Ericksen's type inequalities for constrained Q-tensor models of nematic liquid crystals

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Abstract

This paper considers the four-elastic-constant Landau–de Gennes free-energy which characterizes nematic liquid crystal configurations in the framework of **Q**-tensor theory. The density for the Landau–de Gennes energy functional involves the tensor order parameter **Q** and its spatial detivatives. The order parameter **Q** takes values into the set of 3×3 real symmetric traceless matrices, the **Q**-tensors. The purpose of this review paper is to give an account of the general conditions on the elastic constants which guarantee the coercivity of the free-energy density, and hence the internal consistency of the theory, in the constrained (hard) and soft Landau–de Gennes regimes. This generalizes the well-known Ericksen inequalities among the elastic constants in the classical Oseen–Frank expansion of the free-energy density. We start by recalling some background material about the **Q**-tensor theory of nematic liquid crystals and describing the related order parameter spaces. Next, we consider the constrained (hard) theory of uniaxial and biaxial nematic liquid crystals. We describe the geometric features of the corresponding **Q**-tensor models, providing the Cartesian expression of the elastic invariants, and discuss coercivity conditions and existence results of the minima for the free-energy. We then address the soft theory of biaxial nematics, characterized by requiring the "Lyuksyutov constraint" $\mathrm{tr}(\mathbf{Q}^2) = \mathrm{const}$. We describe the **Q**-tensor model for soft biaxial nematic systems and exploit the geometry of the model and the frame-indifference of the energy density to discuss the question of coercivity of the free-energy density.

1 Introduction

A liquid crystal is a state of matter, called mesomorphic, intermediate between the crystal state and the liquid state, in which the molecules retain preferential orientations relative to one another over large distances [17]. There are many different types of liquid crystals, the main classes being nematics, cholesterics and smectics. In nematic liquid crystals the constituent rod-like molecules have a locally preferred direction.

In the Landau–de Gennes theory of nematic liquid crystals [5, 4, 17, 28, 52], the propensities for alignments of molecules are represented, at each point x of the region Ω of $\mathbb{R}^3$ occupied by the fluid, by a 3×3 real symmetric traceless matrix $\mathbf{Q}(x)$, the so-called **Q**-tensor. The *order parameter* tensor field **Q** contains information about the degree of order and the deviation from isotropy of the liquid crystal at a point in Ω. More specifically, the eigenvectors of **Q** give the directions of preferred orientation of the molecules, while the eigenvalues give the degree of order about these directions [13, 52]. An equilibrium state of a nematic liquid crystal is called a *phase*. In terms of the order parameter, a phase is said to be (1) *isotropic* (I) when **Q** has three equal eigenvalues, i.e., when **Q** vanishes identically, (2) *uniaxial* ($\mathrm{N_U}$) when **Q** has two nonzero equal eigenvalues, and (3) *biaxial* ($\mathrm{N_B}$) when **Q** has three distinct eigenvalues. While the existence of uniaxial nematics has been known for more than a century, the experimental evidence of biaxial nematic liquid crystals is only recent [42]. Transitions from isotropic to uniaxial or biaxial nematic phases are usually connected with the breaking of the $SO(3)$ rotational symmetry of the system [34, 49].

In a general biaxial phase, by the spectral theorem, a tensor order parameter **Q**, i.e., an element of the vector space

$$\mathcal{S}_0 := \{\mathbf{Q} \in \mathbb{M}_{3\times 3} \mid \mathbf{Q}^T = \mathbf{Q}\,,\ \mathrm{tr}(\mathbf{Q}) = 0\} \tag{1.1}$$

can be written in the form [45, 52]

$$\mathbf{Q} = S_1\Big(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\Big) + S_2\Big(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}\mathbf{I}\Big), \tag{1.2}$$

where $S_1, S_2 : \Omega \to \mathbb{R}$ are scalar order parameters and $(\mathbf{n}\,,\ \mathbf{m}\,,\ \boldsymbol{\ell} = \mathbf{n}\times\mathbf{m})$ is a field of orthonormal eigenvectors of $\mathbf{Q}$ corresponding, respectively, to the eigenvalues

$$\lambda_1 = \frac{2S_1 - S_2}{3}, \quad \lambda_2 = \frac{2S_2 - S_1}{3}, \quad \lambda_3 = -\frac{S_1 + S_2}{3}\,. \tag{1.3}$$

Here $\mathbf{I}$ denotes the identity matrix and for a column vector $\mathbf{n}$ the tensor product $\mathbf{n}\otimes\mathbf{n}$ stands for the matrix $\mathbf{n}\mathbf{n}^T$. Equivalently, if $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ denotes the traceless diagonal matrix of the eigenvalues, the representation (1.2) of the symmetric matrix $\mathbf{Q}$ amounts to

$$\mathbf{Q} = \mathbf{G}\boldsymbol{\Lambda}\mathbf{G}^T \tag{1.4}$$

for some rotation matrix $\mathbf{G}\in SO(3)$. Therefore, one has $\mathbf{Q} = \lambda_1\mathbf{n}\otimes\mathbf{n} + \lambda_2\mathbf{m}\otimes\mathbf{m} + \lambda_3\boldsymbol{\ell}\otimes\boldsymbol{\ell}$. (Notice that a different numbering of the eigenvalues would lead to different S_1 and S_2.) According to the above decomposition, a tensor order parameter $\mathbf{Q}$ has five degrees of freedom: two of them specify the degree of order, while the remaining three are needed to specify the principal directions. In the isotropic phase, clearly $S_1 = S_2 = 0$. In the uniaxial phase, either $S_1 = 0\,,\ S_2 \neq 0$, or $S_1 \neq 0\,,\ S_2 = 0$, or $S_1 = S_2$, so that $\mathbf{Q}$ takes the form

$$\mathbf{Q} = s\Big(\mathbf{r}\otimes\mathbf{r} - \frac{1}{3}\mathbf{I}\Big)\,, \quad s : \Omega \to \mathbb{R},\ \mathbf{r} : \Omega \to \mathbb{S}^2\,, \tag{1.5}$$

where s is the only scalar order parameter. The uniaxial representation for $\mathbf{Q}$ is readily obtained from the completeness property of the eigenvectors, i.e.

$$\mathbf{n}\otimes\mathbf{n} + \mathbf{m}\otimes\mathbf{m} + \boldsymbol{\ell}\otimes\boldsymbol{\ell} = \mathbf{I}\,, \qquad \boldsymbol{\ell} := \mathbf{n}\times\mathbf{m}\in\mathbb{S}^2\,. \tag{1.6}$$

A tensor order parameter $\mathbf{Q}$ can be visualized by a rectangular box which is built from the eigensystem of the tensor. The eigenvalues, suitably augmented by $\sqrt{(2/3)\,\mathrm{tr}(\mathbf{Q}^2)}$ to ensure positivity, can be used as the edge lengths of the box. For a uniaxial $\mathbf{Q}$ two edges have the same length, while for a biaxial $\mathbf{Q}$ all three edges are of different lengths.

For a general biaxial phase, the inequality $(\mathrm{tr}(\mathbf{Q}^2))^3 \geq 6(\mathrm{tr}(\mathbf{Q}^3))^2$ holds, with equality satisfied in the uniaxial case only [27, 44]. The eigenvalues of physical $\mathbf{Q}$-tensors are constrained by the inequalities $-1/3 \leq \lambda_i \leq 2/3$, $i = 1, 2, 3$, though from a physical point of view the limiting values $\lambda_i = -1/3$ or $\lambda_i = 2/3$ represent unrealistic configurations (cf. [6, 44] for a discussion of the physical meaning of these constraints).

Free energy. The Landau–de Gennes free-energy is a nonlinear integral functional

$$\mathcal{F}[\mathbf{Q}] := \int_\Omega \psi(\mathbf{Q}, \nabla\mathbf{Q})\,dx$$

of the components of $\mathbf{Q}$ and of its gradient $\nabla\mathbf{Q}$, subject to the appropriate physical symmetries (cf. [5, 7, 17, 52]). In general, the density $\psi = \psi(\mathbf{Q}, \nabla\mathbf{Q})$ is required to be independent of the reference frame, which amounts to the *frame-indifference* condition

$$\psi(\mathbf{Q}, \nabla\mathbf{Q}) = \psi(M\mathbf{Q}M^T, \mathbf{D}^*), \qquad \forall\, M = (M^i_j) \in SO(3)\,, \tag{1.7}$$

where $\mathbf{D}^*$ denotes a third order tensor such that $\mathbf{D}^*_{ijk} = M^i_l M^j_m M^k_p \mathbf{Q}_{lm,p}$, and $\mathbf{Q}_{ij,k}$ denotes the partial derivative $\partial\mathbf{Q}_{ij}/\partial x_k =: \partial_k\mathbf{Q}_{ij}$ (cf. [5]). The summation convention over repeated indices is assumed.

In the absence of external forces, such as electromagnetic fields, and ignoring surface terms, the free energy density ψ is composed of a thermotropic bulk part and an elastic part (cf. [5, 52]),

$$\psi(\mathbf{Q}, \nabla\mathbf{Q}) := \psi_B(\mathbf{Q}) + \psi_E(\mathbf{Q}, \nabla\mathbf{Q}).$$

The bulk energy density $\psi_B(\mathbf{Q})$ is a function of the eigenvalues of $\mathbf{Q}$ and is usually given as a truncated expansion in the scalar invariants $\mathrm{tr}(\mathbf{Q}^2)$ and $\mathrm{tr}(\mathbf{Q}^3)$. It embodies the ordering/disordering effects, which are responsible for the nematic-isotropic (N-I) phase transition. In order to account for a stable biaxial nematic phase, one needs a sixth order truncated expansion such as

$$\begin{aligned}\psi_B(\mathbf{Q}) :&= \frac{A}{2}\,\mathrm{tr}(\mathbf{Q}^2) - \frac{B}{3}\,\mathrm{tr}(\mathbf{Q}^3) + \frac{C}{4}\,\mathrm{tr}(\mathbf{Q}^2)^2 \\ &\quad + \frac{D}{5}\,\mathrm{tr}(\mathbf{Q}^2)\mathrm{tr}(\mathbf{Q}^3) + \frac{E}{6}\,\mathrm{tr}(\mathbf{Q}^2)^3 + \frac{E'}{6}\,\mathrm{tr}(\mathbf{Q}^3)^2,\end{aligned} \tag{1.8}$$

where A, B, C, D, E and E' are material bulk constants (see, for instance, [16, 17, 27]). A most common expression for the free-elastic energy density is [17, 52, 64]

$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) = L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4, \tag{1.9}$$

where the L_i are material constants and the elastic invariants I_i are given by

$$I_1 := \mathbf{Q}_{ij,j}\mathbf{Q}_{ik,k}\,, \quad I_2 := \mathbf{Q}_{ik,j}\mathbf{Q}_{ij,k}\,, \quad I_3 := \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}\,, \quad I_4 := \mathbf{Q}_{lk}\mathbf{Q}_{ij,l}\mathbf{Q}_{ij,k}\,. \tag{1.10}$$

Observe that $I_1 - I_2 = \left(\mathbf{Q}_{ij}\mathbf{Q}_{ik,k}\right)_{,j} - \left(\mathbf{Q}_{ij}\mathbf{Q}_{ik,j}\right)_{,k}$ is a null Lagrangian.

For general $\mathbf{Q}$-tensors, the presence of the cubic term I_4 is responsible for the energy $\mathcal{F}[\mathbf{Q}]$ being unbounded from below [5, 6]. On the other hand, it is known that, if $L_4 = 0$, the elastic part of the energy,

$$\mathcal{F}_E[\mathbf{Q}] := \int_\Omega \psi_E(\mathbf{Q}, \nabla\mathbf{Q})\, dx\,, \tag{1.11}$$

is bounded from below and coercive if and only if the elastic constants L_1, L_2, and L_3 satisfy [16, 38]

$$L_3 > 0\,, \quad -L_3 < L_2 < 2L_3\,, \quad L_1 > -\frac{3}{5}L_3 - \frac{1}{10}L_2\,. \tag{1.12}$$

The Longa–Monselesan–Trebin positivity conditions (1.12) were originally obtained by writing the elastic energy density as a linear combination of irreducible $SO(3)$-invariants, computed using the representation theory of $SO(3)$ on spherical tensors and the Clebsch–Gordan coefficients from the angular momentum theory of quantum mechanics [47]. A more direct proof is proposed in the appendix of [56], where we used the scalar coordinates corresponding to the representation of $\mathbf{Q}$-tensors described in Section 2.3.

