# On the Landau–de Gennes elastic energy of a $Q$-tensor model for soft biaxial nematics

*Domenico Mucci and Lorenzo Nicolodi*

**Abstract**

In the Landau–de Gennes theory of liquid crystals, the propensities for alignments of molecules are represented at each point of the fluid by an element $\mathbf{Q}$ of the vector space $\mathcal{S}_0$ of $3 \times 3$ real symmetric traceless matrices, or $\mathbf{Q}$-tensors. According to Longa and Trebin [25], a biaxial nematic system is called *soft biaxial* if the tensor order parameter $\mathbf{Q}$ satisfies the constraint $\mathrm{tr}(\mathbf{Q}^2) = \mathrm{const}$. After the introduction of a $\mathbf{Q}$-tensor model for soft biaxial nematic systems and the description of its geometric structure, we address the question of coercivity for the most common four-elastic-constant form of the Landau–de Gennes elastic free-energy [4, 20, 35, 38] in this model. For a soft biaxial nematic system, the tensor field $\mathbf{Q}$ takes values in a four-dimensional sphere $\mathbb{S}^4_\rho$ of radius $\rho \leq \sqrt{2/3}$ in the five-dimensional space $\mathcal{S}_0$ with inner product $\langle \mathbf{Q}, \mathbf{P} \rangle = \mathrm{tr}(\mathbf{QP})$. The rotation group $SO(3)$ acts orthogonally on $\mathcal{S}_0$ by conjugation and hence induces an action on $\mathbb{S}^4_\rho \subset \mathcal{S}_0$. This action has generic orbits of codimension one that are diffeomorphic to an eightfold quotient $\mathbb{S}^3/\mathcal{H}$ of the unit three-sphere $\mathbb{S}^3$, where $\mathcal{H} = \{\pm 1, \pm \mathsf{i}, \pm \mathsf{j}, \pm \mathsf{k}\}$ is the quaternion group, and has two degenerate orbits of codimension two that are diffeomorphic to the projective plane $\mathbb{R}P^2$. Each generic orbit can be interpreted as the order parameter space of a constrained biaxial nematic system and each singular orbit as the order parameter space of a constrained uniaxial nematic system [37, 38]. It turns out that $\mathbb{S}^4_\rho$ is a cohomogeneity one manifold, i.e., a manifold with a group action whose orbit space is one-dimensional [1, 19, 34]. Another important geometric feature of the model is that the set $\Sigma_\rho$ of diagonal $\mathbf{Q}$-tensors of fixed norm $\rho$ is a (geodesic) great circle in $\mathbb{S}^4_\rho$ which meets every orbit of $\mathbb{S}^4_\rho$ orthogonally and is then a *section* for $\mathbb{S}^4_\rho$ in the sense of the general theory of canonical forms [42, 43]. We compute necessary and sufficient coercivity conditions for the elastic energy by exploiting the $SO(3)$-invariance of the elastic energy (frame-indifference), the existence of the section $\Sigma_\rho$ for $\mathbb{S}^4_\rho$, and the geometry of the model, which allow us to reduce to a suitable invariant problem on (an arc of) $\Sigma_\rho$. Our approach can ultimately be seen as an application of the general method of reduction of variables, or cohomogeneity method [18, 19].

**Key words:** Landau–de Gennes energy, $\mathbf{Q}$-tensor theory, soft biaxial nematics, liquid crystals, symmetry breaking

**AMS subject classifications:** 82D30, 76A15, 76M30, 49J40, 35A15, 58K70

## 1 Introduction

In the Landau–de Gennes theory of nematic liquid crystals [11, 17, 35], the propensities for alignments of molecules are represented, at each point $x$ of the region $\Omega$ occupied by the fluid, by an element $\mathbf{Q} = \mathbf{Q}(x)$ of the five-dimensional vector space

