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**Equilibrium order parameters of nematic liquid
crystals in the Landau-De Gennes theory**

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Equilibrium order parameters of nematic liquid crystals in the Landau-De Gennes theory

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Abstract

We study equilibrium liquid crystal configurations in three-dimensional domains, within the continuum Landau-De Gennes theory. We obtain explicit bounds for the equilibrium scalar order parameters in terms of the temperature and material-dependent constants. We explicitly quantify the temperature regimes where the Landau-De Gennes predictions match and the temperature regimes where the Landau-De Gennes predictions don't match the probabilistic second-moment definition of the \mathbf{Q} -tensor order parameter. The regime of agreement may be interpreted as the regime of validity of the Landau-De Gennes theory since the Landau-De Gennes theory predicts large values of the equilibrium scalar order parameters - larger than unity, in the low-temperature regime. We discuss a modified Landau-De Gennes energy functional which yields physically realistic values of the equilibrium scalar order parameters in all temperature regimes.

Keywords: Nematic liquid crystals, order parameters, equilibrium configurations, Landau-De Gennes theory

AMS Classification: 35Qxx, 35Jxx, 35Bxx

1 Introduction

Liquid crystals are an intermediate phase of matter between the commonly observed solid and liquid phases [6]. In the simplest liquid crystal phase, the nematic phase, the constituent rod-like molecules translate freely as in a conventional liquid but whilst flowing, tend to align along certain locally preferred directions i.e. they exhibit a certain degree of long-range orientational ordering. Liquid crystals have attracted a lot of interest in recent years because of their unique physical properties and continue to do so because of their diverse applications [12] and their analogies to other physical systems.

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The mathematical theory of nematic liquid crystals is very rich; for a review see [18, 13]. The key ingredient of any mathematical theory for nematic liquid crystals is the definition of an *order parameter* that distinguishes the ordered nematic phase from the disordered isotropic liquid phase. Mean-field liquid crystal theories, such as the Maier-Saupe theory, describe the liquid crystal configuration in terms of a probability distribution function ψ on the unit sphere. The order-parameter, known as the \mathbf{Q} -tensor order parameter, is defined in terms of the second moment of ψ [6, 16]. This *probabilistic second-moment definition* naturally requires \mathbf{Q} to be a symmetric, traceless 3×3 matrix and imposes certain constraints on its eigenvalues, which represent the degree of ordering. The Landau-De Gennes theory, on the other hand, is a continuum theory for nematic liquid crystals and does not contain any information about either ψ or the intermolecular interactions [6, 16]. The \mathbf{Q} -tensor order parameter, within the Landau-De Gennes framework, is a symmetric, traceless 3×3 matrix with no a priori constraints on the eigenvalues. The Landau-De Gennes energy functional is a nonlinear integral functional of \mathbf{Q} and its spatial derivatives and the equilibrium, physically observable configurations correspond to either global or local minimizers of this energy subject to the imposed boundary conditions.

A natural question of interest is - do the equilibrium configurations predicted by the Landau-De Gennes theory agree with the probabilistic second-moment definition of \mathbf{Q} ? We systematically address this question in this paper. We obtain explicit bounds for the scalar order parameters of global energy minimizers, referred to as *equilibrium scalar order parameters*, in terms of the temperature and the material-dependent constants. These bounds quantify (to some extent) the competing effects of the different terms in the Landau-De Gennes energy density. Further, these bounds are compared to the probabilistic second-moment definition of \mathbf{Q} . This allows us to explicitly delineate the regions of agreement and the regions of disagreement and we find that the Landau-De Gennes predictions don't match the probabilistic second-moment definition in the low-temperature regime. In particular, the equilibrium scalar order parameters, within the Landau-De Gennes framework, can take physically unrealistic values (larger than unity) in the low-temperature regime. Our results largely depend on the use of maximum principle type of arguments for nonlinear elliptic systems of partial differential equations and they can be readily extended to more general energy functionals than the ones considered in this paper.

The derivation of the Landau-De Gennes energy density is valid near the isotropic state, close to the nematic-isotropic transition temperature. Therefore, it is well-expected that the predictions are physically unrealistic in the low temperature regime. However, our results show that the Landau-De Gennes predictions fail to be consistent with the probabilistic second-moment definition within a sufficiently small neighbourhood of the nematic-isotropic transition temperature. In principle, one would want to develop a

continuum theory that works for all temperature regimes. In the last part of the paper, we briefly outline a Ginzburg-Landau approach that remedies the flawed predictions in the low temperature regimes. We define a modified Landau-De Gennes energy functional such that the energy density blows up whenever the liquid crystal configuration violates the constraints imposed by the probabilistic second-moment definition of \mathbf{Q} or equivalently whenever the scalar order parameters are physically unrealistic. One deficiency of this approach is that it has no apparent connection with the mean-field microscopic approaches. A different approach has been suggested in [11] and we hope to systematically investigate a microscopic-macroscopic derivation of a continuum energy functional in future work [2].

The paper is organized as follows. In Section 2, we review the probabilistic second-moment definition of the order parameter. In Section 3, we study equilibrium liquid crystal configurations within the continuum Landau-De Gennes theory. In Section 3.1, we consider spatially homogeneous cases whereas in Sections 3.2 and 3.3, we include spatial inhomogeneities into the model and obtain upper bounds for the corresponding equilibrium scalar order parameters. These bounds explicitly define the domain for the equilibrium scalar order parameters in terms of the temperature and the material-dependent parameters. In Section 4, we discuss the main results and conclusions of this paper and suggest future research directions.

2 The Probabilistic Second-Moment Definition

In this section, we briefly review the probabilistic second-moment definition of the \mathbf{Q} -tensor order parameter and the Maier-Saupe mean-field liquid crystal theory. The interested reader is referred to [6, 14, 19] for details and we present the main points here for completeness.

Within the simplest microscopic model, the nematic molecules are modelled by elongated rods where the long molecular axes tend to align along certain locally preferred directions [6, 16]. The state of alignment of the nematic molecules is described by a probability distribution function for the molecular orientations on the unit sphere, $\psi : S^2 \rightarrow \mathbb{R}^+$, since $S^2 \subset \mathbb{R}^3$ is the space of all admissible directions. The probability distribution function, $\psi(\mathbf{p})$, gives the probability of finding molecules oriented in the direction $\mathbf{p} \in S^2$. Then ψ has the following properties - [6, 1] -

$$\begin{aligned} \psi(\mathbf{p}) &\geq 0 \quad \mathbf{p} \in S^2 \\ \psi(\mathbf{p}) &= \psi(-\mathbf{p}) \end{aligned} \tag{1}$$

$$\int_{S^2} \psi(\mathbf{p}) \, d\mathbf{p} = 1. \tag{2}$$

where (1) accounts for the indistinguishability of the states \mathbf{p} and $-\mathbf{p}$ on the unit sphere.

The macroscopic variables are defined in terms of the moments of ψ . The first moment vanishes because of the equivalence between antipodal points, $\mathbf{p} \equiv -\mathbf{p}$. We define the nematic order parameter, the \mathbf{Q} -tensor order parameter, to be the normalized second moment of the probability distribution function as follows [6, 16]-

$$\mathbf{Q} = \int_{S^2} \left(\mathbf{p} \otimes \mathbf{p} - \frac{1}{3} \mathbf{I} \right) \psi(\mathbf{p}) d\mathbf{p} \quad (3)$$

We refer to (3) as the probabilistic second-moment definition of \mathbf{Q} in the rest of the paper. For an isotropic system, where all directions in space are equally likely, the function ψ is a constant i.e.

$$\psi(\mathbf{p}) = \frac{1}{4\pi} \quad \forall \mathbf{p} \in S^2 \quad (4)$$

and consequently, $\mathbf{Q} = 0$. On the other hand, for a perfectly aligned system where the nematic molecules identically align along a pair of unit-vectors $(\mathbf{e}, -\mathbf{e})$, the function ψ is given by -

$$\psi(\mathbf{p}) = \frac{1}{8\pi} (\delta_{S^2}(\mathbf{e}, \mathbf{p}) + \delta_{S^2}(-\mathbf{e}, \mathbf{p})) \quad (5)$$

where δ_{S^2} is the Dirac-delta function on S^2 and the corresponding \mathbf{Q} -tensor is $\mathbf{Q} = (\mathbf{e} \otimes \mathbf{e} - \frac{1}{3} \mathbf{I})$.