Uniaxial theories. In the *constrained* uniaxial case, i.e., when the scalar order parameter s in (1.5) is assumed to be constant, the more common and popular *director* approach to continuum modeling can be used only on simply-connected domains (see [7] for the non simply-connected case). More precisely, in the Oseen–Frank theory [59, 23], a configuration of a uniaxial liquid crystal is described mathematically as a unitary vector field $\mathbf{r}(x)$ in Ω, which represents the direction of preferred molecular alignment. In the Oseen-Frank model, the elastic energy associated to the configuration $\mathbf{r}$ is given by

$$\mathcal{E}(\mathbf{r}, \Omega) := \int_\Omega w(\mathbf{r}, \nabla\mathbf{r})\, dx \tag{1.13}$$

where

$$w(\mathbf{r}, \nabla\mathbf{r}) := K_1(\operatorname{div}\mathbf{r})^2 + K_2(\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 + K_3|\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2 + (K_2+K_4)\left[\operatorname{tr}[(\nabla\mathbf{r})^2] - (\operatorname{div}\mathbf{r})^2\right], \tag{1.14}$$

and the K_i are elastic constants. The energy density $w(\mathbf{r}, \nabla\mathbf{r})$ was derived by Oseen [59] on the basis of a molecular theory, and by Frank [23] as a consequence of Galilean invariance. This energy density, in fact, satisfies the *invariance properties*

$$\begin{aligned} &w(\mathbf{r}, \nabla\mathbf{r}) = w(-\mathbf{r}, -\nabla\mathbf{r}), \\ &w(H\mathbf{r}, H\,\nabla\mathbf{r}\,H^T) = w(\mathbf{r}, \nabla\mathbf{r}), \qquad \forall\, H \in O(3)\,, \end{aligned} \tag{1.15}$$

so that the functional (1.13) is well defined on vector fields in Ω, regardless of the orientation. The first equation in (1.15) accounts for the lack of polarity of nematics, while the second one expresses both the frame indifference and the condition of material symmetry corresponding to the lack of chirality of nematics. Requiring that the second line condition in (1.15) hold for the special orthogonal group only is equivalent to the frame indifference condition (1.7) for constrained uniaxial $\mathbf{Q}$-tensors.

In the constrained (or hard) uniaxial theory, the order parameter space identifies with the projective plane $\mathbb{R}P^2$, see [5, 7, 53], obtained by identification of antipodal points in $\mathbb{S}^2$. In this case, the presence of the cubic term I_4 allows the reduction of the elastic density $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ to the classical Oseen–Frank density [23, 59, 72]. This is achieved (cf. [7, 9, 52]) by formally calculating the energy density (1.9) in terms of $\mathbf{r}$ and $\nabla\mathbf{r}$, see (3.1), and by then choosing the L_i and the K_i, $i = 1, 2, 3, 4$, so that

$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) = w(\mathbf{r}, \nabla\mathbf{r})\,,$$

see (3.2). Relations among L_1, L_2, L_3, and L_4 can be determined so that the corresponding energy density is coercive [7, 20, 38, 68].

The director approach to continuum modeling has been further developed by Ericksen and Leslie [19, 36] in their hydrodynamic theory of nematic liquid crystals, which reduces to the Oseen–Frank theory in the static case. In the more recent *Ericksen theory* [21], also a spatially varying orientational order is taken into account, i.e., the state of the liquid crystal is described by a pair $(s, \mathbf{r}) \in \mathbb{R} \times \mathbb{S}^2$, depending on $x \in \Omega$.

However, although the director representation of uniaxial nematics is quite intuitive, it is not completely appropriate from a physical point of view as it does not respect the inversion symmetry, in which $\mathbf{r}$ and $-\mathbf{r}$ represent the same state. This means that the vector field $\mathbf{r}$ in the Oseen-Frank approach should actually take values in the projective plane $\mathbb{R}P^2$. This problem is overcome by the $\mathbf{Q}$-tensor approach, as the representation (1.5) is invariant under the transformation $\mathbf{r} \mapsto -\mathbf{r}$.

A variational theory that takes into account the *lack of orientability* of $\mathbb{R}P^2$ is discussed by the first author in [53]. In particular, for any Sobolev map $u \in W^{1,2}(\Omega, \mathbb{R}P^2)$, where $\Omega \subset \mathbb{R}^3$ is a simply-connected domain, there exists, up to the action of an element of $\pi_1(\mathbb{R}P^2) = \mathbb{Z}_2$, a unique map $\mathbf{r} \in W^{1,2}(\Omega, \mathbb{S}^2)$ such that $u = \Pi \circ \mathbf{r}$, where $\Pi : \mathbb{S}^2 \to \mathbb{R}P^2$ is the canonical projection map. This lifting property was obtained in a more general setting and with different techniques by Bethuel and Chiron [8], who also showed that the lifting property is no longer true for the Sobolev classes $W^{1,p}$, when $p < 2$.

The lifting problem has been studied using the $\mathbf{Q}$-tensor approach by Ball and Zarnescu in [7], where the orientability problem has been discussed also in the non simply-connected case. They also proved that the existence of a lifting of class $W^{1,2}$ implies the existence of a lifting for the *trace* on the boundary of Ω, in the corresponding fractional Sobolev space $W^{\frac{1}{2},2}$. As for non simply-connected two-dimensional domains, they specialized to the subclass of (1.5) where $\mathbf{r}$ has the third component identically zero. Such subclass of $\mathbf{Q}$-tensors is identified with the real projective line $\mathbb{R}P^1$. In this framework, they showed examples in which the minimum energy in the class of $W^{1,2}$ maps $\mathbf{Q}(\mathbf{r})$ is strictly lower than the minimum energy in the corresponding class $W^{1,2}(\Omega, \mathbb{S}^1)$.

Constrained biaxial theory. The bulk energy $\psi_B(\mathbf{Q})$ in (1.8) is invariant under the $SO(3)$-action by conjugation on the five-dimensional space of $\mathbf{Q}$-tensors, so that the critical points of the bulk energy form an orbit of solutions in the five-dimensional space of $\mathbf{Q}$-tensors. In particular, the $SO(3)$-orbit corresponding to the general case of a biaxial minimizer is a 3-manifold, while in the special case corresponding to a uniaxial minimizer the orbit reduces to a 2-manifold (see Section 2). Clearly, a tensor order parameter taking values in a group orbit has constant scalar order parameters. Actually, in many applications, it suffices to work within the so-called *constrained* (or *hard*) biaxial theory [26, 38, 39], where the scalar order parameters S_1, S_2 are assumed to be independent of position, and hence the tensor order parameter $\mathbf{Q}$ has constant eigenvalues [7]. Equivalently, both the scalar invariants $\mathrm{tr}(\mathbf{Q}^2)$ and $\mathrm{tr}(\mathbf{Q}^3)$ are constant, whence the bulk energy is constant and one only has to consider the elastic free energy. Notice that the condition $(\mathrm{tr}(\mathbf{Q}^2))^3 = 6(\mathrm{tr}(\mathbf{Q}^3))^2 = \mathrm{const}$ corresponds to a constrained uniaxial phase [27, 39].

In the constrained biaxial case, moreover, the order parameter space is diffeomorphic to the eightfold quotient $\mathbb{S}^3/\mathcal{H}$ of the 3-sphere $\mathbb{S}^3$, where $\mathcal{H} = \{\pm 1, \pm \mathsf{i}, \pm \mathsf{j}, \pm \mathsf{k}\}$ is the quaternion group [54, 57]. We refer to Section 2 for the mathematical setting involved and for some background material.

Conditions on L_1, L_2, L_3, and L_4 guaranteeing coercivity of the energy, and hence existence of minimizers, were established by the authors in [54, 55], see also [57]. These results are collected in Section 3.

Soft biaxial theory. Following Gartland [24], in the "low temperature regime" several effects are manifested, including the degree of the orientational order increasing, the potential wells in the bulk term becoming deeper with the barriers between the wells smallers, and correlation length and defect core size becoming smaller as well. The combination of these features serves to penalize biaxiality less, encouraging local biaxiality in the free-energy-minimizing solutions as a way for equilibrium tensor fields to avoid the large free-energy cost of isotropic cores in defects. This is the motivation to analyze this limit rigorously in the papers [15] and [29].

By considering an elastic energy $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ only depending on the third invariant I_3, see (1.9) and (1.10), the scaling analysis in [24] yields to consider the minimization problem of the rescaled (and dimensionless) energy functional

$$\mathcal{G}_\varepsilon(\mathbf{Q},\nabla\mathbf{Q}) := \int_\Omega \Big(\varepsilon^2\,\frac{L}{2}\,|\nabla\mathbf{Q}|^2 - \frac{1}{2}\,\mathrm{tr}(\mathbf{Q}^2) - \varepsilon\,\sqrt{3}\,\mathrm{tr}(\mathbf{Q}^3) + \frac{1}{4}\,\mathrm{tr}(\mathbf{Q}^2)^2\Big)\,dx \tag{1.16}$$

on the Sobolev space $W^{1,2}(\Omega,\mathcal{S}_0)$. In this formula, $0<\varepsilon\ll 1$ is a control parameter, $L:=\xi_{NI}/R$, where $R>0$ is the length scale appropriate to the geometry of the problem domain, and ξ_{NI} is the nematic correlation length at temperature $T=T_{NI}$, the "nematic-isotropic transition temperature", so that $\varepsilon\cdot\xi_{NI}$ agrees with the "temperature-dependent nematic correlation length" ξ_n.

The term $-\frac{1}{2}\,\mathrm{tr}(\mathbf{Q}^2)+\frac{1}{4}\,\mathrm{tr}(\mathbf{Q}^2)^2$ having minimum equal to $-1/4$ at $\mathrm{tr}(\mathbf{Q}^2)=1$, a condition that is verified by the boundary datum when it is assumed in the so-called uniaxial phase 1, for $\varepsilon>0$ small. Therefore, one is led to search for the minimum of $\mathcal{G}_\varepsilon(\mathbf{Q},\nabla\mathbf{Q})$ among maps in $W^{1,2}(\Omega_R,\mathcal{S}_0)$ such that $\mathrm{tr}(\mathbf{Q}^2)=1$. The set of bulk-minimizing tensor order parameters satisfying $\mathrm{tr}(\mathbf{Q}^2)=1$, includes a continuum of biaxial states. Thus the usual penalty from the bulk term for biaxiality vanishes in this limit. This behavior was discovered in [43], and it is at the basis of the so called "Lyuksyutov constraint" $\mathrm{tr}(\mathbf{Q}^2)=\mathrm{const}$, an ansatz used in [33, 43, 62] to obtain approximated energy minimizers deep in the nematic phase. We refer to [29] for a well-explained justification of the Lyuksyutov constraint.

Following Longa and Trebin [39], a biaxial nematic phase is called *soft biaxial* if the tensor order parameter $\mathbf{Q}$ satisfies the constraint $\mathrm{tr}(\mathbf{Q}^2)=\mathrm{const}$ (cf. also [50, 62, 63]). In a soft biaxial phase, although the sum of the squared axis lengths of $\mathbf{Q}$ is fixed, the individual axis lengths are still allowed to vary in space. According to the discussion in [3], soft biaxial nematic systems are difficult to study experimentally. Professor Longa [41] suggested that possible general candidates of soft biaxial systems could be certain micellar systems where the micellar shape is allowed to fluctuate (cf. [40] and references therein). A subclass where in addition to $\mathrm{tr}(\mathbf{Q}^2)=\mathrm{const}$ we also have $\mathrm{tr}(\mathbf{Q}^3)=0$ is important for this case is giving second order isotropic-nematic (I-N) phase transition (cf. the Landau point L in [3, Fig. 6]). From an experimental point of view, it is believed that the proximity of a Landau point L is what makes the isotropic-nematic (I-N) phase transition weakly first order (cf. [27] for details).

In [56], we analyzed a theory for soft-biaxial liquid crystals in the above mentioned sense. After discussing the geometry of the $SO(3)$-action on soft biaxial classes of $\mathbf{Q}$-tensors, we also found necessary and sufficient conditions leading to coercivity of the free-energy functional. These results are collected in Section 4.

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2 Q-tensors and order parameter spaces

In this section we recall some background material and fix notation.

2.1 Quaternions

Following e.g. [18], we let $\mathbb{H}$ be the real non-commutative algebra of quaternions, with the standard basis $\{1,\mathsf{i},\mathsf{j},\mathsf{k}\}$. Multiplication is determined by the rules

$$\mathsf{i}^2=\mathsf{j}^2=\mathsf{k}^2=\mathsf{ijk}=-1$$

which imply $\mathsf{jk}=-\mathsf{kj}=\mathsf{i}$, $\mathsf{ki}=-\mathsf{ik}=\mathsf{j}$, $\mathsf{ij}=-\mathsf{ji}=\mathsf{k}$. The typical quaternion is

$$q=q_0+q_1\mathsf{i}+q_2\mathsf{j}+q_3\mathsf{k},\quad q_0,q_1,q_2,q_3\in\mathbb{R}\,.$$

The real part of q is q_0 and the pure quaternion part is $q_1\mathsf{i}+q_2\mathsf{j}+q_3\mathsf{k}$. The conjugate $\bar q$ and the norm $|q|$ are defined by

$$\bar q=q_0-q_1\mathsf{i}-q_2\mathsf{j}-q_3\mathsf{k}\,,\quad |q|^2=q\bar q=\bar q q=q_0^2+q_1^2+q_2^2+q_3^2$$

hence the multiplicative inverse of any non-zero quaternion is $q^{-1}=\bar q/|q|^2$. As a vector space, $\mathbb{H}$ is identified with $\mathbb{R}^4$ via the usual isomorphism, which in turn induces an isomorphism between the subspace of pure quaternions and $\mathbb{R}^3$. Therefore, the elements $1,\mathsf{i},\mathsf{j},\mathsf{k}$ of $\mathbb{H}$ will be identified with the elements of the canonical basis $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ of $\mathbb{R}^4$, respectively. We will also make use of the decomposition $\mathbb{H} = \mathbb{R} \oplus \mathbb{R}^3 = \mathrm{span}\{1\} \oplus \mathrm{span}\{\mathsf{i}, \mathsf{j}, \mathsf{k}\}$ into the real and imaginary parts, and write $q = (q_0, \mathbf{q})$, where $\mathbf{q} := (q_1, q_2, q_3)$.