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

of all $3 \times 3$ real symmetric traceless matrices, the so-called $\mathbf{Q}$-tensors, with matrix norm $|\mathbf{Q}| := \sqrt{\mathrm{tr}(\mathbf{Q}^2)}$. The tensor field $\mathbf{Q}$, known as the *order parameter* tensor field, contains information about the degree of order and the deviation from isotropy of the liquid crystal at a point in $\Omega$. More specifically, the eigenvectors of $\mathbf{Q}$ give the directions of preferred orientation of the molecules, while the eigenvalues give the degree of order about these directions [9, 35]. An equilibrium state of a nematic liquid crystal is called a *phase*. In terms of the order parameter tensor field $\mathbf{Q}$, a phase is said to be (1) *isotropic* (I) when $\mathbf{Q}$ has three equal eigenvalues (and hence, zero), i.e., when $\mathbf{Q}$ vanishes identically, (2) *uniaxial* ($\mathrm{N_U}$) when $\mathbf{Q}$ has two nonzero equal eigenvalues, and (3) *biaxial* ($\mathrm{N_B}$) when $\mathbf{Q}$ has three distinct eigenvalues. Transitions from isotropic to uniaxial or biaxial nematic phases are usually connected with the breaking of the $SO(3)$ rotational symmetry of the system [21, 32].

In a general biaxial phase, the tensor order parameter $\mathbf{Q}$ can be written as

$$\mathbf{Q} = S_1\Big(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\Big) + S_2\Big(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}\mathbf{I}\Big), \tag{1.1}$$

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

$$\lambda_1 = \frac{2S_1 - S_2}{3}, \quad \lambda_2 = \frac{2S_2 - S_1}{3}, \quad \lambda_3 = -\frac{S_1 + S_2}{3}\,. \tag{1.2}$$

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, $\mathbf{Q} = \lambda_1\mathbf{n}\otimes\mathbf{n} + \lambda_2\mathbf{m}\otimes\mathbf{m} + \lambda_3\boldsymbol{\ell}\otimes\boldsymbol{\ell}$. (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

$$\mathbf{Q} = s\Big(\mathbf{r}\otimes\mathbf{r} - \frac{1}{3}\mathbf{I}\Big)\,, \quad s : \Omega \to \mathbb{R},\ \mathbf{r} : \Omega \to \mathbb{S}^2. \tag{1.3}$$

For a general biaxial phase, $(\mathrm{tr}(\mathbf{Q}^2))^3 \geq 6(\mathrm{tr}(\mathbf{Q}^3))^2$ and equality holds in the uniaxial case only [16, 28]. The eigenvalues of physical $\mathbf{Q}$-tensors are subject to the constraints $-1/3 \leq \lambda_i \leq 2/3$, $i = 1, 2, 3$, though from a physical point of view the limiting values $\lambda_i = -1/3$ or $\lambda_i = 2/3$ represent unrealistic configurations (cf. [4, 28] for a discussion of the physical meaning of these constraints). This implies in particular that the matrix norm of physical $\mathbf{Q}$-tensors is bounded (cf. also Section 2.2).

The Landau–de Gennes free-energy functional is a nonlinear integral functional (cf. [3, 5, 11, 35])

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

of the components of $\mathbf{Q}$ and of its gradient $\nabla\mathbf{Q}$, subject to the appropriate physical symmetries. 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

$$\psi(\mathbf{Q}, \nabla\mathbf{Q}) = \psi(M\mathbf{Q}M^T, \mathbf{D}^*), \qquad \forall\, M = (M^i_j) \in SO(3)\,, \tag{1.4}$$

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. [3]). 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 $\psi$ is composed of a thermotropic bulk part and an elastic part (cf. [3, 35]),

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

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

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

where $A, B, C, D, E$ and $E'$ are material bulk constants (see, for instance, [10, 11, 16]). A most common expression for the free-elastic energy density is [11, 35, 46]

$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) = L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4, \tag{1.5}$$

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

$$I_1 := \mathbf{Q}_{ij,j}\mathbf{Q}_{ik,k}\,, \quad I_2 := \mathbf{Q}_{ik,j}\mathbf{Q}_{ij,k}\,, \quad I_3 := \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}\,, \quad I_4 := \mathbf{Q}_{lk}\mathbf{Q}_{ij,l}\mathbf{Q}_{ij,k}\,. \tag{1.6}$$

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 [3, 4]. On the other hand, it is known that, if $L_4 = 0$, the elastic part of the energy,

$$\mathcal{F}_E[\mathbf{Q}] := \int_\Omega \psi_E(\mathbf{Q}, \nabla\mathbf{Q})\, dx\,, \tag{1.7}$$

is bounded from below and coercive if and only if the elastic constants $L_1$, $L_2$, and $L_3$ satisfy [10, 24]

$$L_3 > 0\,, \quad -L_3 < L_2 < 2L_3\,, \quad L_1 > -\frac{3}{5}L_3 - \frac{1}{10}L_2\,. \tag{1.8}$$

(We will propose a proof of this result in the final appendix of the paper.)