It follows directly from (3) that \mathbf{Q} is a symmetric, traceless 3×3 matrix. From the spectral decomposition theorem, we can express \mathbf{Q} in terms of a triad of orthonormal eigenvectors, $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, and corresponding eigenvalues, $\{\lambda_1, \lambda_2, \lambda_3\}$, subject to the tracelessness condition $\sum_i \lambda_i = 0$.

$$\mathbf{Q} = \lambda_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + \lambda_2 \mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \otimes \mathbf{e}_3 \quad \text{where} \quad \sum_i \lambda_i = 0. \quad (6)$$

Nematic liquid crystals are broadly classified into three main families according to the eigenvalue structure of \mathbf{Q} . A nematic liquid crystal is called isotropic when it has three equal eigenvalues (the tracelessness condition implies that $\mathbf{Q} = 0$), uniaxial when it has a pair of equal non-zero eigenvalues and biaxial when it has three distinct eigenvalues [6, 16]. The eigenvalues measure the degree of orientational ordering along the corresponding eigenvectors and one can verify that the eigenvalues are constrained by the following inequalities -

$$-\frac{1}{3} \leq \lambda_i = \int_{S^2} (\mathbf{p} \cdot \mathbf{e}_i)^2 \psi(\mathbf{p}) d\mathbf{p} - \frac{1}{3} \leq \frac{2}{3}, \quad i = 1 \dots 3 \quad (7)$$

since $0 \leq \int_{S^2} (\mathbf{p} \cdot \mathbf{e}_i)^2 \psi(\mathbf{p}) d\mathbf{p} \leq 1$. If the eigenvalue $\lambda_i = -\frac{1}{3}$ (the lower bound in (7)), then the function ψ is supported on the great circle perpendicular to the corresponding eigenvector \mathbf{e}_i . On the other hand, if $\lambda_i = \frac{2}{3}$

(the upper bound in (7)), then ψ is as in (5) and the liquid crystal molecules line up perfectly along the pair of unit-vectors $(\mathbf{e}_i, -\mathbf{e}_i)$. For example, the liquid crystal state, $(\lambda_1, \lambda_2, \lambda_3) = (\frac{2}{3}, -\frac{1}{3}, -\frac{1}{3})$, is an example of a perfectly ordered state along the eigenvector \mathbf{e}_1 and exhibits *prolate* uniaxial symmetry whereas the liquid crystal state, $(\lambda_1, \lambda_2, \lambda_3) = (-\frac{1}{3}, \frac{1}{6}, \frac{1}{6})$, has the molecules aligned in the plane orthogonal to \mathbf{e}_1 and exhibits *oblate* uniaxial symmetry [8]. From a physical point of view, the limiting values, $\lambda_i = -\frac{1}{3}$ or $\lambda_i = \frac{2}{3}$, represent unrealistic configurations.

The \mathbf{Q} -tensor order parameter can be expressed more concisely in terms of just a pair of eigenvectors $(\mathbf{e}_1, \mathbf{e}_2)$ and a pair of scalar order parameters (s, r) as shown below [16].

$$\mathbf{Q} = s \left(\mathbf{e}_1 \otimes \mathbf{e}_1 - \frac{1}{3} \mathbf{I} \right) + r \left(\mathbf{e}_2 \otimes \mathbf{e}_2 - \frac{1}{3} \mathbf{I} \right), \quad (8)$$

where s, r are linear combinations of the λ_i 's given by

$$\begin{aligned} s &= \lambda_1 - \lambda_3 = 2\lambda_1 + \lambda_2 \\ r &= \lambda_2 - \lambda_3 = \lambda_1 + 2\lambda_2. \end{aligned} \quad (9)$$

The constraints (7) directly translate into constraints for the scalar order parameters (s, r) in (9) and necessarily imply that (s, r) take values inside or on the boundary of the *physical triangle*, T_ψ , illustrated in Figure 1. On each of the boundary segments of T_ψ , one of the eigenvalues λ_i necessarily attains the lower bound in (7). For example, on the boundary segment $s + r = 1$, we have $\lambda_3 = -\frac{1}{3}$. Similarly, every vertex of T_ψ represents a state of perfect alignment along of the eigenvectors of \mathbf{Q} . For example, the vertex $(s, r) = (1, 0)$ represents a state of perfect alignment along the eigenvector \mathbf{e}_1 . We call T_ψ , the physical triangle, on the grounds that the scalar order parameters are appropriately bounded (less than unity) inside T_ψ and the boundary represents physically unrealistic liquid crystal configurations.

For definiteness, we can assume a specific ordering of the eigenvalues such as $\lambda_3 \leq \lambda_2 \leq \lambda_1$. Then λ_1 is necessarily non-negative and λ_3 is necessarily non-positive and the constraints (7) require (s, r) to take values inside a subset of T_ψ , which is referred to as a *fundamental domain* T_f defined below

$$T_f = \{(s, r); 0 \leq s \leq 1, 0 \leq r \leq \min\{s, 1 - s\}\} \subset T_\psi. \quad (10)$$

Analogous remarks apply to the other five possibilities for the ordering of the eigenvalues.

The Maier-Saupe theory is a mean-field theory for uniaxial nematic liquid crystals [6, 17]. The Maier-Saupe free energy has two contributions -

$$I_{MS}[\psi] = \int_{S^2} \psi(\mathbf{p}) \log \psi(\mathbf{p}) \, d\mathbf{p} - \frac{1}{2} U(T) S^2 \quad (11)$$

where $U(T)$ accounts for the intermolecular interactions and is temperature-dependent and S is the uniaxial scalar order parameter. A standard minimization procedure for I_{MS} yields a self-consistent equation for the equilibrium order parameter, $S(T)$, as a function of the temperature. For high temperatures, the isotropic phase $S = 0$ is the global energy minimizer whereas for temperatures below a certain critical temperature T_c , the nematic phase is globally stable and the Maier-Saupe theory predicts a first-order nematic-isotropic phase transition at the critical temperature T_c .

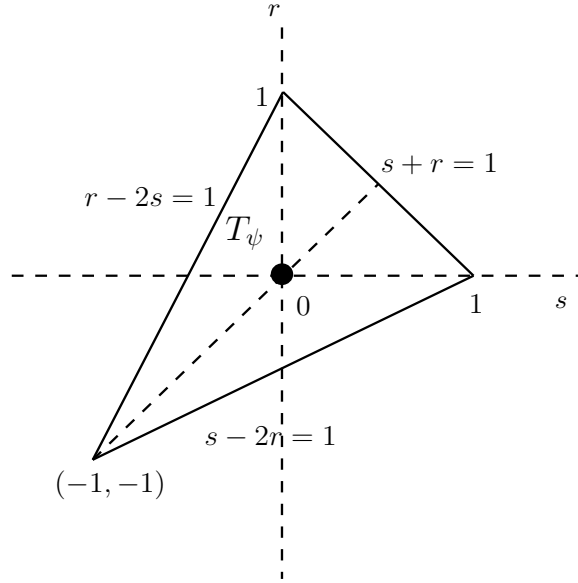


Figure 1: The physical triangle T_ψ . The origin $(s, r) = (0, 0)$ represents the isotropic liquid state; the dotted lines $U = \{(s, r) \in T_\psi : s = 0 \text{ or } r = 0 \text{ or } s = r\} \setminus (0, 0)$ represent uniaxial states and $B = T_\psi \setminus \{U \cup (0, 0)\}$ is the biaxial region.

3 The Landau–De Gennes Theory

In this section, we study equilibrium nematic configurations within the continuum Landau–De Gennes theory. The Landau–De Gennes theory describes the state of a nematic liquid crystal by a macroscopic order parameter - the \mathbf{Q} -tensor order parameter, which is defined in terms of macroscopic quantities such as the magnetic susceptibility [6, 13]. Within the Landau–De Gennes framework, \mathbf{Q} is a symmetric, traceless 3×3 matrix with no a priori bounds on the eigenvalues; in particular, the eigenvalues are not constrained by the inequalities (7).

We work in a three-dimensional setting, take the domain $\Omega \subset \mathbb{R}^3$ to be

bounded and simply-connected with smooth boundary. Let S_0 denote the space of symmetric, traceless 3×3 matrices

$$S_0 = \{ \mathbf{Q} \in \mathbf{M}^{3 \times 3}; \mathbf{Q}_{\alpha\beta} = \mathbf{Q}_{\beta\alpha}, \mathbf{Q}_{\alpha\alpha} = 0 \}. \quad (12)$$

The corresponding matrix norm is defined to be [13]

$$|\mathbf{Q}|^2 = \mathbf{Q}_{\alpha\beta} \mathbf{Q}_{\alpha\beta} \quad \alpha, \beta = 1 \dots 3 \quad (13)$$

and the Einstein summation convention is used here and elsewhere in the paper. We define our admissible space \mathcal{A} to be

$$\mathcal{A} = \{ \mathbf{Q} \in W^{1,2}(\Omega, S_0); \mathbf{Q} = \mathbf{Q}_0 \text{ on } \partial\Omega \} \quad (14)$$

where the Sobolev space $W^{1,2}(\Omega, S_0)$ is given by [10, 7]

$$W^{1,2}(\Omega, S_0) = \left\{ \mathbf{Q} \in S_0; \int_{\Omega} |\mathbf{Q}|^2 + |\nabla \mathbf{Q}|^2 dV < \infty \right\} \quad (15)$$

and \mathbf{Q}_0 is a smooth, *physically realistic* boundary condition in the sense that its scalar order parameters, (s, r) in (9), are inside the physical triangle T_{ψ} .

In the absence of external fields and surface energies, the Landau-De Gennes energy functional, I_{LG} , is given by

$$I_{LG}[\mathbf{Q}] = \int_{\Omega} f_B(\mathbf{Q}) + L|\nabla \mathbf{Q}|^2 dV. \quad (16)$$

Here f_B is the bulk energy density, $L > 0$ is a material-dependent elastic constant,

$$|\nabla \mathbf{Q}|^2 = \mathbf{Q}_{ij,k} \mathbf{Q}_{ij,k} \quad i, j, k = 1 \dots 3$$

is the elastic energy density where $\mathbf{Q}_{ij,k} = \frac{\partial \mathbf{Q}_{ij}}{\partial \mathbf{r}_k}$ denote the first partial derivatives of \mathbf{Q} .

Comment: We work with the simplest form of the elastic energy density - the one-constant elastic energy density in (16). There are more general forms of the elastic energy density, see [16, 5].