There is a diffeomorphism between the unit 3-sphere $\mathbb{S}^3 \subset \mathbb{R}^4$ and the group of unit quaternions,

$$Sp(1) = \{q \in \mathbb{H} \mid |q| = 1\}\,.$$

Let q be a unit quaternion and consider the $\mathbb{R}$-linear transformation $C_q : \mathbb{H} \to \mathbb{H}$, defined by $C_q(w) = qw\bar{q}$, for all $w \in \mathbb{H}$. The map C_q is an isometry, that is, $|C_q(w)| = |w|$, and preserves the decomposition $\mathbb{H} = \mathbb{R} \oplus \mathbb{R}^3$. We now see that it can then be interpreted as a rotation of $\mathbb{R}^3$.

Let $M(q)$ be the 4×4 matrix that represents the linear transformation C_q with respect to the standard basis $\{1, \mathsf{i}, \mathsf{j}, \mathsf{k}\}$. Since C_q is an isometry, $M(q)$ must be an orthogonal matrix, i.e., $M(q) \in O(4)$. The continuity of the determinant and the connectedness of $\mathbb{S}^3$ imply that the determinant of $M(q)$ is positive, so that $M(q) \in SO(4)$. The first column of $M(q)$ is the vector representing the quaternion $q1\bar{q} = q\bar{q} = 1$, that is, $\mathbf{e}_0$. Therefore, $M(q)$ is of the form

$$M(q) = \begin{pmatrix} 1 & 0 \\ 0 & \Phi(q) \end{pmatrix},$$

where $\Phi(q)$ is an element of the special orthogonal group $SO(3)$. The map

$$\Phi : \mathbb{S}^3 \cong Sp(1) \to SO(3), \qquad q \mapsto \Phi(q)$$

is a homomorphism of groups which is surjective and has kernel $\{\pm 1\}$. In particular, two matrices $\Phi(p)$ and $\Phi(q)$ represent the same rotation if and only if $p = \pm q$. The rotation matrix corresponding to the unit quaternion $q = q_0 + q_1\mathsf{i} + q_2\mathsf{j} + q_3\mathsf{k}$ is given explicitly by

$$\Phi(q) = \begin{pmatrix} q_0^2 + q_1^2 - (q_2^2 + q_3^2) & 2(q_1q_2 - q_0q_3) & 2(q_1q_3 + q_0q_2) \\ 2(q_1q_2 + q_0q_3) & q_0^2 + q_2^2 - (q_1^2 + q_3^2) & 2(q_2q_3 - q_0q_1) \\ 2(q_1q_3 - q_0q_2) & 2(q_2q_3 + q_0q_1) & q_0^2 + q_3^2 - (q_1^2 + q_2^2) \end{pmatrix}. \tag{2.1}$$

Since every unit quaternion q is of the form $q = \cos(\theta/2) + \sin(\theta/2)\mathbf{u}$, for a real number θ and a pure unit quaternion $\mathbf{u} = u_1\mathsf{i} + u_2\mathsf{j} + u_3\mathsf{k}$, the matrix $\Phi(q) \in SO(3)$ actually represents a rotation $G(\mathbf{u}, \theta)$ through an angle θ with axis along $\mathbf{u}$,

$$G(\mathbf{u}, \theta) := \begin{pmatrix} u_1^2(1-\cos\theta) + \cos\theta & u_1u_2(1-\cos\theta) - u_3\sin\theta & u_1u_3(1-\cos\theta) + u_2\sin\theta \\ u_1u_2(1-\cos\theta) + u_3\sin\theta & u_2^2(1-\cos\theta) + \cos\theta & u_2u_3(1-\cos\theta) - u_1\sin\theta \\ u_1u_3(1-\cos\theta) - u_2\sin\theta & u_2u_3(1-\cos\theta) + u_1\sin\theta & u_3^2(1-\cos\theta) + \cos\theta \end{pmatrix}. \tag{2.2}$$

In particular, we have:

$$\Phi(\pm 1) = \mathbf{I}, \quad \Phi(\pm\mathsf{i}) = \mathrm{diag}(1, -1, -1)\,, \quad \Phi(\pm\mathsf{j}) = \mathrm{diag}(-1, 1, -1)\,, \quad \Phi(\pm\mathsf{k}) = \mathrm{diag}(-1, -1, 1)\,. \tag{2.3}$$

2.2 Constrained biaxial liquid crystals

In the *constrained Landau–de Gennes theory* [7, 45, 46, 39], the scalar order parameters S_1 and S_2 are required to be constant, so that the structure of the liquid crystal at each point $x \in \Omega$ only depends on the value of the orthonormal vectors $\mathbf{n}$, $\mathbf{m}$ at x. In particular, the eigenvalues in (1.3) are constant. In the constrained uniaxial case, according to (1.5) any tensor order parameter $\mathbf{Q}$ has two degrees of freedom and determines a point $\mathbf{r}$ in the projective plane $\mathbb{R}P^2$. In the constrained biaxial case, $\mathbf{Q}$ has instead three degrees of freedom. We now give some details.

Definition 2.1 *Let us fix three distinct constants $\lambda_1, \lambda_2, \lambda_3 \in (-\frac{1}{3}, \frac{2}{3})$, ordered by $\lambda_1 < \lambda_2 < \lambda_3$, so that $\lambda_1 + \lambda_2 + \lambda_3 = 0$. The space $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ of all elements of $\mathcal{S}_0$ in* (1.1) *of the form* (1.2) *so that* (1.3) *holds is known as the order parameter space of the system.*

Denoting $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$, by (1.4) we thus have

$$\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3) = \left\{\mathbf{Q} \in \mathcal{S}_0 \mid \mathbf{Q} = \mathbf{G}\mathbf{\Lambda}\mathbf{G}^T \text{ for some } \mathbf{G} \in SO(3)\right\}.$$

If one considers the left action of $SO(3)$ on $\mathcal{S}_0$ given by

$$\mathbf{G} \star \mathbf{Q} := \mathbf{G}\mathbf{Q}\mathbf{G}^T, \quad \mathbf{G} \in SO(3), \ \mathbf{Q} \in \mathcal{S}_0, \tag{2.4}$$

then it is clear that $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ is just the orbit of the diagonal matrix $\mathbf{\Lambda}$ with respect to this action. Since the eigenvalues are distinct, the subgroup of $SO(3)$ which fixes $\mathbf{\Lambda}$,

$$SO(3)_{\mathbf{\Lambda}} := \{\mathbf{G} \in SO(3) \mid \mathbf{G} \star \mathbf{\Lambda} = \mathbf{\Lambda}\},$$

that is the isotropy subgroup of $\mathbf{\Lambda}$, is readily seen to be the abelian four-element group

$$D_2 := \{\mathrm{diag}(1,1,1),\ \mathrm{diag}(-1,-1,1),\ \mathrm{diag}(-1,1,-1),\ \mathrm{diag}(1,-1,-1)\}, \tag{2.5}$$

i.e., the dihedral group D_2 which consists of the identity and 180°-rotations about three mutually perpendicular axes. Now, from the theory of homogeneous spaces [11, 70], we know that the coset space $SO(3)/SO(3)_{\mathbf{\Lambda}} = SO(3)/D_2$ can be given a structure of differentiable manifold, so that the bijective map

$$SO(3)/SO(3)_{\mathbf{\Lambda}} \to \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3), \quad [\mathbf{G}] = \mathbf{G}SO(3)_{\mathbf{\Lambda}} \mapsto \mathbf{G} \star \mathbf{\Lambda} = \mathbf{G}\mathbf{\Lambda}\mathbf{G}^T$$

provides $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ with a differentiable structure with this map becoming a diffeomorphism. The coset space $SO(3)/D_2$ is an eightfold quotient of the 3-sphere. In fact, according to (2.3), the preimage of D_2 in $\mathbb{S}^3$ under the 2:1 group homomorphism $\Phi : \mathbb{S}^3 \cong Sp(1) \to SO(3)$ coincides with the non-abelian eight-element quaternion group $\mathcal{H} := \{\pm 1, \pm \mathsf{i}, \pm \mathsf{j}, \pm \mathsf{k}\}$. The parameter space $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ is thus diffeomorphic to the coset space $\mathbb{S}^3/\mathcal{H}$,

$$\mathbb{S}^3/\mathcal{H} \cong Sp(1)/\mathcal{H} = \{p\,\mathcal{H} \mid p \in Sp(1)\}.$$

Remark 2.2 Note that $\mathbb{S}^3/\mathcal{H}$ can be endowed with a unique Riemannian structure so that the canonical projection $\Pi : \mathbb{S}^3 \to \mathbb{S}^3/\mathcal{H}$ is a Riemannian covering map. Moreover, since $\mathbb{S}^3$ is simply connected, Π is the universal covering map and $\pi_1(\mathbb{S}^3/\mathcal{H}) = \mathcal{H}$ acts isometrically on $\mathbb{S}^3$ (see for instance [71]).

Remark 2.3 From (1.3) and the specific ordering $\lambda_1 < \lambda_2 < \lambda_3$ of the eigenvalues in the representation (1.2), it follows that $S_1 < S_2 < 0$. Moreover, according to the analysis in the proof of Proposition 1 in [45], one can conclude indeed that either

$$\frac{S_1}{2} \le S_2 < 0, \quad \text{or} \quad S_2 \le \frac{S_1}{2} < 0 \tag{2.6}$$

and, with the notation from [45], that R_2^- and R_3^+ are the only admissible regions.

2.3 Representation of Q-tensors

The vector space $\mathcal{S}_0$ of $\mathbf{Q}$-tensors, see (1.1), is naturally equipped with inner product $\langle \mathbf{Q}, \mathbf{P} \rangle = \mathrm{tr}(\mathbf{Q}\mathbf{P})$ and norm $|\mathbf{Q}| = \sqrt{\mathrm{tr}(\mathbf{Q}^2)}$. Let $\{\mathbf{E}_i\}_{i=1}^5$ be the ordered orthonormal basis for $\mathcal{S}_0$ given by (cf. [65])

$$\begin{aligned} &\mathbf{E}_1 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad \mathbf{E}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{E}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ &\mathbf{E}_4 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{E}_5 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \end{aligned} \tag{2.7}$$

Then any $\mathbf{Q} \in \mathcal{S}_0$ has a unique representation

$$\mathbf{Q} = \begin{pmatrix} q_1 & q_3 & q_4 \\ q_3 & q_2 & q_5 \\ q_4 & q_5 & -(q_1 + q_2) \end{pmatrix} = \sum_{i=1}^{5} u^i \mathbf{E}_i, \quad \text{where} \quad u^i = \mathrm{tr}(\mathbf{Q}\mathbf{E}_i). \tag{2.8}$$

It easily follows that

$$u^1 = \frac{\sqrt{6}}{2}(q_1 + q_2), \quad u^2 = \frac{\sqrt{2}}{2}(q_1 - q_2), \quad u^i = \sqrt{2} q_i, \quad i = 3, 4, 5 \tag{2.9}$$

and hence

$$q_1 = \frac{1}{\sqrt{6}}u^1 + \frac{1}{\sqrt{2}}u^2\,, \quad q_2 = \frac{1}{\sqrt{6}}u^1 - \frac{1}{\sqrt{2}}u^2\,, \quad q_i = \frac{1}{\sqrt{2}}u^i\,, \quad i = 3,4,5. \tag{2.10}$$

The mapping $\mathbf{T} : \mathcal{S}_0 \to \mathbb{R}^5$, defined by

$$\mathbf{T}(\mathbf{Q}) = \mathbf{T}(u^1\mathbf{E}_1 + \cdots + u^5\mathbf{E}_5) := (u^1, \ldots, u^5) = \mathbf{u}, \tag{2.11}$$

establishes an isometric isomorphism between $\mathcal{S}_0$ (with the inner product $\langle \mathbf{Q}, \mathbf{P}\rangle = \mathrm{tr}(\mathbf{QP})$) and $\mathbb{R}^5$ with the standard inner product $\mathbf{u}\cdot\mathbf{v} = \sum_i u^i v^i$. In particular,

$$\mathrm{tr}(\mathbf{Q}^2) = 2\,(q_1^2 + q_2^2 + q_1q_2 + q_3^2 + q_4^2 + q_5^2) = |\mathbf{T}(\mathbf{Q})|^2 = |\mathbf{u}|^2. \tag{2.12}$$

Following [16], we refer to $(u^1, \ldots, u^5) = \mathbf{u} = \mathbf{T}(\mathbf{Q})$ as the *scalar coordinates* of $\mathbf{Q}$ with respect to the basis $\{\mathbf{E}_i\}_{i=1}^5$. If $\Omega \subset \mathbb{R}^3$ is a smooth bounded domain, the mapping $\mathbf{T}$ defined by (2.11) establishes an isometric isomorphism between the Soboles classes $W^{1,2}(\Omega, \mathbb{R}^5)$ and $W^{1,2}(\Omega, \mathcal{S}_0)$ (cf. [16]). This implies that there is no essential difference between studying the elastic energy $\mathcal{F}_E[\mathbf{Q}]$ or the functional $F_E[\mathbf{T}(\mathbf{Q})] = F_E[\mathbf{u}] := \mathcal{F}_E[\sum_i u^i\mathbf{E}_i]$.