In the *constrained* (or *hard*) uniaxial theory, $\mathbf{Q}$ has a constant scalar order parameter and the order parameter space identifies with the projective plane $\mathbb{R}P^2$ [3, 5, 36]. 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 [14, 41, 51]

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

where the $K_i$ are elastic constants. This is achieved (cf. [5, 6, 35]) by formally calculating the energy density (1.5) in terms of $\mathbf{r}$ and $\nabla\mathbf{r}$ and by then choosing the $L_i$ and the $K_i$, $i = 1, 2, 3, 4$, so that

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

Relations among $L_1$, $L_2$, $L_3$, and $L_4$ can be determined so that the corresponding energy density is coercive [5, 12, 24, 49].

In the *constrained* (or *hard*) biaxial theory [15, 24, 25], it is assumed that the scalar order parameters $S_1$, $S_2$ of $\mathbf{Q}$ are independent of position. This amounts to requiring that the three distinct eigenvalues of $\mathbf{Q}$ are constant or equivalently that both the scalar invariants $\operatorname{tr}(\mathbf{Q}^2)$ and $\operatorname{tr}(\mathbf{Q}^3)$ are constant. In this case, the order parameter space is diffeomorphic to the eightfold quotient $\mathbb{S}^3/\mathcal{H}$ of the three-sphere $\mathbb{S}^3$, where $\mathcal{H} = \{\pm 1, \pm\mathsf{i}, \pm\mathsf{j}, \pm\mathsf{k}\}$ is the quaternion group [37, 39]. 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 [37, 38].

Following Longa and Trebin [25], a biaxial $\mathbf{Q}$-tensor $\mathbf{Q} \in \mathcal{S}_0$ (and the corresponding phase) is called *soft biaxial* if $\operatorname{tr}(\mathbf{Q}^2)$ is a given constant. Accordingly, a *soft biaxial nematic system* (or *system of soft biaxial nematic phases*) is a system whose tensor order parameter $\mathbf{Q}$ is required to satisfy the constraint

$$\operatorname{tr}(\mathbf{Q}^2) = \rho^2, \tag{1.9}$$

for some $\rho > 0$, independent of the position $x \in \Omega$ (cf. also [33, 44, 45]). In a soft biaxial nematic system, 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 [2], soft biaxial nematic systems are difficult to study experimentally. Professor Longa [27] suggested that possible general candidates of soft biaxial systems could be certain micellar systems where the micellar shape is allowed to fluctuate (cf. [26] and the references therein). An important subclass is that where in addition to $\operatorname{tr}(\mathbf{Q}^2) = \text{const}$ also $\operatorname{tr}(\mathbf{Q}^3) = 0$ is required; in fact, this case gives second order isotropic-nematic (I-N) phase transition (cf. the Landau point $L$ in [2, 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. [16] for details).

Let $\mathbb{S}^4_\rho \subset \mathcal{S}_0$ denote the set of biaxial $\mathbf{Q}$-tensors satisfying the soft condition (1.9), i.e.,

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

With respect to the matrix norm $|\mathbf{Q}| = \sqrt{\operatorname{tr}(\mathbf{Q}^2)}$, the set $\mathbb{S}^4_\rho$ can be seen as the four-dimensional sphere of radius $\rho$ in the five-dimensional vector space $\mathcal{S}_0$. Taking into account that the eigenvalues are subject to the constraints $-1/3 \le \lambda_i \le 2/3$, $i = 1, 2, 3$, it follows that $0 < \rho \le \sqrt{2/3}$ (cf. Section 2). This implies that, for a soft biaxial nematic system, the order parameter tensor field $\mathbf{Q}$ takes values in a four-dimensional sphere $\mathbb{S}^4_\rho$ in $\mathcal{S}_0$. The special orthogonal (rotation) group $SO(3)$ acts orthogonally on $\mathcal{S}_0$ by conjugation and hence induces an action on $\mathbb{S}^4_\rho \subset \mathcal{S}_0$. The four-sphere $\mathbb{S}^4_\rho$ acted upon by the symmetry group $SO(3)$ provides a mathematical model of symmetry breaking for soft biaxial nematic systems. The study of the action of $SO(3)$ on $\mathbb{S}^4_\rho$ will answer the question of which subgroups of $SO(3)$ can be symmetry groups of equilibrium states (phases) of the system and will allow the determination of the corresponding order parameters of phases with broken symmetry (cf. Section 2). This will make clear the link between phase transitions and the breaking of the $SO(3)$ symmetry. For a discussion of the general question of symmetry breaking in physical problems invariant under a group $G$, we refer the reader to [21, 29, 31, 32] and the references therein.