The bulk energy density f_B is a scalar function of \mathbf{Q} and it dictates the preferred liquid crystal phase - isotropic, uniaxial or biaxial. We work with the simplest form of f_B that allows for a first-order nematic-isotropic phase transition. This simplest form of f_B is a quartic polynomial in \mathbf{Q} as shown below

$$f_B(\mathbf{Q}) = \frac{a}{2} \text{tr} \mathbf{Q}^2 - \frac{b}{3} \text{tr} \mathbf{Q}^3 + \frac{c}{4} (\text{tr} \mathbf{Q}^2)^2 \text{ with} \quad (17)$$

$$\text{tr} \mathbf{Q}^2 = \mathbf{Q}_{\alpha\beta} \mathbf{Q}_{\alpha\beta}, \text{tr} \mathbf{Q}^3 = \mathbf{Q}_{\alpha\beta} \mathbf{Q}_{\beta\gamma} \mathbf{Q}_{\gamma\alpha} \quad \alpha, \beta, \gamma = 1 \dots 3. \quad (18)$$

Here $b, c > 0$ are material-dependent bulk constants, independent of the temperature, whereas the parameter a scales linearly with the absolute temperature and is given by

$$a = \alpha (T - T^*) \quad (19)$$

where $\alpha > 0$ and T^* is a characteristic liquid crystal temperature [6, 16].

The equilibrium, physically observable configurations correspond to global or local minimizers of the Landau-De Gennes energy functional, I_{LG} , subject to the imposed boundary conditions. In what follows, we first consider spatially homogeneous cases in Section 3.1 and then study global energy minimizers in spatially inhomogeneous cases in Sections 3.2 and 3.3.

3.1 The Bulk Energy Density

Our first proposition concerns the stationary points of the bulk energy density. Proposition 1 is known in the literature [9] and we give an alternative proof here for completeness.

Proposition 1. [1] *The stationary points of the bulk energy density, f_B in (17), are given by either uniaxial or isotropic \mathbf{Q} -tensors of the form*

$$\mathbf{Q} = d \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) \quad (20)$$

where d is a scalar order parameter and \mathbf{n} is one of the eigenvectors of \mathbf{Q} in (6). On comparing (20) with (8), we see that when $\mathbf{n} = \mathbf{e}_1$, the parameter $d = s$ and the scalar order parameter $r = 0$. Similarly, when $\mathbf{n} = \mathbf{e}_2$, the parameter $d = r$ and $s = 0$ whereas when $\mathbf{n} = \mathbf{e}_3$, the order parameters s, r in (8) are equal and are given by $s = r = -d$.

Proof. For a symmetric, traceless matrix \mathbf{Q} of the form (6), $\text{tr} \mathbf{Q}^n = \sum_{i=1}^3 \lambda_i^n$ subject to the tracelessness condition so that the bulk energy density f_B only depends on the eigenvalues λ_1, λ_2 and λ_3 . Then the stationary points of f_B are given by the stationary points of the function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ defined by

$$f(\lambda_1, \lambda_2, \lambda_3) = \frac{a}{2} \sum_{i=1}^3 \lambda_i^2 - \frac{b}{3} \sum_{i=1}^3 \lambda_i^3 + \frac{c}{4} \left(\sum_{i=1}^3 \lambda_i^2 \right)^2 - 2\delta \sum_{i=1}^3 \lambda_i \quad (21)$$

where we have recast f_B in terms of the eigenvalues and introduced a Lagrange multiplier δ for the tracelessness condition.

The equilibrium equations are given by a system of three algebraic equations

$$\frac{\partial f}{\partial \lambda_i} = 0 \Leftrightarrow a\lambda_i - b\lambda_i^2 + c \left(\sum_{k=1}^3 \lambda_k^2 \right) \lambda_i = 2\delta, \quad \text{for } i = 1 \dots 3, \quad (22)$$

together with the tracelessness condition $\sum_i \lambda_i = 0$. The system (22) is equivalent to

$$(\lambda_i - \lambda_j) \left[a - b(\lambda_i + \lambda_j) + c \sum_{k=1}^3 \lambda_k^2 \right] = 0 \quad 1 \leq i < j \leq 3. \quad (23)$$

Let $\{\lambda_i\}$ be a solution of the system (22) with three distinct eigenvalues $\lambda_1 \neq \lambda_2 \neq \lambda_3$. We consider equation (23) for the pairs (λ_1, λ_2) and (λ_1, λ_3) . This yields two equations

$$\begin{aligned} a - b(\lambda_1 + \lambda_2) + c \sum_{k=1}^3 \lambda_k^2 &= 0 \\ a - b(\lambda_1 + \lambda_3) + c \sum_{k=1}^3 \lambda_k^2 &= 0 \end{aligned} \quad (24)$$

from which we obtain

$$-b(\lambda_2 - \lambda_3) = 0, \quad (25)$$

contradicting our initial hypothesis $\lambda_2 \neq \lambda_3$. We, thus, conclude that a stationary point of f_B must have at least two equal eigenvalues and therefore correspond to either an uniaxial or isotropic liquid crystal state. In particular, there are no biaxial stationary points for the particular choice of f_B in (17). \square

By virtue of Proposition 1, it suffices to consider uniaxial \mathbf{Q} -tensors of the form

$$\mathbf{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) \quad \mathbf{n} \in S^2$$

whilst computing the stationary points of f_B . For such \mathbf{Q} -tensors, f_B is a quartic polynomial in the uniaxial scalar order parameter s and the stationary points are the roots of the algebraic equation given below

$$\frac{df_B}{ds} = \frac{1}{27} (18as - 6bs^2 + 12cs^3) = 0. \quad (26)$$

There are precisely three stationary points;

$$s = 0 \quad \text{and} \quad s_{\pm} = \frac{b \pm \sqrt{b^2 - 24ac}}{4c} \quad (27)$$

where

$$f_B(0) = 0 \quad \text{and} \quad f_B(s_{\pm}) = \frac{s_{\pm}^2}{54} (9a - bs_{\pm}), \quad (28)$$

and $f_B(s_-) > f_B(s_+)$. Hence, the global bulk energy minimizer is either the isotropic state $\mathbf{Q} = 0$ or the ordered nematic state

$$\mathbf{Q} = s_+ \left(\mathbf{e} \otimes \mathbf{e} - \frac{1}{3} \mathbf{I} \right) \quad (29)$$

where \mathbf{e} is the eigenvector with the largest eigenvalue.

A natural question is - for which temperature ranges does the global bulk energy minimizer lie inside the physical triangle T_ψ i.e. for which

temperature regimes does s_+ , which is the stable nematic stationary point, take values in the physical range

$$0 \leq s_+ = \frac{b + \sqrt{b^2 - 24ac}}{4c} \leq 1?$$

One can directly verify that $s_+ \in [0, 1]$ if and only if

$$\frac{1}{3}(b - 2c) \leq a \leq \frac{b^2}{24c}, \quad (30)$$

or equivalently, in terms of the absolute temperature T if and only if

$$\frac{1}{3\alpha}(b - 2c) + T^* \leq T \leq \frac{b^2}{24\alpha c} + T^*. \quad (31)$$

For the common liquid crystal material MBBA, the values of the characteristic bulk constants are given in the literature [15, 16]

$$\begin{aligned} \alpha &= 0.42 \times 10^3 J/m^3 \text{ } ^\circ C, \quad b = 0.64 \times 10^4 J/m^3, \quad c = 0.35 \times 10^4 J/m^3 \\ T^* &= 45^\circ C \quad T_c = 46^\circ C \end{aligned} \quad (32)$$

where T_c is the nematic-isotropic transition temperature. We substitute these values into (30) and (31) and find that $s_+ > 1$ for $T < 44.52^\circ C$ i.e. s_+ moves outside the physical range within a $2^\circ C$ - neighbourhood of the nematic-isotropic transition temperature.

We recall that there are three characteristic temperatures predicted by the quartic form of f_B in (17): (i) $a = 0$, below which the isotropic state loses its stability (ii) the nematic-isotropic transition temperature, $a = \alpha(T_c - T^*) = \frac{b^2}{27c}$, for which $f_B(s_+) = f_B(0)$ and (iii) $a = \frac{b^2}{24c}$ above which the ordered nematic stationary points are no longer defined in (27). We provide a pictorial representation for the stationary points of f_B for ease of comparison with T_ψ . We define the *bulk triangle*, $\Delta(T)$, to be the convex hull of the stationary points of f_B in the order-parameter (s, r) - plane. For $-\alpha T^* \leq a < -\frac{b^2}{3c}$, $\Delta(T)$ is an isosceles triangle with its vertices at the points $\{(2|s_-|, 0), (0, 2|s_-|), (-2|s_-|, -2|s_-|)\}$ whereas for $-\frac{b^2}{3c} \leq a \leq \frac{b^2}{24c}$, $\Delta(T)$ is an isosceles triangle with its vertices at the points $\{(s_+, 0), (0, s_+), (-s_+, -s_+)\}$. For $a > \frac{b^2}{24c}$, $\Delta(T)$ collapses to the origin since $s = 0$ is the unique critical point in the high-temperature regime. In Figures 2 and 3, we illustrate $\Delta(T)$ for all temperature regimes.