Remark 2.4 Assume that the map $\Omega \ni x \mapsto \mathbf{Q}(x) \in \mathcal{S}_0$ is smooth. By the above identifications, using (2.8), (2.9) and (2.10), we compute

$$\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k} = |\nabla\mathbf{Q}|^2 = 2\left(|\nabla q_1|^2 + |\nabla q_2|^2 + \nabla q_1 \bullet \nabla q_2 + |\nabla q_3|^2 + |\nabla q_4|^2 + |\nabla q_5|^2\right), \tag{2.13}$$

where

$$\left(|\nabla q_1|^2 + |\nabla q_2|^2 + \nabla q_1 \bullet \nabla q_2\right) = \frac{1}{2}\left(|\nabla u^1|^2 + |\nabla u^2|^2\right)$$

and

$$|\nabla q_j|^2 = \frac{1}{2}\,|\nabla u^j|^2\,, \qquad j = 3,4,5$$

so that

$$|\nabla\mathbf{Q}(x)| = |\nabla\mathbf{u}(x)|\,, \quad x \in \Omega\,. \tag{2.14}$$

Remark 2.5 For $\mathbf{Q} \in \mathcal{S}_0$ with eigenvalues $\lambda_1, \lambda_2, \lambda_3$, then $\mathrm{tr}(\mathbf{Q}^2) = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = -2(\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3)$ and hence

$$\det(\mathbf{Q} - t\mathbf{I}) = -t^3 + \frac{\mathrm{tr}(\mathbf{Q}^2)}{2}\,t + \det\mathbf{Q}\,, \quad t \in \mathbb{R}\,.$$

From the Cayley–Hamilton theorem, it follows that

$$\mathbf{Q}^3 - \frac{\mathrm{tr}(\mathbf{Q}^2)}{2}\,\mathbf{Q} - (\det\mathbf{Q})\,\mathbf{I} = 0. \tag{2.15}$$

Taking the trace yields $\mathrm{tr}(\mathbf{Q}^3) = 3\det\mathbf{Q}$, which implies that the characteristic equation reads

$$t^3 - \frac{\mathrm{tr}(\mathbf{Q}^2)}{2}\,t - \frac{\mathrm{tr}(\mathbf{Q}^3)}{3} = 0\,. \tag{2.16}$$

Using (2.15), it easily follows that the invariants $\mathrm{tr}(\mathbf{Q}^k)\,,\, k \geq 4$, can be expressed as polynomials in $\mathrm{tr}(\mathbf{Q}^2)$ and $\mathrm{tr}(\mathbf{Q}^3)$ [5, 27]. Moreover, it follows from (2.16) that the invariants $\mathrm{tr}(\mathbf{Q}^2)$ and $\mathrm{tr}(\mathbf{Q}^3)$ are constant if and only if the eigenvalues $\lambda_1\,, \lambda_2\,, \lambda_3$ of $\mathbf{Q}$ are constant, which amounts to the requirement that the system is constrained (hard). Finally, note that the characteristic equation (2.16) has real roots if and only if $(\mathrm{tr}(\mathbf{Q}^2))^3 \geq 6(\mathrm{tr}(\mathbf{Q}^3))^2$ and has two equal roots when $(\mathrm{tr}(\mathbf{Q}^2))^3 = 6(\mathrm{tr}(\mathbf{Q}^3))^2$.

2.4 Plane representation of diagonal Q-tensors

Let $\mathbf{Q} = \mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ be a diagonal $\mathbf{Q}$-tensor. According to our previous notation,

$$\mathbf{u} = \mathbf{T}(\mathbf{\Lambda}) = (\mathbf{x}, \mathbf{y}, 0, 0, 0),$$

where

$$\mathbf{x} := \frac{\sqrt{6}}{2}\,(\lambda_1+\lambda_2)\,, \quad \mathbf{y} := \frac{\sqrt{2}}{2}\,(\lambda_1-\lambda_2). \tag{2.17}$$

By (2.10), we have the inverse formulas

$$\lambda_1 = \frac{\sqrt{2}}{2}\left(\frac{\mathbf{x}}{\sqrt{3}}+\mathbf{y}\right), \quad \lambda_2 = \frac{\sqrt{2}}{2}\left(\frac{\mathbf{x}}{\sqrt{3}}-\mathbf{y}\right), \quad \lambda_3 = -\frac{2}{\sqrt{6}}\,\mathbf{x}\,. \tag{2.18}$$

The physical constraints $-1/3 \le \lambda_i \le 2/3$ on the eigenvalues imply that the point $(\mathbf{x},\mathbf{y})$ in the $\mathbf{xy}$-plane associated with $\mathbf{Q}=\mathbf{\Lambda}$ lies in the interior or on the boundary of the *physical triangle* (cf. [13, 44])

$$\lhd := \left\{(\mathbf{x},\mathbf{y}) \in \mathbb{R}^2 \mid -(\mathbf{x}/\sqrt{3}+\sqrt{2}/3) \le \mathbf{y} \le (\mathbf{x}/\sqrt{3}+\sqrt{2}/3)\,, \quad -2/\sqrt{6} \le \mathbf{x} \le 1/\sqrt{6}\right\},$$

an equilateral triangle with edges of length $\sqrt{2}$ and vertices at $(-2/\sqrt{6},0)$, $(1/\sqrt{6},\pm\sqrt{2}/2)$ (cf. Figure 1).

Moreover, we have

$$\lambda_1 = c_1 \iff \frac{\mathbf{x}}{\sqrt{3}}+\mathbf{y} = \sqrt{2}\,c_1\,, \quad \lambda_2 = c_2 \iff \frac{\mathbf{x}}{\sqrt{3}}-\mathbf{y} = \sqrt{2}\,c_2\,, \quad \lambda_3 = c_3 \iff \mathbf{x} = -\frac{\sqrt{6}}{2}\,c_3\,.$$

Therefore, the *uniaxial* phases are

$$\lambda_1=\lambda_2 \iff \mathbf{y}=0\,, \quad \lambda_1=\lambda_3 \iff \mathbf{y}=-\sqrt{3}\,\mathbf{x}\,, \quad \lambda_2=\lambda_3 \iff \mathbf{y}=\sqrt{3}\,\mathbf{x} \tag{2.19}$$

and the so-called *maximal biaxial* phases are

$$\lambda_1 = 0 \iff \mathbf{y} = -\frac{\mathbf{x}}{\sqrt{3}}\,, \quad \lambda_2 = 0 \iff \mathbf{y} = \frac{\mathbf{x}}{\sqrt{3}}\,, \quad \lambda_3 = 0 \iff \mathbf{x} = 0\,. \tag{2.20}$$

In particular, observe that for a physical $\mathbf{Q}$-tensor, the bounds on the eigenvalues imply that

$$\mathrm{tr}(\mathbf{Q}^2) = \lambda_1^2+\lambda_2^2+\lambda_3^2 = \mathbf{x}^2+\mathbf{y}^2 \le \frac{2}{3}. \tag{2.21}$$

As explained in Section 4.1 below, up to the action by conjugation of an element of $SO(3)$, we may assume a specific order of the eigenvalues. If, for instance, $\lambda_1 \ge \lambda_2 \ge \lambda_3$, the point $(\mathbf{x},\mathbf{y})$ representing $\mathbf{Q}$ takes value in a subset $\lhd_f$ of $\lhd$,

$$\lhd_f := \left\{(\mathbf{x},\mathbf{y}) \in \mathbb{R}^2 \mid 0 \le \mathbf{x} \le 1/\sqrt{6},\, 0 \le \mathbf{y} \le \sqrt{3}\mathbf{x}\right\}$$

referred to as the *fundamental domain* (cf. for example [44]).

Remark 2.6 In this representation, the diagonal $\mathbf{Q}$-tensors satisfying the condition $\mathrm{tr}(\mathbf{Q}^2) \equiv \rho^2$, for some positive constant ρ, correspond to the points of the intersection between $\lhd$ and the circle $\mathbb{S}^1_\rho$ of radius ρ centered at the origin in the $\mathbf{xy}$-plane. In particular, we have (cf. Figure 1):

- if $\rho^2 < 1/6$, the circle $\mathbb{S}^1_\rho$ is contained in the interior of $\lhd$;
- if $\rho^2 = 1/6$, the circle $\mathbb{S}^1_{1/\sqrt{6}}$ is tangent to the boundary of $\lhd$ at the middle points $(\frac{-1}{2\sqrt{6}},\frac{\pm\sqrt{2}}{4})$, $(\frac{1}{\sqrt{6}},0)$ of the edges;
- if $1/6 < \rho^2 < 2/3$, the circle $\mathbb{S}^1_\rho$ intersects the boundary of $\lhd$ at three couples of points $(\mathbf{x},\mathbf{y})$ whose first coordinate is, respectively,

$$\mathbf{x} = \mathbf{x}_-(\rho) := -\frac{1}{2\sqrt{6}} - \frac{\sqrt{6\rho^2-1}}{2\sqrt{2}}\,, \quad \mathbf{x} = \mathbf{x}_+(\rho) := -\frac{1}{2\sqrt{6}} + \frac{\sqrt{6\rho^2-1}}{2\sqrt{2}}\,, \quad \mathbf{x} = \frac{1}{\sqrt{6}}\,;$$

- if $\rho^2 = 2/3$, the circle $\mathbb{S}^1_{\sqrt{2/3}}$ intersects the boundary of $\lhd$ at the vertices $(\frac{-2}{\sqrt{6}},0)$, $(\frac{1}{\sqrt{6}},\frac{\pm\sqrt{2}}{2})$;

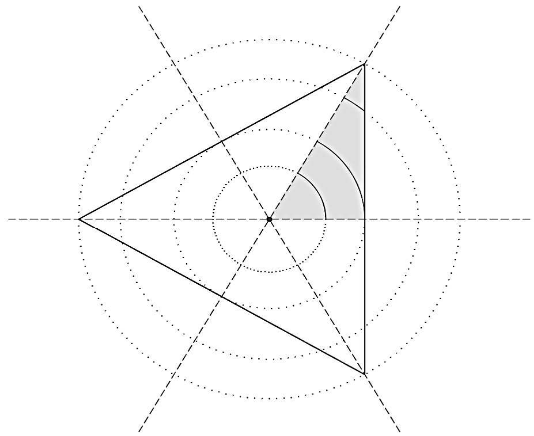

Figure 1: The *physical triangle* $\lhd$ and the *fundamental domain* $\lhd_f$ (shaded region) in the $\mathbf{xy}$-plane. The origin $(0,0)$ represents the isotropic phase. The dashed lines $U = \{(\mathbf{x},\mathbf{y}) \in \lhd \mid \mathbf{y} = 0 \text{ or } \mathbf{y} = -\sqrt{3}\mathbf{x} \text{ or } \mathbf{y} = \sqrt{3}\mathbf{x}\} \setminus \{(0,0)\}$ represent uniaxial phases; the set $B = \lhd \setminus (U \cup \{(0,0)\})$ represent biaxial phases. The points on the dotted circumferences inside or on the boundary of $\lhd$, not on U, represent soft biaxial phases.

- if $\rho^2 > 2/3$, the circle $\mathbb{S}^1_\rho$ does not intersect the triangle $\lhd$.

Remark 2.7 Using the notation (2.17) and (2.18), we have

$$\operatorname{tr}(\mathbf{Q}^3) = 3\lambda_1\lambda_2\lambda_3 = \frac{\mathbf{x}}{\sqrt{6}}\,(3\mathbf{y}^2 - \mathbf{x}^2)$$

so that the function $\mathbf{Q} \mapsto \operatorname{tr}(\mathbf{Q}^3)$ is bounded in $\mathbb{S}^4_\rho$. More precisely, it turns out that for any choice of $0 < \rho^2 \leq 2/3$

$$|\operatorname{tr}(\mathbf{Q}^3)| \leq \frac{\rho^3}{\sqrt{6}} \quad \forall\, \mathbf{Q} \in \mathbb{S}^4_\rho\,.$$

3 Constrained theory of biaxial liquid crystals

Let $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ be the set of all constrained biaxial $\mathbf{Q}$-tensors of the form (1.2) with distinct constant eigenvalues $\lambda_1,\lambda_2,\lambda_3$. By using the model described in Section 2.2, a configuration of a biaxial nematic liquid crystal is described by a map from Ω to $\mathbb{S}^3/\mathcal{H}$, as opposed to the constrained uniaxial case where the order parameter space is $\mathbb{R}P^2$.