The purposes of this paper are twofold. The first is to describe the geometric features of the above $\mathbf{Q}$-tensor model for soft biaxial nematic systems. The second purpose is to address the question of coercivity for the Landau–de Gennes elastic free-energy (1.7), exploiting from the outset the geometry of the model and the frame-indifference of the energy density.

Description of results and organization of the paper. In Section 2, after recalling some background material about the $\mathbf{Q}$-tensor theory of nematic liquid crystals, we discuss the basic geometric structure of the $\mathbf{Q}$-tensor model for soft biaxial nematic systems introduced above. This is achieved by studying the action of $SO(3)$ on the four-sphere $\mathbb{S}^4_\rho$. More precisely, the action of $SO(3)$ on $\mathbb{S}^4_\rho$ has generic orbits of codimension one which are diffeomorphic to an eightfold quotient $\mathbb{S}^3/\mathcal{H}$ of the unit three-sphere $\mathbb{S}^3$, where $\mathcal{H}$ is the quaternion group, and has two degenerate orbits of codimension two which are diffeomorphic to the projective plane $\mathbb{R}P^2$. It turns out that $\mathbb{S}^4_\rho$ is a *cohomogeneity one* manifold, i.e., a manifold with a group action whose orbit space is one-dimensional (cf. [1, 19, 34]). Each generic orbit can be interpreted as the order parameter space of a constrained biaxial nematic system, while each singular orbit can be interpreted as the order parameter space of a constrained uniaxial nematic system (cf. [37, 38]). From a differential geometric point of view, the generic orbits can be seen as examples of isoparametric hypersurfaces (cf. Sections 2.4 and 2.5), while each degenerate orbit can be seen as a Veronese surface, i.e., as a minimally embedded projective plane with constant curvature in $\mathbb{S}^4_\rho$ (cf. Sections 2.4 and 2.6). An additional geometric feature of the model is that the set $\Sigma_\rho$ of diagonal $\mathbf{Q}$-tensors of fixed norm $\rho$ is a (geodesic) great circle in $\mathbb{S}^4_\rho$ which meets every orbit of $\mathbb{S}^4_\rho$ orthogonally. Thus $\Sigma_\rho$ is a *section* for $\mathbb{S}^4_\rho$ in the sense of the general theory of canonical forms (cf. [42, 43]).

In Section 3, we compute necessary and sufficient conditions for the positivity of the elastic energy density (1.5) of a soft biaxial nematic system when $L_4 = 0$. For this we exploit both the $SO(3)$-invariance of the elastic energy density (frame-indifference) and the geometric properties of the $\mathbf{Q}$-tensor model for soft biaxial nematic systems, which allow us to reduce to a suitable invariant problem on (an arc of) the section $\Sigma_\rho$. More precisely, we show that if $\rho^2 = \operatorname{tr}(\mathbf{Q}^2)$ is sufficiently small, namely $0 < \rho^2 \le 1/6$, then there exists a constant $\nu > 0$, such that

$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) \ge \nu\, |\nabla\mathbf{Q}|^2$$

for all admissible $\mathbf{Q}$ if and only if the constants $L_1$, $L_2$, and $L_3$ satisfy the same conditions (1.8) established in [10] and [24] for general biaxial $\mathbf{Q}$-tensors. This is the content of Theorem 3.3. Notice that, for $0 < \rho^2 \le 1/6$, the order parameter space of soft biaxial nematic systems agrees with the whole four-sphere $\mathbb{S}^4_\rho$ (cf. Remark 2.3). Interestingly enough, the soft biaxial condition has no effect on the coercivity conditions when $0 < \rho^2 \le 1/6$. Instead, sharper conditions are obtained if $1/6 < \rho^2 \le 2/3$. This case is discussed in Remark 3.5 and especially in Proposition 3.6. Finally, using the fact that the energy density $I_1 - I_2$ is a null-Lagrangian, the coercivity of the elastic energy functional (1.7) under Dirichlet-type boundary conditions is discussed in Corollary 3.7, when $0 < \rho^2 \le 1/6$.