3.2 The One-constant Elastic Energy Density

In this section, we study global minimizers of the Landau-De Gennes energy functional, I_{LG} in (16),

$$I_{LG}[\mathbf{Q}] = \int_{\Omega} f_B(\mathbf{Q}) + L|\nabla \mathbf{Q}|^2 dV$$

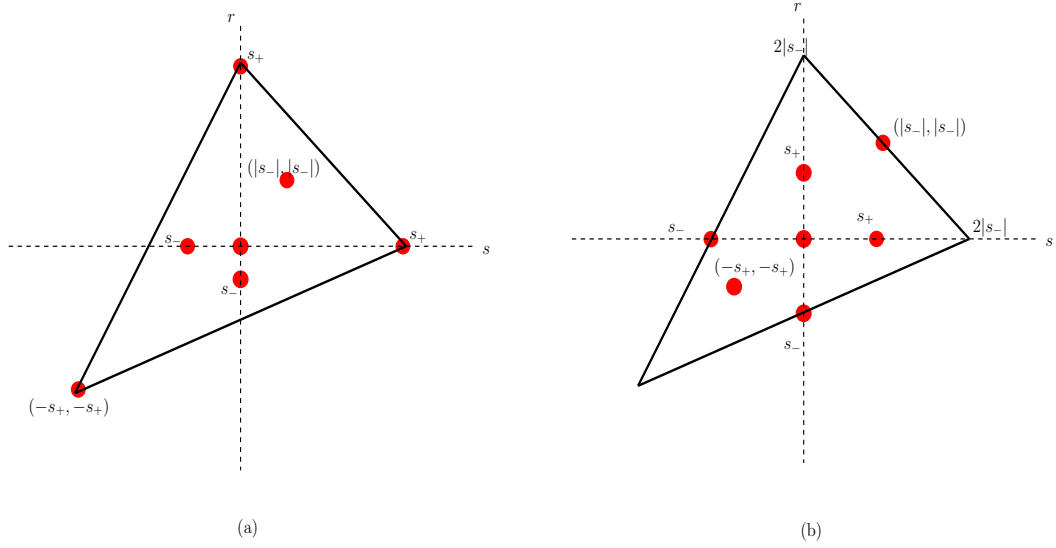


Figure 2: (a) The triangle $\triangle(T)$ for $-\frac{b^2}{3c\alpha} + T^* \leq T < T^*$. The red marked points label the stationary points of f_B in this temperature regime. (b) The triangle $\triangle(T)$ for $T < -\frac{b^2}{3c\alpha} + T^*$.

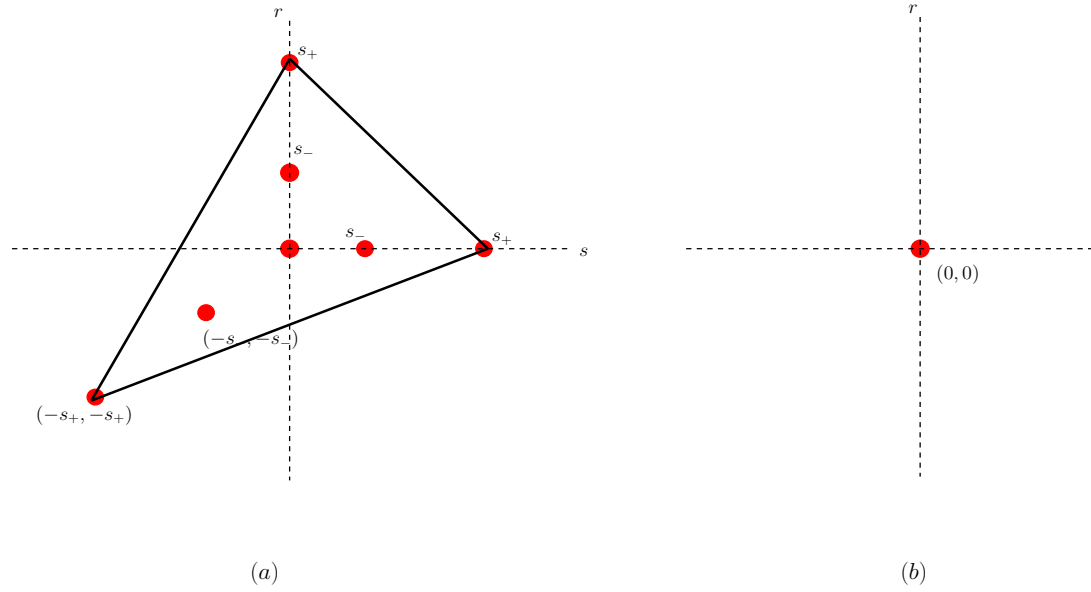


Figure 3: The triangle $\triangle(T)$ for $T^* \leq T < \frac{b^2}{24\alpha c} + T^*$. The stationary point $s_- > 0$ in this temperature regime. (b) The triangle $\triangle(T)$ shrinks to the origin for $T > \frac{b^2}{24\alpha c} + T^*$, since the isotropic state $(s, r) = (0, 0)$ is the unique stationary point in this temperature regime.

and obtain explicit bounds for the equilibrium scalar order parameters, (s, r) in (9). These bounds quantify the effect of the elastic energy density on the bulk energy minima and can also be compared to the probabilistic bounds in (7).

3.2.1 Existence and regularity of minimizers

There exists a global minimizer, \mathbf{Q}^* , of I_{LG} in the admissible class \mathcal{A} , where \mathcal{A} has been defined in (14). This is a ready consequence of the direct methods in the calculus of variations [4, 5]. Indeed, one can check that I_{LG} satisfies the following coerciveness estimate [5]

$$I_{LG}[\mathbf{Q}] \geq \alpha_c \|\mathbf{Q}\|_{W^{1,2}(\Omega)}^2 \quad (33)$$

where $\alpha_c > 0$ and the $W^{1,2}$ -norm, $\|\mathbf{Q}\|_{W^{1,2}(\Omega)}$, is given by

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

The Landau-De Gennes energy density is convex in the gradient $\nabla \mathbf{Q}$ and therefore I_{LG} is weakly lower semicontinuous [7]. The coerciveness and weak lower semicontinuity of I_{LG} guarantee that the infimum energy is actually achieved i.e. there exists a $\mathbf{Q}^* \in \mathcal{A}$ with the property

$$I_{LG}[\mathbf{Q}^*] = \inf_{\mathbf{Q} \in \mathcal{A}} I_{LG}[\mathbf{Q}]. \quad (34)$$

The global minimizer \mathbf{Q}^* is a weak solution of the corresponding Euler-Lagrange equations, which is a system of nonlinear elliptic partial differential equations as shown below -

$$2L\Delta \mathbf{Q}_{\alpha\beta} = a\mathbf{Q}_{\alpha\beta} + b \left(\frac{1}{3} \text{tr} \mathbf{Q}^2 \delta_{\alpha\beta} - \mathbf{Q}_{\alpha p} \mathbf{Q}_{p\beta} \right) + c (\mathbf{Q}_{pq})^2 \mathbf{Q}_{\alpha\beta} \quad \alpha, \beta = 1 \dots 3. \quad (35)$$

We use standard results from the theory of elliptic partial differential equations to deduce that \mathbf{Q}^* is actually a classical solution of the system (35) and \mathbf{Q}^* is smooth and analytic everywhere in Ω [10]. Given smooth boundary conditions, \mathbf{Q}^* is also smooth up to the boundary.

3.2.2 Upper bounds for the order parameters

The global minimizer \mathbf{Q}^* can be expressed in terms of a pair of eigenvectors $(\mathbf{n}^*, \mathbf{m}^*)$ and the scalar order parameters (s^*, r^*) , as in (8),

$$\mathbf{Q}^* = s^* \left(\mathbf{n}^* \otimes \mathbf{n}^* - \frac{1}{3} \mathbf{I} \right) + r^* \left(\mathbf{m}^* \otimes \mathbf{m}^* - \frac{1}{3} \mathbf{I} \right) \quad (36)$$

and

$$|\mathbf{Q}^*|^2 = \frac{2}{3} (s^{*2} + r^{*2} - s^* r^*). \quad (37)$$

We partition the (s, r) -plane into three regions: (a) $R_1 = \{(s, r) | s, r \geq 0\}$ - the top quadrant, (b) $R_2 = \{(s, r) | s \leq 0; r \geq s\}$ and (c) $R_3 = \{r \leq 0; r \leq s\}$. In R_1 , we have the inequalities

$$\frac{1}{6} (s^* + r^*)^2 \leq |\mathbf{Q}^*|^2 \leq \frac{2}{3} (s^* + r^*)^2. \quad (38)$$

Similarly, for R_2 , we have that

$$\frac{1}{6} (r^* - 2s^*)^2 \leq |\mathbf{Q}^*|^2 \leq \frac{2}{3} (r^* - 2s^*)^2 \quad (39)$$

and for R_3 ,

$$\frac{1}{6} (s^* - 2r^*)^2 \leq |\mathbf{Q}^*|^2 \leq \frac{2}{3} (s^* - 2r^*)^2. \quad (40)$$

For every $\eta > 0$, we define the bounded region $\Sigma_\eta = \{(s^*, r^*) ; |\mathbf{Q}^*| \leq \eta\}$ in the (s, r) -plane. Let T_η be the isosceles triangle in the (s, r) -plane with its vertices at the points - $\{(\eta, 0), (0, \eta), (-\eta, -\eta)\}$. Then it follows immediately from (38), (39) and (40) that

$$T_{\sqrt{\frac{3}{2}} \eta} \subset \Sigma_\eta \subset T_{\sqrt{6} \eta} \quad (41)$$

so that $T_{\sqrt{6}\eta} \subseteq T_\psi$ necessarily implies that $\Sigma_\eta \subset T_\psi$. Our first result in this section is an explicit upper bound for the norm of a global energy minimizer in the low-temperature regime $a \leq \frac{b^2}{24c}$ and as the preceding discussion shows, this upper bound allows us to define the admissible domain for the equilibrium scalar order parameters.

