right)\mathrm{d}\mathbf{x}. \tag{5.4}$$

Analogously, one can ask the following problem.

Problem 1 For the local minimizers of Landau-de Gennes energy

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

the level sets of each component of $\mathbf{Q}$ are hyperplanes.

This problem concerns about a five-components system, which may lead to high complexity. In the proof of Theorem 4.1, by restricting $\mathbf{Q} = \mathrm{diag}\big\{ -\frac{1}{3}(S+T), -\frac{1}{3}(S-T), \frac{2}{3}S \big\}$, we obtain a two-components system as below, which seems not only much simpler but also mathematically interesting even for 1-dimension case:

$$-S'' + S - 3S^2 + T^2 + \frac{2S(3S^2 + T^2)}{3} = 0, \tag{5.5}$$

$$-T'' + T + 6ST + \frac{2T(3S^2 + T^2)}{3} = 0, \tag{5.6}$$

with boundary conditions

$$S(-\infty) = T(\pm\infty) = 0, \; S(+\infty) = 1. \tag{5.7}$$

First, we conjecture the uniqueness of solution to the system (5.5)–(5.7).

Problem 2(a) The system (5.5)–(5.7) has only one solution $S(x) = S^*(x)$, $T(x) = 0$.

One may write the above conjecture in complex form.

Problem 2(b) The equation

$$\begin{aligned} &-z'' + z - 3\bar{z}^2 + 2|z|^2 z = 0, \qquad z \in \mathbb{C}, \\ &z(-\infty) = 0, \quad z(+\infty) = 1, \end{aligned}$$

has only one solution $z(x) = S^*(x)$.

We also make the following De Giorgi Type conjecture for the above two components system whose form seems much simpler than Problem 1.

Problem 1* For the local minimizers of

$$\mathcal{F}(S, T) = \int_{\mathbb{R}^3} \Big(\frac{1}{2}|\nabla S|^2 + \frac{1}{6}|\nabla T|^2 + \frac{1}{6}(3S^2 + T^2) - S(S^2 - T^2) + \frac{1}{18}(3S^2 + T^2)^2 \Big) \mathrm{d}\mathbf{x},$$

the level sets of S and T are hyperplane.

In addition, we can ask the following De Giorgi Type conjecture for the higher dimensional case. For more information on De Giorgi conjecture, we refer the reader to [1,14] and the references therein.

Problem 3 *(the generalized De Giorgi conjecture)* Let $\mathbf{Q} : \mathbb{R}^n \to \mathcal{S}_0$ be a smooth entire solution of the Euler–Lagrange equation

$$-\Delta\mathbf{Q} + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2\mathbf{Q} + 3|\mathbf{Q}|^2\mathbf{I} = 0, \quad \mathbf{x} \in \mathbb{R}^n.$$

If $\frac{\partial Q_{ij}}{\partial x_n} > 0$, then all level sets $\{\mathbf{x} \in \mathbb{R}^n : Q_{ij}(\mathbf{x}) = \vartheta\}(\vartheta \in \mathbb{R})$ are hyperplanes. In particular, the most interesting problem goes to the case when $n = 2$ or 3.

The case of $L \neq 0$ is much more complicated. A main distinct feature in this case is that the anchoring alignment at $+\infty$ will make a significant effect on the behavior of minimizers in one-dimensional case, as we have seen in Sect. 4.2. A uniaxial solution $\mathbf{Q} = S\,\mathrm{diag}\big\{-\frac{1}{3}, -\frac{1}{3}, \frac{2}{3}\big\}$ to the Euler–Lagrange equation for homeotropic anchoring boundary condition has been found and the stability is studied there. The behavior of equilibrium solutions with plannar and tilt anchoring boundary conditions remains to be open. For this, let us consider a special order tensor depending only on x_3 of the form

$$\mathbf{Q} = \begin{pmatrix} -\frac{(S+T)}{2}\cos^2\theta + S\cos^2\theta & 0 & -\frac{(3S+T)}{4}\sin 2\theta \\ 0 & -\frac{(S-T)}{2} & 0 \\ -\frac{3(3S+T)}{4}\sin 2\theta & 0 & -\frac{(S+T)}{2}\sin^2\theta + S\cos^2\theta \end{pmatrix} \tag{5.8}$$

with the boundary condition

$$S(-\infty) = T(\pm\infty) = 0,\;\; S(+\infty) = 1, \theta(+\infty) = \theta_0. \tag{5.9}$$

Here we restrict ourselves to the case that the molecular director is parallel to x_1–x_3 plane and the function θ measures the angle between the molecular director and the positive x_3-axis. Let

$$\mathcal{A} = \Big\{\mathbf{Q} : \mathbf{Q} \text{ satisfies (5.8) and (5.9)}, S, T, \theta \in W^{1,2}(\mathbb{R})\Big\}.$$

Problem 4 *(planar anchoring condition)* Let $\theta_0 = \frac{\pi}{2}$ and $\mathbf{Q}$ be a global minimizer of

$$\mathcal{F}_L(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}} \left\{\frac{1}{6}|\mathbf{Q}'|^2 + \frac{L}{4}\sum_{i=1}^{3}(Q'_{i3})^2 + \frac{1}{6}\mathrm{Tr}\mathbf{Q}^2 - \mathrm{Tr}\mathbf{Q}^3 + \frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2\right\} \mathrm{d}x_3 \tag{5.10}$$

in $\mathcal{A}$. Let (S, T, θ) represent the global minimizer $\mathbf{Q}$. An interesting problem is to prove that S is monotonically increasing and $\theta(-\infty) = 0$. Does $\mathcal{F}$ also have a unique minimizer in $\mathcal{A}$?

Problem 5 *(tilt anchoring condition)* Let $0 < \theta_0 < \frac{\pi}{2}$. Does a global minimizer $\mathbf{Q} \in \mathcal{A}$ of energy (5.10) satisfy $\theta(-\infty) = 0$? and does (5.10) have a unique minimizer? and what are the profiles for S, T, θ corresponding the global minimizer?

Even for the homeotropic anchoring case, solutions for the 1-D problem are not clearly understood yet. One may ask the following questions.

Problem 6 Can we find all solutions to system

$$-\frac{1+L}{2}S'' + \frac{S}{2} - \frac{3S^2}{2} + \frac{T^2}{2} + \frac{S(3S^2+T^2)}{3} = 0, \tag{5.11}$$

$$-\frac{1}{6}T'' + \frac{T}{6} + ST + \frac{T(3S^2+T^2)}{9} = 0, \tag{5.12}$$

with boundary condition $S(+\infty) = 1, T(+\infty) = S(-\infty) = T(-\infty) = 0$?

In the proof of Theorem 4.2, we know that for all $L > -2/3$, the solution $S = S^*(\cdot/\sqrt{1+L}), T = 0$ is stable for the energy (4.13), and it may be the only solution.

Finally, we state the De Giorgi type conjecture for $L \neq 0$.

Problem 7 For all local minimizers of the Landau-de Gennes energy

$$\mathcal{F}_L(\mathbf{Q}, \nabla\mathbf{Q}) = \int_{\mathbb{R}^3} \left\{\frac{1}{6}|\nabla\mathbf{Q}|^2 + \frac{L}{4}Q_{ij,j}Q_{ik,k} + \frac{1}{6}\mathrm{Tr}\mathbf{Q}^2 - \mathrm{Tr}\mathbf{Q}^3 + \frac{1}{4}(\mathrm{Tr}\mathbf{Q}^2)^2\right\}\mathrm{d}\mathbf{x},$$

the level sets of each component of $\mathbf{Q}$ are hyperplanes.

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