Remark 3.1 We recall that in the constrained uniaxial case, the elastic invariants I_i in (1.10) satisfy:

$$\begin{aligned} I_1 &= s^2\big((\operatorname{div}\mathbf{r})^2 + |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2\big)\,, \quad I_2 = s^2\big(|\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2 + \operatorname{tr}[(\nabla\mathbf{r})^2]\big)\,,\\ I_3 &= 2s^2\big(\operatorname{tr}[(\nabla\mathbf{r})^2] + (\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 + |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2\big)\,,\\ I_4 &= 2s^3\Big(\frac{2}{3}|\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2 - \frac{1}{3}\operatorname{tr}[(\nabla\mathbf{r})^2] - \frac{1}{3}(\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2\Big)\,, \end{aligned} \tag{3.1}$$

see [54] for a proof. As a consequence, compare [7], choosing

$$\begin{aligned} K_1 &:= L_1s^2 + L_2s^2 + 2L_3s^2 - \frac{2}{3}L_4s^3\,, \quad K_2 := 2L_3s^2 - \frac{2}{3}L_4s^3\,,\\ K_3 &:= L_1s^2 + L_2s^2 + 2L_3s^2 + \frac{4}{3}L_4s^3\,, \quad K_4 := L_2s^2 \end{aligned} \tag{3.2}$$

it turns out that the energy density $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ in (1.9) agrees with the Oseen-Frank energy density $w(\mathbf{r},\nabla\mathbf{r})$ of *nematic liquid crystals*, see (1.14). We also recall that necessary and sufficient conditions for

$$w(\mathbf{r},\nabla\mathbf{r}) \geq \nu\,|\nabla\mathbf{r}|^2 \qquad \text{for some } \nu > 0$$

are the classical *Ericksen inequalities* [20, 68]

$$2K_1 > K_2 + K_4\,, \quad K_3 > 0\,, \quad K_2 > |K_4|\,, \tag{3.3}$$

see [55] for a proof. By using the formulas (3.2), they can be rewritten in terms of the coefficients L_i as

$$2L_1 + L_2 + 2L_3 > \frac{2}{3}L_4 s\,, \quad L_1 + L_2 + 2L_3 + \frac{4}{3}L_4 s > 0\,, \quad 2L_3 - \frac{2}{3}L_4 s > |L_2|\,. \tag{3.4}$$

In the constrained biaxial case, following the representation described in Section 2.3, the Landau–de Gennes elastic free-energy density $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ is expressed as a density on maps $q:\Omega\to\mathbb{S}^3$, depending on q and its first derivatives. For this purpose, in [54] we identified the conditions on a generic energy density $f:\mathbb{S}^3\times\mathbb{M}_{4\times 3}\to[0,+\infty)$, in order that:

(1) f is independent of arbitrary superposed rigid rotations (frame indifference condition);

(2) f is well defined on the class of configuration maps $\Omega\to\mathbb{S}^3/\mathcal{H}$ (residual symmetry condition).

As for condition (1), we have the following.

Definition 3.2 *An energy density* $f:\mathbb{S}^3\times\mathbb{M}_{4\times 3}\to[0,+\infty)$ *satisfies the* frame invariance condition *if, for any* $q\in\mathbb{S}^3$,

$$f(w,H) = f(qw, L(q)H\Phi(q)^T) \qquad \forall\,(w,H)\in\mathbb{S}^3\times\mathbb{M}_{4\times 3}\,, \tag{3.5}$$

where $L(q)$ *denotes the orthogonal matrix representing the real linear map on* $\mathbb{H}$ *defined by* $w\mapsto q\,w$, *with respect to the standard basis* $\{1,\mathsf{i},\mathsf{j},\mathsf{k}\}$, *and* $\Phi:\mathbb{S}^3\to SO(3)$ *is the 2:1 group homomorphism given in* (2.1).

The frame invariance and the frame indifference conditions are in fact related as follows.

Theorem 3.3 ([54]) *For constrained biaxial nematics, the frame invariance condition* (3.5) *is equivalent to the frame invariance* (1.7) *in the sense of* $\mathbf{Q}$*-tensors.*

As a consequence, we have the following useful result, see [55].

Lemma 3.4 *If the condition* (3.5) *holds and if* $f(q_0,H)\geq 0$ *for a given* $q_0\in\mathbb{S}^3$ *and all* $H\in\mathbb{M}_{4\times 3}$ *such that* $H^Tq_0=0$, *then* $f(q,H)\geq 0$ *for any* $q\in\mathbb{S}^3$ *and all* $H\in\mathbb{M}_{4\times 3}$ *such that* $H^Tq=0$.

Condition (2) has to do with a specific physical symmetry of the material associated with the group $\mathcal{H}$. It corresponds to the "head-to-tail" symmetry in the uniaxial case. In order to deal with a functional defined on maps taking values in the coset space $\mathbb{S}^3/\mathcal{H}$, we also introduce the following symmetry condition.

Definition 3.5 *An energy density* $f:\mathbb{S}^3\times\mathbb{M}_{4\times 3}\to[0,+\infty)$ *is said to satisfy the* residual symmetry property *if, for any* $q\in\mathcal{H}$, *one has*

$$f(w,H) = f(qw, L(q)H) \qquad \forall\,(w\,,H)\in\mathbb{S}^3\times\mathbb{M}_{4\times 3}\,. \tag{3.6}$$

The above symmetry property, in fact, is the counterpart of the property in the first line of (1.15), that is satisfied by the energy density of uniaxial nematic liquid crystals in the sense of Oseen–Frank [25, 36].

Therefore, conditions (3.5) and (3.6) are necessary for a map $f:\mathbb{S}^3\times\mathbb{M}_{4\times 3}\to[0,+\infty)$ representing an energy density for constrained biaxial nematic states.

The main steps in our discussion are the following.

1. Compute the Cartesian expressions for the elastic invariants I_1, I_2, I_3, and I_4.
2. Use the Cartesian expressions for I_1, I_2, I_3, and I_4 and the identification of $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ with $\mathbb{S}^3/\mathcal{H}$ to express the energy density $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ in terms of maps $q:\Omega\to\mathbb{S}^3$ and their derivatives, so that

$$\psi_E(\mathbf{Q}(q(x)),\nabla\mathbf{Q}(q(x))) = f_E(q(x),\nabla q(x)) \qquad \forall\,x\in\Omega,$$

for a suitably constructed energy density model $f_E(q,\nabla q)$ satisfying the required invariance conditions.

3. Use the frame indifference to determine necessary and sufficient conditions on the elastic constants L_i for the (pointwise) expression of the energy density model $f_E(q, \nabla q)$ to be a positive definite quadratic function of ∇q.
4. Apply the above results to the question of coercivity for the energy functional $\mathcal{F}_E[\mathbf{Q}]$.
5. Apply the above results to the question of existence of minimizers for the energy functional $\mathcal{F}_E[\mathbf{Q}]$.

Each of these points is now discussed separately.

1. Cartesian expressions. For a constrained biaxial $\mathbf{Q}$ of the form (1.2), with distinct constant eigenvalues $\lambda_1, \lambda_2, \lambda_3$, in [54, 55] we derived the following Cartesian expressions for the elastic invariants I_1, I_2, I_3, and I_4 in terms of the gradient, the divergence, and the curl of the orthonormal eigenvector fields $(\mathbf{n}, \mathbf{m}, \boldsymbol{\ell})$ associated with $\mathbf{Q}$, namely:

$$\begin{aligned}
I_1(\mathbf{Q}, \nabla\mathbf{Q}) &= S_1(S_1 - S_2)\big((\operatorname{div}\mathbf{n})^2 + |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\big) \\
&\quad + S_2(S_2 - S_1)\big((\operatorname{div}\mathbf{m})^2 + |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\big) \\
&\quad + S_1S_2\big((\operatorname{div}\boldsymbol{\ell})^2 + |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\big)\,, \\
I_2(\mathbf{Q}, \nabla\mathbf{Q}) &= S_1(S_1 - S_2)\big(\operatorname{tr}[(\nabla\mathbf{n})^2] + |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\big) \\
&\quad + S_2(S_2 - S_1)\big(\operatorname{tr}[(\nabla\mathbf{m})^2] + |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\big) \\
&\quad + S_1S_2\big(\operatorname{tr}[(\nabla\boldsymbol{\ell})^2] + |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\big)\,, \\
I_3(\mathbf{Q}, \nabla\mathbf{Q}) &= 2S_1(S_1 - S_2)|\nabla\mathbf{n}|^2 + 2S_2(S_2 - S_1)|\nabla\mathbf{m}|^2 + 2S_1S_2|\nabla\boldsymbol{\ell}|^2\,, \\
I_4(\mathbf{Q}, \nabla\mathbf{Q}) &= 3^{-1}\,S_1(2S_1 - S_2)(S_2 - S_1)\,\big(\operatorname{tr}[(\nabla\mathbf{n})^2] + (\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2\big) \\
&\quad + 3^{-1}\,S_1(S_1 - S_2)(4S_1 - 5S_2)\,|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 \\
&\quad + 3^{-1}\,S_2(2S_2 - S_1)(S_1 - S_2)\,\big(\operatorname{tr}[(\nabla\mathbf{m})^2] + (\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2\big) \\
&\quad + 3^{-1}\,S_2(S_2 - S_1)(S_1 + 4S_2)\,|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2 \\
&\quad + 3^{-1}\,S_1S_2(S_1 + S_2)\,\big(\operatorname{tr}[(\nabla\boldsymbol{\ell})^2] + (\boldsymbol{\ell}\cdot\operatorname{curl}\boldsymbol{\ell})^2\big) \\
&\quad + 3^{-1}\,S_1S_2(S_2 - 5S_1)\,|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2 \\
&\quad + 2S_1S_2(S_1 - S_2)\,[(\mathbf{m}\cdot\operatorname{curl}\mathbf{n})^2 + (\boldsymbol{\ell}\cdot\operatorname{curl}\mathbf{m})^2 + (\mathbf{n}\cdot\operatorname{curl}\boldsymbol{\ell})^2]\,,
\end{aligned} \tag{3.7}$$

The important fact about these Cartesian expressions for I_1, I_2, I_3, I_4, is that they are written, up to a divergence term, using only the twelve independent quadratic first order invariants

$$\begin{array}{ccc}
|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\,, & |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\,, & |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\,, \\
(\operatorname{div}\mathbf{n})^2\,, & (\operatorname{div}\mathbf{m})^2\,, & (\operatorname{div}\boldsymbol{\ell})^2\,, \\
(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2\,, & (\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2\,, & (\boldsymbol{\ell}\cdot\operatorname{curl}\boldsymbol{\ell})^2\,, \\
(\mathbf{m}\cdot\operatorname{curl}\mathbf{n})^2\,, & (\boldsymbol{\ell}\cdot\operatorname{curl}\mathbf{m})^2\,, & (\mathbf{n}\cdot\operatorname{curl}\boldsymbol{\ell})^2\,,
\end{array}$$

which appear in the expansion up to second order of the elastic free-energy density of a constrained biaxial system [26, 39, 66].

2. Energy density model. Next, using the identification of the order parameter space $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ with the homogeneous space $\mathbb{S}^3/\mathcal{H}$, to any unit quaternion $q \in \mathbb{S}^3$ there corresponds a tensor order parameter $\mathbf{Q}(q) := \mathbf{G}(q)\boldsymbol{\Lambda}\mathbf{G}(q)^T$, where $\boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$ and $\mathbf{G}(q) = \Phi(q)$ is the orthogonal matrix having $\mathbf{n}(q)$, $\mathbf{m}(q)$, and $\boldsymbol{\ell}(q)$ as column vectors, the function $\Phi : \mathbb{S}^3 \to SO(3)$ being the universal covering map of $SO(3)$ (cf. Section 2.1, Eq. (2.1)). This, together with the Cartesian expressions above, allows us to express $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ in terms of maps $q : \Omega \to \mathbb{S}^3$ and their derivatives. Namely, there exists a function $f_E : \mathbb{S}^3 \times \mathbb{M}_{4\times 3} \to [0, +\infty]$, such that

$$\psi_E(\mathbf{Q}(q(x)), \nabla\mathbf{Q}(q(x))) = f_E(q(x), \nabla q(x)) \qquad \forall\, x \in \Omega\,.$$

Therefore, the function $f_E(q, \nabla q)$ may be interpreted as the elastic energy density model for the configuration maps $q : \Omega \to \mathbb{S}^3/\mathcal{H}$ of a constrained biaxial nematic system, and the corresponding energy functional is well defined, for instance, on Sobolev maps $q : \Omega \to \mathbb{S}^3/\mathcal{H}$.

In principle, using the Cartesian expression for ψ_E and the above identifications, we could explicitly compute f_E arguing as in [54], where we computed f_3 such that $I_3(\mathbf{Q}(q), \nabla\mathbf{Q}(q)) = f_3(q, \nabla q)$. However, for our purposes, such computations are not needed.

3. Coercivity conditions. For any given map $q : \Omega \to \mathbb{S}^3$, we then determine necessary and sufficient conditions on the elastic constants L_i for the (pointwise) expression of the energy density model $f_E(q, \nabla q)$ to be a positive definite quadratic function of ∇q. Actually, we find necessary and sufficient conditions on the L_i under which the function f_E satisfies $f_E(q, H) > 0$, for any given $q \in \mathbb{S}^3$ and all 4×3 matrices $H \neq 0$ such that $H^T q = 0$. This is achieved by first studying the positivity of the form $f_E(p_0, \cdot)$ at a fixed pole $p_0 \in \mathbb{S}^3$ and by then exploiting the frame invariance condition (3.5) and Lemma 3.4 to prove the positivity for any $q \in \mathbb{S}^3$.

Notice that the positivity of $f_E(q, \nabla q)$ holds true also for maps in $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$ by the lifting result of Bethuel–Chiron. In particular, for each Sobolev map $q \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$, the corresponding map $\Omega \ni x \mapsto \mathbf{Q}(q(x))$ belongs to the Sobolev class $W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))$. Moreover, the diffeomorphism $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3) \cong \mathbb{S}^3/\mathcal{H}$ establishes a bijective correspondence between $W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))$ and $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$, see e.g. [54] for details. Finally, using the Nash–Moser isometric embedding of the Riemannian homogeneous manifold $\mathbb{S}^3/\mathcal{H}$ into some Euclidean space $\mathbb{R}^N$, the elements $\mathbf{Q}$ of $W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))$ are identified with the Sobolev functions w in $W^{1,2}(\Omega, \mathbb{R}^N)$ such that $w(x) \in \mathbb{S}^3/\mathcal{H}$, for a.e. $x \in \Omega$.