Theorem 1. *Let $\mathbf{Q}^* \in \mathcal{A}$ be a global minimizer for the energy functional I_{LG} , where \mathcal{A} and I_{LG} have been defined in (14) and (16) respectively. We work in the temperature regime $a \leq \frac{b^2}{24c}$ and make the following assumption about the boundary condition \mathbf{Q}_0 ,*

$$|\mathbf{Q}_0(\mathbf{r})| < \min \left\{ \frac{b + \sqrt{b^2 - 24ac}}{4\sqrt{6}c}, \frac{1}{\sqrt{6}} \right\} \quad \mathbf{r} \in \partial\Omega, \quad (42)$$

where $|\mathbf{Q}|$ has been defined in (13). The condition (42) is equivalent to requiring that the boundary order parameters are contained inside T_ψ and the bulk triangles $\triangle(T)$ defined in Section 3.1. Then \mathbf{Q}^* obeys the following global upper bound on $\bar{\Omega}$ -

$$|\mathbf{Q}^*(\mathbf{r})| \leq \frac{b + \sqrt{b^2 - 24ac}}{2\sqrt{6}c} \quad \text{for } \mathbf{r} \in \bar{\Omega}. \quad (43)$$

Proof. We assume that the contrary holds i.e. the subset $\Omega^* = \left\{ \mathbf{r} \in \Omega; |\mathbf{Q}^*(\mathbf{r})| > \frac{b+\sqrt{b^2-24ac}}{2\sqrt{6c}} \right\} \subset \Omega$ has positive measure. The subset Ω^* clearly does not intersect $\partial\Omega$ since the boundary condition \mathbf{Q}_0 obeys this upper bound from assumption (42).

We define a perturbation, $\tilde{\mathbf{Q}}$, of the global minimizer \mathbf{Q}^* as follows –

$$\tilde{\mathbf{Q}}(\mathbf{r}) = \begin{cases} \mathbf{Q}^*(\mathbf{r}), & \mathbf{r} \in \Omega \setminus \Omega^*, \\ \frac{\Gamma}{|\mathbf{Q}^*(\mathbf{r})|} \mathbf{Q}^*(\mathbf{r}), & \mathbf{r} \in \Omega^* \end{cases} \quad (44)$$

where

$$\Gamma = \frac{b + \sqrt{b^2 - 24ac}}{2\sqrt{6c}}. \quad (45)$$

We note from (27) that

$$\Gamma = \sqrt{\frac{2}{3}} s_+ \quad (46)$$

by definition. It is evident from (44) that $\tilde{\mathbf{Q}}$ agrees with \mathbf{Q}^* everywhere outside Ω^* and hence belongs to our admissible space. Moreover, $\tilde{\mathbf{Q}}$ has constant norm on the set Ω^* i.e. $|\tilde{\mathbf{Q}}(\mathbf{r})| = \Gamma$ for $\mathbf{r} \in \Omega^*$.

We obtain an upper bound for the free energy difference

$$I_{LG}[\tilde{\mathbf{Q}}] - I_{LG}[\mathbf{Q}^*] = \int_{\Omega^*} f_B(\tilde{\mathbf{Q}}) + L|\nabla\tilde{\mathbf{Q}}|^2 - (f_B(\mathbf{Q}^*) + L|\nabla\mathbf{Q}^*|^2) dV \quad (47)$$

where f_B is as in (17).

We can explicitly compute $|\nabla\tilde{\mathbf{Q}}|^2$ as shown below ,

$$|\nabla\tilde{\mathbf{Q}}(\mathbf{r})|^2 = \left(\frac{\Gamma}{|\mathbf{Q}^*(\mathbf{r})|} \right)^2 \left(|\nabla\mathbf{Q}^*|^2 - \frac{1}{|\mathbf{Q}^*|^2} (\mathbf{Q}_{pq}^* \mathbf{Q}_{pq,k}^*) (\mathbf{Q}_{ij,k}^* \mathbf{Q}_{ij,k}^*) \right) \leq |\nabla\mathbf{Q}^*(\mathbf{r})|^2 \quad (48)$$

since $\left(\frac{\Gamma}{|\mathbf{Q}^*(\mathbf{r})|} \right)^2 < 1$ on Ω^* by definition.

Consider the function $G : [0, \infty) \rightarrow \mathbb{R}$ defined by

$$G(u) = -u^2 \left(\frac{a}{2} - \frac{b}{3\sqrt{6}}u + \frac{c}{4}u^2 \right). \quad (49)$$

We estimate the bulk energy density difference in terms of the function G as follows

$$\begin{aligned} f_B(\tilde{\mathbf{Q}}) - f_B(\mathbf{Q}^*) &= \frac{a}{2} \text{tr}\tilde{\mathbf{Q}}^2 - \frac{b}{3} \text{tr}\tilde{\mathbf{Q}}^3 + \frac{c}{4} (\text{tr}\tilde{\mathbf{Q}}^2)^2 - \left(\frac{a}{2} \text{tr}\mathbf{Q}^{*2} - \frac{b}{3} \text{tr}\mathbf{Q}^{*3} + \frac{c}{4} (\text{tr}\mathbf{Q}^{*2})^2 \right) = \\ &= \frac{a}{2} (\Gamma^2 - |\mathbf{Q}^*|^2) - \frac{b}{3} \frac{\text{tr}\mathbf{Q}^{*3}}{|\mathbf{Q}^*|^3} (\Gamma^3 - |\mathbf{Q}^*|^3) + \frac{c}{4} (\Gamma^4 - |\mathbf{Q}^*|^4) \leq G(|\mathbf{Q}^*|) - G(\Gamma). \end{aligned} \quad (50)$$

In the last step of (50), we use the equality

$$\text{tr} \tilde{\mathbf{Q}}^3 = \Gamma^3 \frac{\text{tr} \mathbf{Q}^{*3}}{|\mathbf{Q}^*|^3},$$

$(\Gamma^3 - |\mathbf{Q}^*|^3) < 0$ on Ω^* and the inequality

$$\frac{\text{tr} \mathbf{Q}^{*3}}{|\mathbf{Q}^*|^3} \leq \frac{1}{\sqrt{6}}, \quad (51)$$

from Lemma 1. One can readily verify that $G(u)$ attains a local maximum for $u = \Gamma$ and $G'(u) < 0$ for all $u > \Gamma$. Therefore,

$$G(|\mathbf{Q}^*|) - G(\Gamma) < 0, \quad (52)$$

since $|\mathbf{Q}^*| > \Gamma$ on Ω^* by definition.

We substitute (48), (50) and (52) into (47) to obtain

$$I_{LG}[\tilde{\mathbf{Q}}] - I_{LG}[\mathbf{Q}^*] < 0, \quad (53)$$

contradicting the absolute energy minimality of \mathbf{Q}^* . We thus conclude that Ω^* is empty and

$$|\mathbf{Q}^*(\mathbf{r})| \leq \Gamma = \frac{b + \sqrt{b^2 - 24ac}}{2\sqrt{6}c} \quad (54)$$

for all points $\mathbf{r} \in \bar{\Omega}$. \square

Lemma 1. Let $\beta(\mathbf{Q})$ be defined as follows -

$$\beta(\mathbf{Q}) = 1 - 6 \frac{(\text{tr} \mathbf{Q}^3)^2}{(\text{tr} \mathbf{Q}^2)^3} \quad \mathbf{Q} \in S_0. \quad (55)$$

Then $0 \leq \beta(\mathbf{Q}) \leq 1$.

Proof. The quantity $\beta(\mathbf{Q})$ is known as the biaxiality parameter in the liquid crystal literature and it is well-known that $\beta(\mathbf{Q}) \in [0, 1]$ [15]. We present a simple proof here for completeness.

Since $6 \frac{(\text{tr} \mathbf{Q}^3)^2}{(\text{tr} \mathbf{Q}^2)^3} \geq 0$, the inequality $\beta(\mathbf{Q}) \leq 1$ is trivial. To show $\beta(\mathbf{Q}) \geq 0$, we use the representation (8) to express $\text{tr} \mathbf{Q}^3$ and $\text{tr} \mathbf{Q}^2$ in terms of the order parameters s and r .

$$\begin{aligned} \text{tr} \mathbf{Q}^3 &= \frac{1}{9} (2s^3 + 2r^3 - 3s^2r - 3sr^2) \\ \text{tr} \mathbf{Q}^2 &= \frac{2}{3} (s^2 + r^2 - sr) \end{aligned} \quad (56)$$

A straightforward calculation shows that

$$(\text{tr} \mathbf{Q}^3)^2 = \frac{1}{81} (4s^6 + 4r^6 - 12s^5r - 12sr^5 + 26s^3r^3 - 3s^4r^2 - 3s^2r^4)$$

and

$$(\text{tr} \mathbf{Q}^2)^3 = \frac{8}{27} (s^6 + r^6 - 3s^5r - 3sr^5 - 7s^3r^3 + 6s^2r^4 + 6s^4r^2).$$

One can then directly verify that

$$(\text{tr} \mathbf{Q}^2)^3 - 6 (\text{tr} \mathbf{Q}^3)^2 = 2s^2r^2 (s - r)^2 \geq 0 \quad (57)$$

as required. \square

As a further illustration, let us assume that there exists an uniaxial global energy minimizer in the admissible space, \mathcal{A} in (14), where the boundary condition \mathbf{Q}_0 is of the form

$$\mathbf{Q}_0 = s_0 \left(\mathbf{n}_0 \otimes \mathbf{n}_0 - \frac{1}{3} \mathbf{I} \right), \quad \mathbf{n}_0 : \partial\Omega \rightarrow S^2 \quad (58)$$

and $0 < s_0 < \min \{s_+, 1\}$ is a positive constant. Then we have

Lemma 2. *Let \mathbf{Q}_u be an uniaxial global minimizer of I_{LG} in the admissible space \mathcal{A} , with a smooth, uniaxial and physically realistic boundary condition \mathbf{Q}_0 , as in (58). Then \mathbf{Q}_u is necessarily of the form*

$$\mathbf{Q}_u = s_u \left(\mathbf{n}_u \otimes \mathbf{n}_u - \frac{1}{3} \mathbf{I} \right) \quad (59)$$

for some function $s_u : \bar{\Omega} \rightarrow \mathbb{R}$ and unit-vector field $\mathbf{n}_u : \bar{\Omega} \rightarrow S^2$. The equilibrium scalar order parameter is non-negative everywhere and obeys the following inequalities

$$0 \leq s_u(\mathbf{r}) \leq s_+ \quad \mathbf{r} \in \bar{\Omega}. \quad (60)$$

Proof. We prove Lemma 2 by contradiction. Let $\Omega^* = \{\mathbf{r} \in \Omega; s_u(\mathbf{r}) < 0\}$ be a measurable interior subset of Ω . The subset Ω^* does not intersect $\partial\Omega$ by virtue of our choice of \mathbf{Q}_0 in (58). Consider the perturbation

$$\tilde{\mathbf{Q}}_u(\mathbf{r}) = \begin{cases} \mathbf{Q}_u(\mathbf{r}), & \mathbf{r} \in \Omega \setminus \Omega^*, \\ -\mathbf{Q}_u, & \mathbf{r} \in \Omega^*. \end{cases} \quad (61)$$

Then $\tilde{\mathbf{Q}}_u \in \mathcal{A}$ and $\tilde{\mathbf{Q}}_u$ coincides with \mathbf{Q}_u everywhere outside Ω^* . We explicitly estimate the free energy difference, $I_{LG}[\tilde{\mathbf{Q}}_u] - I_{LG}[\mathbf{Q}_u]$, as shown below

$$\begin{aligned} I_{LG}[\tilde{\mathbf{Q}}_u] - I_{LG}[\mathbf{Q}_u] &= \int_{\Omega^*} f_B(\tilde{\mathbf{Q}}_u) + L|\nabla \tilde{\mathbf{Q}}_u|^2 - (f_B(\mathbf{Q}_u) + L|\nabla \mathbf{Q}_u|^2) dV = \\ &= \int_{\Omega^*} \frac{2b}{3} \text{tr} \mathbf{Q}_u^3 dV = \int_{\Omega^*} \frac{4b}{27} s_u^3 dV < 0 \end{aligned} \quad (62)$$

since $\text{tr} \mathbf{Q}_u^3 = \frac{2}{9} s_u^3$, $s_u < 0$ on Ω^* by assumption and $b > 0$. This contradicts the absolute energy minimality of \mathbf{Q}_u . Hence, Ω^* is empty and $s_u \geq 0$ everywhere in Ω .

The upper bound in (60) follows directly from (43) i.e.

$$|\mathbf{Q}_u| = \sqrt{\frac{2}{3}} |s_u| \leq \sqrt{\frac{2}{3}} s_+ \quad (63)$$

and since $s_u \geq 0$, we have that $0 \leq s_u \leq s_+$ from (63). Lemma 2 now follows. \square

Remark: We are not guaranteed the existence of a uniaxial global energy minimizer in our admissible space. We assume the existence of \mathbf{Q}_u in Lemma 2. A more technically precise formulation of the problem would be to minimize I_{LG} in the restricted class of uniaxial \mathbf{Q} -tensors

$$\mathcal{A}_u = \left\{ \mathbf{Q} \in W^{1,2}(\Omega; S_0); \mathbf{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) \text{ a.e. in } \Omega \right\}$$

where s is a real-valued function and \mathbf{n} is a unit-vector field, subject to uniaxial boundary conditions. In this case, one can prove the existence of a uniaxial global minimizer \mathbf{Q}_u in the restricted class \mathcal{A}_u and the statement of Lemma 2 still holds. However, the proof is technically more involved and we omit the details for brevity.

Given the explicit upper bound Γ in (43) for the norm of a global energy minimizer, the corresponding equilibrium scalar order parameters are confined to the bounded region $\Sigma_\Gamma = \{(s, r); |\mathbf{Q}^*| \leq \Gamma\}$ in the (s, r) -plane. We define the elastic triangle $\triangle_{el}(T)$ to be the triangle $T_{\sqrt{6}\Gamma}$, where $T_{\sqrt{\frac{3}{2}}\Gamma} \subset \Sigma_\Gamma \subset T_{\sqrt{6}\Gamma}$ in (41). The elastic triangle can be explicitly specified in terms of the temperature and the material-dependent bulk constants. One can directly verify that $\Sigma_\Gamma \subset \triangle_{el}(T) \subseteq T_\psi$ if and only if

$$\frac{b-c}{6\alpha} + T^* \leq T \leq \frac{b^2}{24\alpha c} + T^*. \quad (64)$$

and $\Sigma_\Gamma \supset T_{\sqrt{\frac{3}{2}}\Gamma} \supseteq T_\psi$ if and only if

$$T \leq \frac{1}{3\alpha} (b - 2c) + T^*. \quad (65)$$

In other words, for temperatures $T \in [0, \frac{1}{3\alpha} (b - 2c) + T^*)$, the equilibrium order parameters may move outside the physical triangle. For the liquid crystal material MBBA, $\Sigma_\Gamma \supset T_\psi$ for $T < 44.52^\circ\text{C}$ i.e. the Landau-De Gennes predictions fail to be consistent with the probabilistic second-moment definition of \mathbf{Q} within a 2°C -neighbourhood of the nematic-isotropic transition temperature.

3.3 Maximum principle approach

In this section, we carry out a parallel analysis in the high-temperature regime $a > \frac{b^2}{24c}$ and extend our analysis to more general Landau-De Gennes energy functionals, where f_B is a general even polynomial in the \mathbf{Q} -tensor components.

Theorem 2. *Let \mathbf{Q}^* be a global minimizer of I_{LG} in the admissible class \mathcal{A} , where I_{LG} and \mathcal{A} have been defined in (16) and (14) respectively, in the temperature regime $a > \frac{b^2}{24c}$. Then the function $|\mathbf{Q}^*| : \bar{\Omega} \rightarrow \mathbb{R}$ attains its maximum on the domain boundary. In particular, if the boundary condition \mathbf{Q}_0 satisfies*

$$|\mathbf{Q}_0(\mathbf{r})| < \frac{1}{\sqrt{6}} \quad \mathbf{r} \in \partial\Omega, \quad (66)$$

then the scalar order parameters of \mathbf{Q}^ are contained inside T_ψ , for this high-temperature regime.*

Proof. The proof proceeds by contradiction. We work in the temperature regime $a > \frac{b^2}{24c}$ and assume that the function $|\mathbf{Q}^*| : \bar{\Omega} \rightarrow \mathbb{R}$ attains a strict maximum at an interior point $\mathbf{r}^* \in \Omega$, where $|\mathbf{Q}^*(\mathbf{r}^*)| > 0$.

The global minimizer \mathbf{Q}^* is a classical smooth solution of the Euler-Lagrange equations

$$2L\Delta\mathbf{Q}_{\alpha\beta} = a\mathbf{Q}_{\alpha\beta} + b\left(\frac{1}{3}\text{tr}\mathbf{Q}^2\delta_{\alpha\beta} - \mathbf{Q}_{\alpha p}\mathbf{Q}_{p\beta}\right) + c(\mathbf{Q}_{pq})^2\mathbf{Q}_{\alpha\beta} \quad L > 0, \alpha, \beta = 1 \dots 3. \quad (67)$$

Therefore, the function $|\mathbf{Q}^*|^2 : \bar{\Omega} \rightarrow \mathbb{R}$ is also a smooth function and we necessarily have that

$$\Delta|\mathbf{Q}^*|^2 \leq 0 \quad \text{at } \mathbf{r}^* \in \Omega, \quad (68)$$

according to our hypothesis [7]. We compute $\Delta|\mathbf{Q}^*|^2$ at this interior maximum point. One can readily show that

$$L\Delta|\mathbf{Q}^*|^2 = 2L(|\nabla\mathbf{Q}^*|^2 + \mathbf{Q}_{ij}^*\mathbf{Q}_{ij,kk}^*). \quad (69)$$

We substitute the Euler-Lagrange equations (67) into (69) to obtain the following

$$\begin{aligned} L\Delta|\mathbf{Q}^*|^2 &= 2L|\nabla\mathbf{Q}^*|^2 + \left(a|\mathbf{Q}^*|^2 - b\text{tr}(\mathbf{Q}^*)^3 + c|\mathbf{Q}^*|^4\right) + \frac{b}{3}(\text{tr}\mathbf{Q}^{*2})\mathbf{Q}_{ii}^* \\ &= 2L|\nabla\mathbf{Q}^*|^2 + a\text{tr}\mathbf{Q}^{*2} - b\text{tr}\mathbf{Q}^{*3} + c(\text{tr}\mathbf{Q}^{*2})^2, \end{aligned} \quad (70)$$

since $\mathbf{Q}_{ii}^* = 0$.