Remark 3.6 In [54], we proved coercivity for the integral $\mathcal{I}_3(\mathbf{Q}) := \int_\Omega I_3(\mathbf{Q}, \nabla\mathbf{Q})\, dx$, by using the model for constrained biaxial nematic systems discussed in Sections 2.1 and 2.2. On account of the expression for I_3 in (3.7), we showed that

$$I_3(\mathbf{Q}, \nabla\mathbf{Q}) \geq 8\, S^2\, |\nabla(u, \mathbf{v})|^2, \qquad \mathbf{Q} = \mathbf{Q}(u, \mathbf{v}),$$

where, according to the alternative in (2.6), by assuming $S_1 < S_2 < 0$, we have set

$$S := \begin{cases} S_2 & \text{if} \quad \dfrac{S_1}{2} \leq S_2 < 0 \\ S_1 & \text{if} \quad S_2 \leq \dfrac{S_1}{2} < 0 \end{cases} \qquad S \neq 0\,. \tag{3.8}$$

4. Coercivity of the energy functional. In [55], we proved the following.

Theorem 3.7 *In the constrained biaxial case, if $L_4 \neq 0$, the quadratic form $L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4$ is positive definite if and only if the following system holds, according to the sign of L_4:*

i) $L_4 \geq 0$ *and*

$$\begin{cases} L_1 + L_2 + 2L_3 + \dfrac{2}{3}\, L_4(2S_1 - S_2) > 0 \\ L_2^2 + 2L_1L_2 + (L_1 + L_2)\Big(4L_3 + \dfrac{2}{3}\, L_4(S_1 + S_2)\Big) + 4L_3^2 + \dfrac{4}{9} L_4^2(2S_1 - S_2)(2S_2 - S_1) + \dfrac{4}{3} L_3L_4(S_1 + S_2) > 0 \\ 3L_3 + L_4(2S_1 - S_2) > 0 \\ 4L_3^2 + \dfrac{4}{9} L_4^2(2S_1 - S_2)(2S_2 - S_1) + \dfrac{4}{3} L_3L_4(S_1 + S_2) - L_2^2 > 0 \\ 4L_3^3 + L_2^3 - 3L_3L_2^2 - \dfrac{4}{27} L_4^3(2S_1 - S_2)(2S_2 - S_1)(S_1 + S_2) - \dfrac{4}{3} L_3L_4^2\big[S_1^2 - S_1S_2 + S_2^2\big] > 0\,. \end{cases}$$

ii) $L_4 \leq 0$ *and*

$$\begin{cases} L_1 + L_2 + 2L_3 - \dfrac{2}{3}\, L_4(S_1 + S_2) > 0 \\ L_2^2 + 2L_1L_2 + (L_1 + L_2)\Big(4L_3 - \dfrac{2}{3}\, L_4(2S_1 - S_2)\Big) + 4L_3^2 - \dfrac{4}{9} L_4^2(2S_2 - S_1)(S_1 + S_2) - \dfrac{4}{3} L_3L_4(2S_1 - S_2) > 0 \\ 3L_3 - L_4(S_1 + S_2) > 0 \\ 4L_3^2 - \dfrac{4}{9} L_4^2(2S_2 - S_1)(S_1 + S_2) - \dfrac{4}{3} L_3L_4(2S_1 - S_2) - L_2^2 > 0 \\ 4L_3^3 + L_2^3 - 3L_3L_2^2 - \dfrac{4}{27} L_4^3(2S_1 - S_2)(2S_2 - S_1)(S_1 + S_2) - \dfrac{4}{3} L_3L_4^2\big[S_1^2 - S_1S_2 + S_2^2\big] > 0\,. \end{cases}$$

The necessary and sufficient conditions of Theorem 3.7 can be interpreted as the constrained biaxial counterpart of the classical Ericksen inequalities, see (3.3) and (3.4). Notice moreover that if $L_4 = 0$, the positivity conditions in i) and ii) are both equivalent to

$$L_2 + L_3 > 0\,, \quad 2L_3 - L_2 > 0 \quad \text{and} \quad 2L_1 + L_2 + 2L_3 > 0\,.$$

Remark 3.8 By (2.6), the coefficients $L_4(2S_1 - S_2)$ and $L_4(S_1 + S_2)$ are both negative when $L_4 > 0$, and both positive when $L_4 < 0$, whereas the sign of $L_4(2S_2 - S_1)$ depends on the two regimes described in (2.6), according to the sign of L_4. Also, it turns out that independently of the sign of L_4, the last three conditions in the above two systems i) and ii) are equivalent. Finally, in both cases the necessary condition $L_3 > 0$ is satisfied.

As a consequence of the previous discussion, we have the following.

Theorem 3.9 *For a constrained biaxial nematic system, let* $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ *be of the form* (1.9)*, for constants* $L_1, L_2, L_3, L_4 \in \mathbb{R}$*. Then, there exists* $\nu > 0$ *such that*

$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) \geq \nu|\nabla\mathbf{Q}|^2, \quad \text{for all} \quad \mathbf{Q} \in W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)),$$

if and only if the constants L_1, L_2, L_3 *, and* L_4 *satisfy the conditions established in Theorem* 3.7*.*

Assume now that the admissible $\mathbf{Q}$ for the functional $\mathcal{F}[\mathbf{Q}]$ satisfy Dirichlet boundary conditions given as follows [17, 22, 37]. Let $\Omega \subset \mathbb{R}^3$ be a bounded and simply connected domain with smooth boundary $\partial\Omega$. For a smooth function $\varphi : \Omega \cup \partial\Omega \to \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$, we define the class $W^{1,2}_\varphi$ of admissible tensor fields by

$$W^{1,2}_\varphi := \left\{ \mathbf{Q} \in W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)) \,:\, \mathbf{Q}_{|\partial\Omega} = \varphi_{|\partial\Omega} \right\},$$

where equality is understood in the sense of traces. Therefore, for each $\mathbf{Q} \in W^{1,2}_\varphi$, the contribution to the energy of a divergence term is a real constant c_φ, only depending on φ.

In [55], we also found sufficient conditions on the coefficients L_i under which there exists a positive constant $\nu > 0$, such that

$$\psi_E(\mathbf{Q}(q), \nabla\mathbf{Q}(q)) = f_E(q, \nabla q) \geq \nu\,|\nabla q|^2 + \text{divergence term} \tag{3.9}$$

yielding to the coercivity of the elastic energy functional $\mathbf{Q} \mapsto \mathcal{F}_E[\mathbf{Q}]$, see (1.11), in the class $W^{1,2}_\varphi$.

The above mentioned sufficient conditions for the constrained biaxial case, can be seen as the counterpart of the analogous conditions for the constrained uniaxial case, compare e.g. [25, Section 5.1], which in terms of the coefficients L_i read

$$L_1 + L_2 + 2L_3 > \frac{2}{3}L_4 s\,, \quad L_1 + L_2 + 2L_3 + \frac{4}{3}L_4 s > 0\,, \quad 2L_3 - \frac{2}{3}L_4 s > 0\,.$$

5. Existence of minimizers. Now, since in the constrained theory the bulk part of the free-energy is constant,

$$\int_\Omega \psi_B(\mathbf{Q})\, dx = c_B\,, \quad \text{for all} \quad \mathbf{Q} \in W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))\,,$$

if the L_i satisfy the inequalities established in Theorem 3.7, there exist constants $K > \nu > 0$ such that

$$c_B + \nu \int_\Omega |\nabla\mathbf{Q}|^2\, dx \leq \mathcal{F}[\mathbf{Q}] \leq c_B + K \int_\Omega |\nabla\mathbf{Q}|^2\, dx\,, \quad \text{for all} \quad \mathbf{Q} \in W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))\,.$$

In a similar way, if the L_i satisfy the inequalities yielding to (3.9), there exist constants $K > \nu > 0$ such that

$$c_B + c_\varphi + \nu \int_\Omega |\nabla\mathbf{Q}|^2\, dx \leq \mathcal{F}[\mathbf{Q}] \leq c_B + c_\varphi + K \int_\Omega |\nabla\mathbf{Q}|^2\, dx\,, \quad \text{for all} \quad \mathbf{Q} \in W^{1,2}_\varphi\,.$$

Next, arguing as in [16, Section 4], it follows that the functional $\mathcal{F}[\mathbf{Q}]$ is convex in $\nabla\mathbf{Q}$ (and continuous in the strong $W^{1,2}$-topology) and hence weakly sequentially lower semicontinuous in $W^{1,2}$. Moreover, both classes $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$ and $W^{1,2}_{\varphi}$ are nonempty and closed under sequential weak convergence. Therefore, by compactness of the target manifold $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$, existence of minimizers for $\mathcal{F}[\mathbf{Q}]$ is guaranteed by the direct method of the calculus of variations (see, for instance, [25], Chapter 1.1). We can thus state the following existence results.

Theorem I *Let* $\Omega\subset\mathbb{R}^3$ *be a bounded, simply connected domain with smooth boundary* $\partial\Omega$*. Let the elastic constants* L_1, L_2, L_3*, and* L_4 *satisfy the inequalities established in Theorem* 3.7*. Then, the functional* $\mathcal{F}[\mathbf{Q}]$ *attains a minimum on* $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$*.*

Theorem II *Let* $\Omega\subset\mathbb{R}^3$ *be a bounded, simply connected domain with smooth boundary* $\partial\Omega$*. Let the elastic constants* L_1, L_2, L_3*, and* L_4 *satisfy the inequalities yielding to* (3.9)*. Let* $\varphi:\Omega\cup\partial\Omega\to\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ *be smooth. Then, the functional* $\mathcal{F}[\mathbf{Q}]$ *attains a minimum on* $W^{1,2}_{\varphi}$*.*

Open questions. There are several interesting open questions still to be investigated. A first problem would be that of finding the necessary and sufficient conditions in Theorem II. Another interesting question would be that of determining the precise inequalities which guarantee coercivity under the so-called *partial* Dirichlet boundary conditions or the physically relevant *conical anchoring* conditions proposed in [5].

4 Soft biaxial nematic systems

According to the terminology introduced by Longa and Trebin [39], a biaxial nematic phase is called *soft biaxial* if the corresponding tensor order parameter $\mathbf{Q}$ satisfies the additional constraint $\mathrm{tr}(\mathbf{Q}^2)=\mathrm{const}$.

If $\mathrm{tr}(\mathbf{Q}^2)=\rho^2$ for some $\rho>0$, by (2.12) the vector $\mathbf{u}=\mathbf{T}(\mathbf{Q})$ belongs to the 4-sphere $\mathbb{S}^4_\rho$ of radius ρ in $\mathbb{R}^5$. Let $\mathbb{S}^{(4)}_\rho$ be the space of matrices in $\mathcal{S}_0$ with norm ρ,

$$\mathbb{S}^{(4)}_\rho := \{\mathbf{Q}\in\mathcal{S}_0 \mid \mathrm{tr}(\mathbf{Q}^2)=\rho^2\}.$$

If $\mathbb{S}^{(4)}_\rho$ is endowed with the metric given by the inner product on $\mathcal{S}_0$ and $\mathbb{S}^4_\rho$ with its usual round metric, the mapping $\mathbf{T}$ defined in (2.11) induces an isometry $\mathbb{S}^{(4)}_\rho\cong\mathbb{S}^4_\rho$. Taking into account the constraints $\lambda_1,\lambda_2,\lambda_3\in[-1/3,2/3]$ on the eigenvalues, by (2.21), we have that $0<\mathrm{tr}(\mathbf{Q}^2)\le 2/3$. Thus if $0<\rho^2\le 2/3$, the tensor order parameter of a soft biaxial nematic system takes values in the class $\mathbb{S}^{(4)}_\rho$.

Furthermore, denoting with $W^{1,2}(\Omega,\mathbb{S}^{(4)}_\rho)$ the class of $W^{1,2}$-maps $\Omega\ni x\mapsto\mathbf{Q}(x)$ such that $\mathbf{Q}(x)\in\mathbb{S}^{(4)}_\rho$ for a.e. $x\in\Omega$, we deduce that the Sobolev class $W^{1,2}(\Omega,\mathbb{S}^{(4)}_\rho)$ is isometric to the Sobolev class

$$W^{1,2}(\Omega,\mathbb{S}^4_\rho) := \{\mathbf{u}\in W^{1,2}(\Omega,\mathbb{R}^5)\,:\,|\mathbf{u}(x)|=\rho \text{ for a.e. } x\in\Omega\},$$

and that actually

$$\int_\Omega |\nabla\mathbf{Q}|^2\,dx = \int_\Omega |\nabla\mathbf{u}|^2\,dx\,,\quad \mathbf{u}(x):=\mathbf{T}(\mathbf{Q}(x))\,,\quad x\in\Omega\,.$$

In the following, we shall identify the two spaces $\mathbb{S}^{(4)}_\rho\cong\mathbb{S}^4_\rho$ and denote them indistinctly by $\mathbb{S}^4_\rho$.

Remark 4.1 By Remark 2.6, we deduce that there is a 1:1 correspondence between the points of $\mathbb{S}^4_\rho$ and the possible physical configurations of the system if and only if $0<\rho^2\le 1/6$, a physical condition we shall assume in the sequel. This yields that for $0<\rho^2\le 1/6$, the order parameter space of soft biaxial nematic liquid crystals agrees with the 4-sphere $\mathbb{S}^4_\rho$.