Consider the function $G : S_0 \rightarrow \mathbb{R}$ defined by

$$G(\mathbf{Q}) = a\text{tr}\mathbf{Q}^2 - b\text{tr}\mathbf{Q}^3 + c(\text{tr}\mathbf{Q}^2)^2. \quad (71)$$

Then G is bounded from below by

$$G(\mathbf{Q}) \geq h(|\mathbf{Q}|) = a|\mathbf{Q}|^2 - \frac{b}{\sqrt{6}}|\mathbf{Q}|^3 + c|\mathbf{Q}|^4$$

from Lemma 1. The function $h : \bar{\Omega} \rightarrow \mathbb{R}$ has its global minimum at the isotropic state, $\mathbf{Q} = 0$, and

$$h(|\mathbf{Q}|) > 0 \quad \mathbf{Q} \neq 0$$

in the temperature regime $a > \frac{b^2}{24c}$. This implies that

$$G(\mathbf{Q}^*) > 0 \quad \text{at } \mathbf{r}^* \in \Omega$$

and consequently $\Delta|\mathbf{Q}^*|^2(\mathbf{r}^*) > 0$ from (70). This contradicts our hypothesis and Theorem 2 now follows.

In particular, if the boundary condition \mathbf{Q}_0 satisfies the hypothesis (66), then the global energy minimizer \mathbf{Q}^* satisfies the inequality

$$|\mathbf{Q}^*(\mathbf{r})| < \frac{1}{\sqrt{6}} \quad (72)$$

on $\bar{\Omega}$. From (41), this is sufficient to ensure that \mathbf{Q}^* is physically realistic, in the sense that its scalar order parameters do not take values outside T_ψ . \square

Theorem 2 shows that in the high temperature regime $a > \frac{b^2}{24c}$, the norm of a global energy minimizer attains its maximum on the boundary. The isotropic state $\mathbf{Q} = 0$ is the global minimizer of the bulk energy density, f_B , in this high-temperature regime and it is not surprising that we observe a dissipation of order in the interior. However, it is interesting that there are no local fluctuations in the interior i.e. there are no interior regions where $|\mathbf{Q}^*|$ experiences a local increase compared to the boundary norm - $\max_{\mathbf{r} \in \partial\Omega} |\mathbf{Q}_0(\mathbf{r})|$. Therefore, Theorem 2 suggests a monotonic decrease in order as we move away from the boundary and it would be interesting to analytically estimate the characteristic length scale of order decay for this problem.

Our methods readily extend to a more general bulk energy density, $f_{B,n}$, which is a polynomial of even degree ' n ' in the \mathbf{Q} -tensor invariants i.e. $\text{tr}\mathbf{Q}^2$ and $\text{tr}\mathbf{Q}^3$ [16] with $n \geq 4$ (since $f_{B,n}$ has to be minimally quartic to allow a first-order nematic-isotropic phase transition). We take $f_{B,n}$ to be

$$f_{B,n} = a_2(T)\text{tr}\mathbf{Q}^2 - a_3\text{tr}\mathbf{Q}^3 + a_4(\text{tr}\mathbf{Q}^2)^2 + \dots + \sum_{m,p \in \mathbb{Z}^+; 2m+3p=n} a_{m,p} (\text{tr}\mathbf{Q}^2)^m (\text{tr}\mathbf{Q}^3)^p \quad (73)$$

where \mathbb{Z}^+ denotes the set of non-negative integers, $a_3, a_4 > 0$ and

$$a_{\frac{n}{2},0} > \sum_{m,p \in \mathbb{Z}^+; p \geq 1; 2m+3p=n} |a_{m,p}|. \quad (74)$$

The first coefficient $a_2(T)$ has a linear dependence on the absolute temperature by analogy with (19) whereas the remaining coefficients $\{a_3, a_4, \dots, \{a_{m,p}\}\}$ are taken to be temperature-independent, material-dependent bulk constants.

We define the corresponding Landau-De Gennes energy functional to be

$$I_n[\mathbf{Q}] = \int_{\Omega} f_{B,n}(\mathbf{Q}) + L|\nabla \mathbf{Q}|^2 dV \quad (75)$$

and our admissible space is

$$\mathcal{A}_n = \{\mathbf{Q} \in W^{1,n}(\Omega; S_0); \mathbf{Q} = \mathbf{Q}_0 \text{ on } \partial\Omega\} \quad (76)$$

where the Sobolev space $W^{1,n}$ is defined to be [7]

$$W^{1,n}(\Omega; S_0) = \left\{ \mathbf{Q} \in S_0; \int_{\Omega} |\mathbf{Q}|^n + |\nabla \mathbf{Q}|^n dV < \infty \right\} \quad (77)$$

and \mathbf{Q}_0 is a smooth, physically realistic boundary condition in the sense of (66). We have the following result by analogy with Theorem 1.

Proposition 2. *Let \mathbf{Q}^* be a global minimizer of I_n in the admissible space \mathcal{A}_n . Then*

$$|\mathbf{Q}^*| \leq \max \left\{ C(a_2, a_3, a_4, \dots, \{a_{m,p}\}), \max_{\mathbf{r} \in \partial\Omega} |\mathbf{Q}_0| \right\} \quad \text{on } \bar{\Omega} \quad (78)$$

where C is a positive constant that only depends on the absolute temperature and the bulk coefficients and is independent of the elastic constant L in (75).

Proof. The existence of a global energy minimizer, \mathbf{Q}^* , for I_n in the space \mathcal{A}_n , follows from the direct methods in the calculus of variations and we can use standard results in elliptic regularity to deduce that \mathbf{Q}^* is smooth everywhere in Ω . Consider the function $|\mathbf{Q}^*|^2 : \Omega \rightarrow \mathbb{R}^+$ and assume that it attains its maximum at the interior point $\mathbf{r}^* \in \Omega$.

The global minimizer \mathbf{Q}^* is a classical solution of the Euler-Lagrange equations

$$2L\mathbf{Q}_{ij,kk} = \frac{\partial f_{B,n}}{\partial \mathbf{Q}_{ij}} - \frac{1}{3} \frac{\partial f_{B,n}}{\partial \mathbf{Q}_{kk}} \delta_{ij} \quad (79)$$

where the second term is a Lagrange multiplier accounting for tracelessness. We multiply both sides of (79) by \mathbf{Q}_{ij} and use $\Delta|\mathbf{Q}|^2 = 2(|\nabla \mathbf{Q}|^2 + \mathbf{Q}_{ij}\mathbf{Q}_{ij,kk})$ to get

$$L\Delta|\mathbf{Q}|^2 = \mathbf{Q}_{ij} \frac{\partial f_{B,n}}{\partial \mathbf{Q}_{ij}} + 2L|\nabla \mathbf{Q}|^2. \quad (80)$$

Then

$$\Delta|\mathbf{Q}^*|^2 \leq 0 \text{ at } \mathbf{r}^* \in \Omega \quad (81)$$

from our hypothesis.

We note that $\mathbf{Q}_{ij} \frac{\partial f_{B,n}}{\partial \mathbf{Q}_{ij}}$ is a polynomial of degree ' n' ' in \mathbf{Q} and from Lemma 1 and (74), we have that

$$\mathbf{Q}_{ij} \frac{\partial f_{B,n}}{\partial \mathbf{Q}_{ij}} \geq K(|\mathbf{Q}|)$$

where

$$K(|\mathbf{Q}|) = a_2 |\mathbf{Q}|^2 - \frac{a_3}{\sqrt{6}} |\mathbf{Q}|^3 + \dots + \left(a_{\frac{n}{2},0} - \sum_{m,p \in \mathbb{Z}^+; p \geq 1; 2m+3p=n} |a_{m,p}| \right) |\mathbf{Q}|^n. \quad (82)$$

The function $K : \Omega \rightarrow \mathbb{R}$ is a polynomial of degree ' n' ', has ' n' ' zeros $\{|\mathbf{Q}_1|, |\mathbf{Q}_n|, \dots, |\mathbf{Q}_n|\}$ where $|\mathbf{Q}_1| \leq |\mathbf{Q}_2| \leq \dots \leq |\mathbf{Q}_n|$ and K is a monotonically increasing function of $|\mathbf{Q}|$ for $|\mathbf{Q}| > |\mathbf{Q}_n|$.

If $|\mathbf{Q}^*(\mathbf{r}^*)| > |\mathbf{Q}_n|$, then we necessarily have that $\Delta |\mathbf{Q}^*|^2 > 0$ at \mathbf{r}^* (from (80)), contradicting the hypothesis (81). We, thus, conclude that

$$|\mathbf{Q}^*| \leq |\mathbf{Q}_n| \quad \text{on } \Omega \quad (83)$$

where $|\mathbf{Q}_n| = C(a_2, a_3, a_4, \dots, \{a_{m,p}\})$ can be explicitly expressed in terms of the bulk coefficients. Proposition 2 now follows from combining (83) and the maximum norm of \mathbf{Q}_0 on the boundary. \square

The explicit upper bound (78) allows us to define the admissible domain for the equilibrium scalar order parameters as in Section 3.2. For certain choices of the bulk coefficients, this domain is larger than T_ψ and consequently, the equilibrium scalar order parameters may take values outside the physical triangle.