4.1 Structure of the $SO(3)$-action on $\mathbb{S}^4_\rho$

In this subsection, we describe the basic structure of the action of $SO(3)$ on the 4-sphere $\mathbb{S}^4_\rho$. Following Section 2.2, the rotation group $SO(3)$ induces an action on the 4-sphere $\mathbb{S}^4_\rho\subset\mathcal{S}_0$ of radius ρ, for any fixed $\rho\le\sqrt{2/3}$. Therefore, every point in $\mathbb{S}^4_\rho$ is conjugate to a diagonal matrix in

$$\Sigma_\rho = \left\{\mathbf{\Lambda}=\mathrm{diag}(\lambda_1,\lambda_2,\lambda_3)\mid \lambda_1+\lambda_2+\lambda_3=0,\ \lambda_1^2+\lambda_2^2+\lambda_3^2=\rho^2\right\},$$

which amounts to saying that $SO(3)\star\Sigma_\rho = \mathbb{S}^4_\rho$. Every $SO(3)$-orbit passes through a diagonal matrix $\mathbf{\Lambda}\in\Sigma_\rho$ and the isotropy subgroup $SO(3)_{\mathbf{\Lambda}}$ only depends on the number of distinct eigenvalues.

In the generic case in which there are three distinct eigenvalues $\lambda_1,\ \lambda_2,\ \lambda_3$,[1] the isotropy subgroup at $\mathbf{\Lambda}$ is $H = S(O(1)\times O(1)\times O(1)) \cong \mathbb{Z}_2\times\mathbb{Z}_2$, the subgroup of diagonal matrices with entries ±1 and with determinant one, i.e., the dihedral group D_2, see (2.5). Consequently, the generic orbit $SO(3)\star\mathbf{\Lambda} = \{\mathbf{G}\star\mathbf{\Lambda} \mid \mathbf{G}\in SO(3)\}$ of the action is diffeomorphic to $SO(3)/H$, which can be seen as the eightfold quotient $\mathbb{S}^3/\mathcal{H}$, where $\mathcal{H} := \{\pm1,\ \pm\mathsf{i},\ \pm\mathsf{j},\ \pm\mathsf{k}\}$. The generic orbits have the highest possible dimension.

In the degenerate cases in which there are two (nonzero) equal eigenvalues, the isotropy subgroup at $\mathbf{\Lambda}$ is isomorphic to the infinite dihedral group D_∞ generated by the rotations around a fixed axis and 180^o-rotations about an axis orthogonal to it. The group D_∞ is actually isomorphic to $O(2)$, which implies that each (degenerate) orbit through $\mathbf{\Lambda}$ is diffeomorphic to the real projective plane $\mathbb{R}P^2$.

Remark 4.2 If $\mathbf{P},\mathbf{Q}\in\mathbb{S}^4_\rho$ are on the same $SO(3)$-orbit, their isotropy subgroups are conjugate. More precisely, if $\mathbf{P} = \mathbf{G}\star\mathbf{Q}$, for some $\mathbf{G}\in SO(3)$, then $SO(3)_{\mathbf{P}} = \mathbf{G}SO(3)_{\mathbf{Q}}\mathbf{G}^{-1}$. The isotropy subgroups $SO(3)_{\mathbf{P}}$ at points $\mathbf{P}\in\mathbb{S}^4_\rho$ which belong to an orbit $SO(3)\star\mathbf{Q}$ form a conjugacy class $(SO(3)_{\mathbf{Q}})$ called the *isotropy type* of the orbit $SO(3)\star\mathbf{Q}$. However, notice that if $\mathbf{P},\mathbf{Q}\in\mathbb{S}^4_\rho$ have conjugate isotropy subgroups, i.e., if there exists $\mathbf{G}\in SO(3)$ such that $SO(3)_{\mathbf{P}} = \mathbf{G}SO(3)_{\mathbf{Q}}\mathbf{G}^{-1}$, then they need not have the same orbit. By definition, they are said to be on the same *stratum* and the corresponding orbits $SO(3)\star\mathbf{P}$ and $SO(3)\star\mathbf{Q}$ are said to be of the *same isotropy type*. The stratum of a point $\mathbf{Q}\in\mathbb{S}^4_\rho$ is the union of all orbits of points having isotropy subgroups that are conjugate to $SO(3)_{\mathbf{Q}}$, i.e., it is the union of all orbits of isotropy type $(SO(3)_{\mathbf{Q}})$. Note that orbits of the same type are diffeomorphic. From the above discussion, it follows that $\mathbb{S}^4_\rho$ has two orbit types and that it can be partitioned into two strata: one consists of the two degenerate orbits, the other one of the generic orbits. For more details on the theory of G-manifolds, we refer the reader to [10, 61]. For some physical applications of the theory, see also [48, 49].

Let $\mathbf{E}_1,\mathbf{E}_2$ be the first two vectors of the orthonormal basis $\{\mathbf{E}_i\}_{i=1}^5$ given in (2.7). Let $\mathbf{\Lambda}:\mathbb{R}\to\mathbb{S}^4_\rho\subset\mathcal{S}_0$ be the periodic parameterized curve, with period $2\pi\rho$, defined by

$$\mathbf{\Lambda}(t) := \rho\cos(t/\rho)\mathbf{E}_1 + \rho\sin(t/\rho)\mathbf{E}_2, \quad t\in\mathbb{R}\,.$$

The image of $\mathbf{\Lambda}$ coincides with the set Σ_ρ of all diagonal matrices in $\mathbb{S}^4_\rho$ and it is the *great circle* of $\mathbb{S}^4_\rho$ obtained by intersecting $\mathbb{S}^4_\rho$ with the 2-dimensional linear subspace $\Pi := \mathrm{span}\{\mathbf{E}_1,\mathbf{E}_2\}$ of $\mathcal{S}_0$ spanned by $\mathbf{E}_1$ and $\mathbf{E}_2$. In particular, as a constant (unit) speed parametrization of a great circle, the curve $\mathbf{\Lambda}:\mathbb{R}\to\mathbb{S}^4_\rho$ is a geodesic of $\mathbb{S}^4_\rho$ (cf. [58, p. 103]).

Every matrix $\mathbf{Q}\in\mathbb{S}^4_\rho\subset\mathcal{S}_0$ is related by conjugation to some diagonal matrix $\mathbf{\Lambda}(t)$. Now, under the action of the matrix $\mathbf{G}(\mathbf{e}_3,\pi/2)$, see (2.2), which represents a rotation through $\pi/2$ about the z-axis, the diagonal matrix $\mathbf{\Lambda}(t)$ is taken to $\mathbf{G}(\mathbf{e}_3,\pi/2)\star\mathbf{\Lambda}(t) = \mathbf{G}(\mathbf{e}_3,\pi/2)\mathbf{\Lambda}(t)\mathbf{G}(\mathbf{e}_3,\pi/2)^T = \mathbf{\Lambda}(-t)$.[2] Next, consider the rotations about the axis in the direction of the unit vector $\mathbf{e} := \frac{1}{\sqrt{3}}(\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3)$. Under the matrices $\mathbf{G}(\mathbf{e},\pm2\pi/3)$, the diagonal matrix $\mathbf{\Lambda}(t)$ is taken to $\mathbf{G}(\mathbf{e},\pm2\pi/3)\star\mathbf{\Lambda}(t) = \mathbf{\Lambda}(t\mp\frac{2\pi}{3})$, respectively.

This implies that the parameter $t\in\mathbb{R}$ can be restricted to the closed interval $I = [0,\frac{\pi}{3}\rho]$. This interval cannot be further reduced, since the function $\det\mathbf{\Lambda}(t) = -\frac{\rho^3}{3\sqrt{6}}\cos(3t/\rho)$ is invertible on the interval I. Therefore, *the geodesic segment* $\mathbf{\Lambda}:[0,\frac{\pi}{3}\rho]\to\mathbb{S}^4_\rho$ *intersects each* $SO(3)$*-orbit of* $\mathbb{S}^4_\rho$ *exactly once.* As a consequence, the orbit space $\mathbb{S}^4_\rho/SO(3)$ is homeomorphic to the closed interval $[0,\frac{\pi}{3}\rho]$.

Remark 4.3 Observe that for $t\in[0,\frac{\pi}{3}\rho]$, $\mathbf{\Lambda}(t) = \mathrm{diag}(\lambda_1,\lambda_2,\lambda_3)$ with $\lambda_1\geq\lambda_2\geq\lambda_3$. In particular, this yields the well-known fact that any $\mathbf{Q}\in\mathbb{S}^4_\rho$ is equivalent under the $SO(3)$-action to a diagonal matrix $\mathrm{diag}(\lambda_1,\lambda_2,\lambda_3)$ with $\lambda_1\geq\lambda_2\geq\lambda_3$.

For $t\in(0,\frac{\pi}{3}\rho)$, the diagonal matrix $\mathbf{\Lambda}(t)$ has distinct eigenvalues $\lambda_1>\lambda_2>\lambda_3$ and the orbit of $\mathbf{\Lambda}(t)$ is diffeomorphic to the eightfold quotient $\mathbb{S}^3/\mathcal{H}$. In particular, we have that $\mathbf{\Lambda}(\frac{\pi}{6}\rho) = \frac{\rho}{\sqrt{2}}\mathrm{diag}(1,0,-1)$, which corresponds to a maximally biaxial phase (cf. (2.20)). Instead, the isotropy group at $\mathbf{\Lambda}_- := \mathbf{\Lambda}(0) = \rho\mathbf{E}_1$ is $K^- = S(O(2)\times O(1))$. The degenerate orbit $B_- := SO(3)/K^-$ through $\mathbf{\Lambda}_-$ is the set of all symmetric matrices with two equal positive eigenvalues which identifies with the real projective plane $\mathbb{R}P^2$. The tangent space T_- to the orbit B_- is $T_- = \mathrm{span}(\mathbf{E}_4,\mathbf{E}_5)$ and its orthogonal complement is $T_-^\perp = \mathrm{span}(\mathbf{E}_2,\mathbf{E}_3)$. Thus,

[1] Observe that this conditions holds on an open and dense subset.
[2] Note that $\mathbf{\Lambda}(-t)$ is obtained from $\mathbf{\Lambda}(t)$ by interchanging the first two eigenvalues.

$\mathbf{\Lambda}(t)$ is an arclength parameterized geodesic starting at $\mathbf{\Lambda}_-$ which is orthogonal to the orbit B_- and hence to all orbits through $\mathbf{\Lambda}(t)$ (cf. [61]). Similarly, the isotropy group at $\mathbf{\Lambda}_+ := \mathbf{\Lambda}(\frac{\pi}{3}\rho) = \frac{\rho}{\sqrt{6}}\,\mathrm{diag}(2,-1,-1)$ is $K^+ = S(O(1)\times O(2))$ and the degenerate orbit $B_+ = SO(3)/K^+$ through $\mathbf{\Lambda}_+$ is the set of all symmetric matrices with two equal negative eigenvalues which again identifies with $\mathbb{R}P^2$. Therefore, *on the geodesic segment* $\mathbf{\Lambda} : [0, \frac{\pi}{3}\rho] \to \mathbb{S}^4_\rho$, *the orbits of* $\mathbf{\Lambda}(0)$ *and* $\mathbf{\Lambda}(\frac{\pi}{3}\rho)$ *are 2-dimensional, while the orbits of* $\mathbf{\Lambda}(t)$, $t \in (0, \frac{\pi}{3}\rho)$, *are 3-dimensional.*

The action of $SO(3)$ on $\mathbb{S}^4_\rho$ just described is the well-known *cohomogeneity one action* of $SO(3)$ on $\mathbb{S}^4_\rho$ (cf. [30, 31]). This action has two orbits of codimension two which are isolated among codimension one orbits of the same type. In accordance with the basic structure of cohomogeneity one actions (cf., for example, [1, 2, 10, 51]), if $\pi : \mathbb{S}^4_\rho \to \mathbb{S}^4_\rho/SO(3) \cong [0, \frac{\pi}{3}\rho]$ is the orbit projection, the inverse images of the interior points are the *principal* or *regular* orbits, while the two *singular* orbits correspond to the inverse images of the endpoints, namely $B_- = \pi^{-1}(0)$ and $B_+ = \pi^{-1}(\frac{\pi}{3}\rho)$. In addition, the great circle Σ_ρ meets every orbit of $\mathbb{S}^4_\rho$ orthogonally and is a *section* or *canonical form* for $\mathbb{S}^4_\rho$, in the sense of the general theory of canonical forms developed by Palais and Terng (cf. [60, 61]).

Remark 4.4 If r denotes the rotation by $2\pi/3$ of the circle $\Sigma_\rho \subset \Pi$ induced by $\mathbf{G}(\mathbf{e}, 2\pi/3)$ and if m is the reflection about a diameter of Σ_ρ induced by $\mathbf{G}(\mathbf{e}_3, \pi/2)$, then it is easily seen that r has order three, m has order two, and that r and m generate the six-element group $\Delta_3 := \{1, r, r^2, m, rm, r^2m\}$, which is the symmetry group of the equilateral triangle. The group Δ_3 is isomorphic to the subgroup of $SO(3)$ that takes Σ_ρ into itself.

Remark 4.5 From a differential geometric point of view, the principal orbits of the $SO(3)$-action on the 4-sphere $\mathbb{S}^4_\rho$ are homogeneous hypersurfaces in $\mathbb{S}^4_\rho$. As such, they have constant principal curvatures and are therefore examples of the so-called *isoparametric hypersurfaces* [12, 31, 60, 61]. On the other hand, each singular orbit is a concrete realization of a minimal embedding of the real projective plane with constant curvature into $\mathbb{S}^4_\rho$, the so-called *Veronese surface* (cf. [30, 31, 35, 69]). The two singular orbits are antipodal to each other at distance $\frac{\pi}{3}\rho$. Explicit immersions of the orbits as submanifolds of the Euclidean 4-sphere $\mathbb{S}^4_\rho$ in $\mathbb{R}^5$ are provided below via the isometric isomorphism $\mathbf{T}$ defined in (2.11).

Remark 4.6 Observe that the image $\mathbf{T}(\mathbf{\Lambda}([0, \frac{\pi}{3}\rho]))$ of the geodesic arc $\mathbf{\Lambda}([0, \frac{\pi}{3}\rho])$ under $\mathbf{T}$ corresponds, in the $\mathbf{xy}$-plane, to the intersection of the fundamental domain $\lhd_f$ with $\mathbb{S}^1_\rho = \mathbf{T}(\Sigma_\rho)$ (cf. Section 2.4, Figure 1).

Principal orbits. Any 3-dimensional principal $SO(3)$-orbit in $\mathbb{S}^4_\rho$ can be interpreted as the order parameter space of a constrained biaxial nematic system, see Section 2.2. Therefore, using the expressions (1.2) and (2.8), we compute

$$q_1 = S_1\,(\mathbf{n}_1^2 - 1/3) + S_2(\mathbf{m}_1^2 - 1/3)\,, \quad q_2 = S_1\,(\mathbf{n}_2^2 - 1/3) + S_2(\mathbf{m}_2^2 - 1/3)\,,$$
$$q_3 = S_1\,\mathbf{n}_1\mathbf{n}_2 + S_2\,\mathbf{m}_1\mathbf{m}_2\,, \quad q_4 = S_1\,\mathbf{n}_1\mathbf{n}_3 + S_2\,\mathbf{m}_1\mathbf{m}_3\,, \quad q_5 = S_1\,\mathbf{n}_2\mathbf{n}_3 + S_2\,\mathbf{m}_2\mathbf{m}_3\,,$$

where $\mathbf{n}$ and $\mathbf{m}$ are the first two columns of the rotation matrix $\mathbf{G}(\mathbf{u}, \theta)$ in (2.2), respectively, and hence

$$\mathbf{T}(\mathbf{Q}) = \frac{\sqrt{2}}{2}\begin{pmatrix} \sqrt{3}\left(S_1(\mathbf{n}_1^2 + \mathbf{n}_2^2) + S_2(\mathbf{m}_1^2 + \mathbf{m}_2^2) - \dfrac{2}{3}\,(S_1 + S_2)\right) \\ \left(S_1(\mathbf{n}_1^2 - \mathbf{n}_2^2) + S_2(\mathbf{m}_1^2 - \mathbf{m}_2^2)\right) \\ 2\left(S_1\,\mathbf{n}_1\mathbf{n}_2 + S_2\,\mathbf{m}_1\mathbf{m}_2\right) \\ 2\left(S_1\,\mathbf{n}_1\mathbf{n}_3 + S_2\,\mathbf{m}_1\mathbf{m}_3\right) \\ 2\left(S_1\,\mathbf{n}_2\mathbf{n}_3 + S_2\,\mathbf{m}_2\mathbf{m}_3\right) \end{pmatrix}^T$$

compare (2.11), with

$$\mathrm{tr}(\mathbf{Q}^2) = \rho^2(\lambda_1, \lambda_2) = 2\,(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2) = \frac{2}{3}\,(S_1^2 + S_2^2 - S_1S_2)\,.$$

The map $\mathbf{T} : \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3) \to \mathbb{S}^4_\rho$ gives rise to an isometric immersion of the 3-dimensional order parameter space $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3) \cong \mathbb{S}^3/\mathcal{H}$ into the 4-sphere $\mathbb{S}^4_\rho$ of radius $\rho(\lambda_1, \lambda_2)$. This immersion is a homogeneous isoparametric hypersurface [12, 31, 60, 67].

SINGULAR ORBITS. In the constrained uniaxial case, the tensor field $\mathbf{Q}$ takes the form (1.5), where s is a constant, and the order parameter space of the system identifies with the real projective plane $\mathbb{R}P^2$. In this case, we compute

$$\mathbf{T}(\mathbf{Q}) = s\,\frac{\sqrt{2}}{2}\left(\sqrt{3}\left(\mathbf{r}_1^2+\mathbf{r}_2^2-\frac{2}{3}\right),\, \mathbf{r}_1^2-\mathbf{r}_2^2,\, 2\mathbf{r}_1\mathbf{r}_2,\, 2\mathbf{r}_1\mathbf{r}_3,\, 2\mathbf{r}_2\mathbf{r}_3\right),$$

and $\operatorname{tr}(\mathbf{Q}^2)=2s^2/3$. Writing in spherical coordinates $\mathbf{r}_1=\cos\alpha\sin\beta$, $\mathbf{r}_2=\sin\alpha\sin\beta$, $\mathbf{r}_3=\cos\beta$, we have

$$\mathbf{T}(\mathbf{Q}) = s\,\frac{\sqrt{2}}{2}\left(\sqrt{3}\left(\sin^2\beta-\frac{2}{3}\right),\, \cos(2\alpha)\sin^2\beta,\, \sin(2\alpha)\sin^2\beta,\, \cos\alpha\sin(2\beta),\, \sin\alpha\sin(2\beta)\right).$$

The mapping $\mathbf{T}$ can be interpreted as giving an embedding $\mathbf{T}:\mathbb{R}P^2\to\mathbb{S}^4_\rho$ of the real projective plane $\mathbb{R}P^2$ into the 4-sphere $\mathbb{S}^4_\rho$ of radius $\rho=\sqrt{2s^2/3}$. The image $\mathbf{T}(\mathbb{R}P^2)$ is the *Veronese surface*, which is a minimal surface in $\mathbb{S}^4_\rho$ (cf. [35, 69] for more details).

4.2 Coercivity conditions

In this subsection, we study the coercivity properties of the elastic free-energy density (1.9) in the soft biaxial case, assuming first that $L_4=0$. For this purpose, we shall exploit the constraint $\mathbf{Q}\in\mathbb{S}^4_\rho$, the existence of the section Σ_ρ for $\mathbb{S}^4_\rho$ and the frame-indifference condition.

Since $\mathbb{S}^4_\rho = SO(3)\star\Sigma_\rho$ (cf. Section 4.1), any element $\mathbf{Q}\in\mathbb{S}^4_\rho$ can be written in the form $\mathbf{Q}=\mathbf{G}\mathbf{\Lambda}\mathbf{G}^T$ for some $\mathbf{G}\in SO(3)$, where $\mathbf{\Lambda}=\operatorname{diag}(\lambda_1,\lambda_2,\lambda_3)\in\Sigma_\rho$. Now, if $\mathbf{D}$ denotes the third order tensor defined by $\mathbf{D}_{ijk}=\mathbf{Q}_{ij,k}$ and $M=\mathbf{G}^T$, the frame-indifference condition (1.7) yields that

$$\psi(\mathbf{Q},\mathbf{D})=\psi(\mathbf{\Lambda},\mathbf{D}^*)\,,\quad \text{where}\quad \mathbf{D}^*_{ijk}=\mathbf{G}^l_i\mathbf{G}^m_j\mathbf{G}^p_k\mathbf{D}_{lmp}\,. \tag{4.1}$$

Actually, this condition holds for any point $\mathbf{Q}$ on the orbit of $\mathbf{\Lambda}$.

Next, if $\mathbf{u}\in W^{1,2}(\Omega,\mathbb{S}^4_\rho)$, we know that the constrain $|\mathbf{u}(x)|=\rho$ implies the orthogonality condition

$$\mathbf{u}\cdot\partial_k\mathbf{u}=0\quad\forall\,k=1,2,3\,.$$

By condition (4.1), we then may and do assume that $\mathbf{u}(x)=\mathbf{T}(\mathbf{\Lambda})$, where $\mathbf{\Lambda}=\operatorname{diag}(\lambda_1,\lambda_2,\lambda_3)$ is the diagonal matrix of the eigenvalues of $\mathbf{Q}(x)$, so that $2\,(\lambda_1^2+\lambda_2^2+\lambda_1\lambda_2)=\rho^2$. We thus have (cf. Section 2.4)

$$\mathbf{u}(x)=\mathbf{T}(\mathbf{\Lambda})=\frac{\sqrt{2}}{2}\left(\sqrt{3}\,(\lambda_1+\lambda_2),\,(\lambda_1-\lambda_2),\,0,\,0,\,0\right)$$

and the orthogonality condition becomes

$$\sqrt{3}\,(\lambda_1+\lambda_2)\partial_k u^1+(\lambda_1-\lambda_2)\partial_k u^2=0\quad\forall\,k=1,2,3\,.$$

Finally, in the case $\lambda_1\neq\lambda_2$, the above condition is equivalent to

$$\partial_k u^2=\frac{\sqrt{3}}{3}\,\mathbf{t}\,\partial_k u^1\,,\quad \mathbf{t}:=3\,\frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}=\frac{S_1+S_2}{S_2-S_1}\,.$$

Now, if $0<\rho^2\le 1/6$, the parameter $\mathbf{t}$ takes each real value. The case $1/6<\rho^2\le 2/3$ has to be treated separately, as in that case the parameter $\mathbf{t}$ has a smaller range. In fact, e.g. in the limiting case $\rho^2=2/3$, the set of $\mathbf{Q}$-tensors $\mathbb{S}^4_\rho$ reduces to the uniaxial phases with $\operatorname{tr}(\mathbf{Q}^2)=2/3$.

If $L_4=0$ and if $0<\rho^2\le 1/6$, the conditions (1.12) of Longa–Monselesan–Trebin [38] and Davis–Gartland [16] are necessary and sufficient for coercivity:

Theorem 4.7 *Assume that $0<\rho^2\le 1/6$ and $L_4=0$. Then the elastic energy density (1.9) is positive definite in the soft biaxial class $\mathbb{S}^4_\rho$ if and only if the following conditions hold:*

$$2L_3>L_2\,,\quad L_3+L_2>0\,,\quad 10L_1+L_2+6L_3>0\,.$$

Assume now that the admissible $\mathbf{Q}$ for the functional $\mathcal{F}[\mathbf{Q}]$ satisfy Dirichlet boundary conditions as before. More precisely, we let $\Omega \subset \mathbb{R}^3$ be a bounded and simply connected domain with smooth boundary $\partial\Omega$. For a smooth function $\varphi : \Omega \cup \partial\Omega \to \mathbb{S}^4_\rho$, we define the class

$$\widetilde{W}^{1,2}_\varphi := \left\{ \mathbf{Q} \in W^{1,2}(\Omega, \mathbb{S}^4_\rho) \, : \, \mathbf{Q}_{|\partial\Omega} = \varphi_{|\partial\Omega} \right\} .$$

Corollary 4.8 *If* $0 < \rho^2 \leq 1/6$ *and* $L_4 = 0$*, then the elastic energy functional* (1.11) *is coercive on the admissible set* $\widetilde{W}^{1,2}_\varphi$ *if and only if*

$$\begin{cases} L_3 > 0 & \textit{in case} \quad L_1 + L_2 \geq 0 \\ 2L_2 + 2L_2 + 3L_3 > 0 & \textit{in case} \quad L_1 + L_2 < 0 \, . \end{cases}$$

The fourth elastic invariant. We now consider the elastic energy (1.9) with $L_4 \neq 0$. Contrary to the general biaxial case, we now see that even if $L_4 \neq 0$, in the soft biaxial case we can find necessary and sufficient conditions for the positivity.

Theorem 4.9 *Assume that* $0 < \rho^2 \leq 1/6$ *and* $L_1 = L_2 = 0$*. Then the elastic energy density* (1.9) *is positive definite in the soft biaxial class* $\mathbb{S}^4_\rho$ *if and only if the following condition holds:*

$$\sqrt{6}\, L_3 > 2\rho \, |L_4| \, .$$

Obtaining necessary and sufficient conditions for the elastic energy density (1.9), when all the physical coefficients L_i are non-trivial, implies a great effort, even in the simpler case $0 < \rho^2 \leq 1/6$. However, by putting together the conditions from Theorem 4.7, Corollary 4.8, and Theorem 4.9, we readily obtain a range of sufficient conditions to positivity in the soft biaxial regime.

Corollary 4.10 *Assume that* $0 < \rho^2 \leq 1/6$*. Then the elastic energy density* (1.9) *is positive definite in the soft biaxial class* $\mathbb{S}^4_\rho$ *if the following condition are satisfied for some coefficient* $\alpha \in (0,1)$ *:*

$$2(1-\alpha)\, L_3 > L_2 \, , \quad (1-\alpha)\, L_3 + L_2 > 0 \, , \quad 10L_1 + L_2 + 6(1-\alpha)\, L_3 > 0 \, , \quad \alpha \sqrt{6}\, L_3 > 2\rho \, |L_4| \, .$$

Similarly, the elastic energy functional (1.11) *is coercive on the admissible set* $\widetilde{W}^{1,2}_\varphi$ *if (and only if)* $L_3 > 0$*, in case* $L_1 + L_2 \geq 0$*, and provided that:*

$$2L_2 + 2L_2 + (1-\alpha)\, L_3 > 0 \, , \quad \alpha \sqrt{6}\, L_3 > 2\rho \, |L_4|$$

for some coefficient $\alpha \in (0,1)$*, in case* $L_1 + L_2 < 0$*.*

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