4 Discussion

We have studied qualitative properties of global minimizers of the Landau-De Gennes energy functional, I_{LG} , in smooth three-dimensional geometries with Dirichlet boundary conditions. We have obtained an explicit upper bound for the norm of a global energy minimizer in terms of the temperature and material-dependent bulk constants, independent of the elastic constant. In particular, we have defined two triangles in the order-parameter, (s, r) -plane: (a) the bulk triangle $\Delta(T)$ which accounts for the stationary points of f_B (b) the elastic triangle $\Delta_{el}(T)$ which accounts for the effects of the elastic energy density and $\Delta(T) \subset \Delta_{el}(T)$. The equilibrium scalar order parameters take values inside or on the boundary of $\Delta_{el}(T)$ and the distance $D(T)$ between $\Delta_{el}(T)$ and $\Delta(T)$ scales as

$$D(T) \leq s_+ = \frac{b + \sqrt{b^2 - 24ac}}{4c}. \quad (84)$$

This, in effect, quantifies the effect of elastic perturbations on the bulk energy minimizers. Secondly, this explicit bound is also compared to the probabilistic bounds in (7) and we find that the equilibrium scalar order parameters may move outside the physical triangle T_ψ and take physically unrealistic values larger than unity, in the low-temperature regime. For the liquid crystal material MBBA, the Landau-De Gennes predictions fail to be physically realistic within a 2°C -neighbourhood of the nematic-isotropic transition temperature.

A natural question is - how can we reconcile the differences between the Landau-De Gennes predictions and the probabilistic second-moment definition of \mathbf{Q} in the low-temperature regime? The Landau-De Gennes bulk energy density, f_B , has no term that enforces the probabilistic bounds in (7) or penalizes configurations that lie outside T_ψ . A first-step in this direction is to use a Ginzburg-Landau approach [3]. We define a modified Landau-De Gennes energy functional, F_ϵ , as shown below

$$F_\epsilon[\mathbf{Q}] = \int_{\Omega} f_B(\mathbf{Q}) + f_\epsilon(|\mathbf{Q}|) + L|\nabla\mathbf{Q}|^2 dV \quad (85)$$

where

$$f_\epsilon(|\mathbf{Q}|) = \begin{cases} 0, & |\mathbf{Q}| \leq \frac{1}{\sqrt{6}}, \\ \frac{1}{\epsilon^2} (|\mathbf{Q}|^2 - \frac{1}{6})^2, & |\mathbf{Q}| > \frac{1}{\sqrt{6}}, \end{cases} \quad (86)$$

f_B is as in (17) and $\epsilon > 0$ is a small positive parameter. We can obtain an explicit upper bound for the norm of a global energy minimizer using a maximum principle approach as shown below.

Proposition 3. *Let \mathbf{Q}^* be a global minimizer of F_ϵ in the admissible space \mathcal{A} in (14). Then*

$$|\mathbf{Q}^*| \leq \max \left\{ \frac{1}{\sqrt{6}}, \frac{b\epsilon^2}{\sqrt{6}(8+2\epsilon^2c)} + \frac{\sqrt{64+16\epsilon^2(c-6a)+\epsilon^4(b^2-24ac)}}{\sqrt{6}(8+2\epsilon^2c)}, \max_{\mathbf{r} \in \partial\Omega} |\mathbf{Q}_0| \right\} \quad \text{on } \bar{\Omega} \quad (87)$$

where a, b, c are the bulk constants in f_B in (17).

Proof. The existence of a global energy minimizer \mathbf{Q}^* follows from the direct methods in the calculus of variations and we use standard arguments in elliptic regularity to deduce that \mathbf{Q}^* is smooth everywhere in Ω , up to the boundary. Then $|\mathbf{Q}^*|^2 : \Omega \rightarrow \mathbb{R}^+$ is a smooth function and we assume that it attains its maximum at an interior point $\mathbf{r}^* \in \Omega$ and $|\mathbf{Q}^*(\mathbf{r}^*)| > \frac{1}{\sqrt{6}}$ (i.e. $f_\epsilon \neq 0$ at \mathbf{r}^* from (86)). It follows that

$$\Delta|\mathbf{Q}^*|^2 \leq 0 \quad \text{at } \mathbf{r}^* \in \Omega.$$

The global minimizer \mathbf{Q}^* is a classical solution of the Euler-Lagrange equations

$$2L\Delta\mathbf{Q}_{\alpha\beta} = a\mathbf{Q}_{\alpha\beta} + b\left(\frac{1}{3}\text{tr}\mathbf{Q}^2\delta_{\alpha\beta} - \mathbf{Q}_{\alpha p}\mathbf{Q}_{p\beta}\right) + c(\mathbf{Q}_{pq})^2\mathbf{Q}_{\alpha\beta} + \frac{4\mathbf{Q}_{\alpha\beta}}{\epsilon^2}\left(|\mathbf{Q}|^2 - \frac{1}{6}\right). \quad (88)$$

Repeating the same arguments as in the proof of Theorem 2, we have the following inequality

$$L\Delta|\mathbf{Q}|^2 \geq M(|\mathbf{Q}|) = a|\mathbf{Q}|^2 - \frac{b}{\sqrt{6}}|\mathbf{Q}|^3 + c|\mathbf{Q}|^4 + \frac{4|\mathbf{Q}|^2}{\epsilon^2}\left(|\mathbf{Q}|^2 - \frac{1}{6}\right).$$

We study the function $M : \Omega \rightarrow \mathbb{R}$ above. This function has precisely three zeros:

$$\begin{aligned} |\mathbf{Q}| &= 0 \\ |\mathbf{Q}| &= \frac{b\epsilon^2}{\sqrt{6}(8+2\epsilon^2c)} \pm \frac{\sqrt{64+16\epsilon^2(c-6a)+\epsilon^4(b^2-24ac)}}{\sqrt{6}(8+2\epsilon^2c)} \end{aligned} \quad (89)$$

and $M(|\mathbf{Q}|) > 0$ for $|\mathbf{Q}| > \frac{b\epsilon^2}{\sqrt{6}(8+2\epsilon^2c)} + \frac{\sqrt{64+16\epsilon^2(c-6a)+\epsilon^4(b^2-24ac)}}{\sqrt{6}(8+2\epsilon^2c)}$. Therefore, we must have

$$|\mathbf{Q}^*(\mathbf{r}^*)| \leq \frac{b\epsilon^2}{\sqrt{6}(8+2\epsilon^2c)} + \frac{\sqrt{64+16\epsilon^2(c-6a)+\epsilon^4(b^2-24ac)}}{\sqrt{6}(8+2\epsilon^2c)}$$

in order to have $\Delta|\mathbf{Q}^*|^2 \leq 0$ at $\mathbf{r}^* \in \Omega$.

We, thus, conclude that

$$|\mathbf{Q}^*| \leq \max \left\{ \frac{1}{\sqrt{6}}, \frac{b\epsilon^2}{\sqrt{6}(8+2\epsilon^2c)} + \frac{\sqrt{64+16\epsilon^2(c-6a)+\epsilon^4(b^2-24ac)}}{\sqrt{6}(8+2\epsilon^2c)}, \max_{\mathbf{r} \in \partial\Omega} |\mathbf{Q}_0| \right\} \quad \text{on } \bar{\Omega} \quad (90)$$

where the second term accounts for the maximum of $|\mathbf{Q}_0|$ on $\partial\Omega$. \square

In the limit $\epsilon \rightarrow 0$ and for a physically realistic boundary condition \mathbf{Q}_0 satisfying (66), the upper bound (87) reduces to

$$|\mathbf{Q}^*| \leq \frac{1}{\sqrt{6}} + O(\epsilon) \quad \text{on } \bar{\Omega} \quad (91)$$

and consequently, the equilibrium scalar order parameters take values within T_ψ for all temperature regimes. Further, one can show that the stationary points of the modified bulk energy density

$$f_{B,\epsilon}(\mathbf{Q}) = f_B(\mathbf{Q}) + f_\epsilon(|\mathbf{Q}|)$$

are either isotropic or uniaxial \mathbf{Q} -tensors as in Proposition 1 and $f_{B,\epsilon}$ also predicts a first-order nematic-isotropic phase transition. Therefore, the modified Landau-De Gennes energy functional F_ϵ reproduces all the qualitative

features of I_{LG} in (16), whilst respecting the probabilistic bounds (7) in the limit $\epsilon \rightarrow 0^+$, for all temperature regimes.

However, the Ginzburg-Landau approach in (85) does not contain any information about the probabilistic second-moment definition of \mathbf{Q} in (3). A more systematic approach is given in [11] where they define a modified bulk energy density Ψ_B from the Maier-Saupe free energy I_{MS} in (11).

$$\Psi_B(\mathbf{Q}) = \inf_{\psi \in \mathcal{A}_{\mathbf{Q}}} \int_{S^2} \psi(\mathbf{p}) \log \psi(\mathbf{p}) \, d\mathbf{p} - \frac{1}{2} U(T) |\mathbf{Q}|^2 \quad (92)$$

where

$$\mathcal{A}_{\mathbf{Q}} = \left\{ \psi \in L^1(S^2; \mathbb{R}^+); \, \mathbf{Q} = \int_{S^2} \left(\mathbf{p} \otimes \mathbf{p} - \frac{1}{3} \mathbf{I} \right) \psi(\mathbf{p}) \, d\mathbf{p} \right\} \quad (93)$$

is the space of all probability distribution functions ψ that have a fixed normalized second moment \mathbf{Q} , as in (3)¹.

The first term in (92) is the entropy contribution, where we minimize the integral over all probability distribution functions that have a fixed second moment \mathbf{Q} . This term diverges whenever the probabilistic bounds in (7) are violated and enforces the equilibrium scalar order parameters to lie strictly inside T_ψ . The second term in (92) is simply the Maier-Saupe interaction energy. The uniaxial case is treated in [11]. We plan to study the biaxial case and include spatial inhomogeneities into this model. This will be reported in future work [2].

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¹ $\psi \in L^1(S^2; \mathbb{R}^+)$ simply means that $\int_{S^2} \psi(\mathbf{p}) \, d\mathbf{p}$ is well-defined

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