In Section 4, we prove a necessary and sufficient condition for the positivity of the (simplest form of the) elastic energy density $\psi_E$ of a soft biaxial nematic system when $L_4 \ne 0$. More precisely, we have the following (cf. Theorem 4.1).

**Theorem** *Assume that $0 < \rho^2 \le 1/6$. The elastic energy density (1.5) with $L_1 = L_2 = 0$ is positive definite in the soft biaxial class $\mathbb{S}^4_\rho$ if and only if the following condition holds:*

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

The above condition clarifies the role played by the soft biaxial constraint in the coercivity issue when the elastic energy density $\psi_E$ contains the cubic term $I_4$, which explicitly depends on $\mathbf{Q}(x)$ and hence on the eigenvalues of $\mathbf{Q}$ (cf. Equation (4.2)). As we already observed, for general $\mathbf{Q}$-tensors the energy $\mathcal{F}[\mathbf{Q}]$ need not be bounded from below when $L_4 \neq 0$ (cf. [3, 4]). As a consequence, sufficient conditions for the positivity of the elastic energy density (1.5) (and for the coercivity of the elastic energy functional (1.7) under Dirichlet-type boundary conditions) are obtained in Corollary 4.3. Finding necessary conditions when all the physical constants $L_i$ are nonzero, requires quite involved computations.

Finally, in the appendix, we reobtain the necessary and sufficient conditions (1.8) for the positivity of the elastic energy density $\psi_E = L_1 I_1 + L_2 I_2 + L_3 I_3$ in the case of general biaxial $\mathbf{Q}$-tensors. To make the calculations we use appropriate coordinates corresponding to the representation of $\mathbf{Q}$-tensors given in Section 2.1. Originally, conditions (1.8) were obtained in [24] by writing the elastic energy $\psi_E$ 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 [30].

**Acknowledgments**. We would like to thank Professor Lech Longa for his kind interest. The authors would also like to thank the anonymous referees for their useful comments and suggestions.

This research was partially supported by PRIN 2010-2011 "Calcolo delle Variazioni" (D.M.) and by PRIN 2010-2011 "Varietà reali e complesse: geometria, topologia e analisi armonica" (L.N.). The authors are members of the "Gruppo Nazionale per l'Analisi Matematica, la Probabilità e le loro Applicazioni" (GNAMPA) (D.M.) and of the "Gruppo Nazionale per le Strutture Algebriche, Geometriche e le loro Applicazioni" (GNSAGA) (L.N.) of the Istituto Nazionale di Alta Matematica "F. Severi" (INdAM).

## 2 A model for soft biaxial nematics

In this section, we recall some background material about the $\mathbf{Q}$-tensor theory of nematic liquid crystals and describe the basic geometric structure and properties of a $\mathbf{Q}$-tensor model for the order parameter space of a soft biaxial nematic system.

### 2.1 Representation of Q-tensors

Let $\mathcal{S}_0$ be the vector space of $3 \times 3$ real symmetric traceless matrices, or $\mathbf{Q}$-tensors,

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

with inner product $\langle \mathbf{Q}, \mathbf{P} \rangle = \operatorname{tr}(\mathbf{QP})$ and norm $|\mathbf{Q}| = \sqrt{\operatorname{tr}(\mathbf{Q}^2)}$. Let $\{\mathbf{E}_i\}_{i=1}^5$ be the ordered orthonormal basis for $\mathcal{S}_0$ given by (cf. [47])

$$\begin{aligned}
&\mathbf{E}_1 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \qquad \mathbf{E}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathbf{E}_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
&\mathbf{E}_4 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \mathbf{E}_5 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.
\end{aligned} \tag{2.1}$$

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

$$\mathbf{Q} = \begin{pmatrix} q_1 & q_3 & q_4 \\ q_3 & q_2 & q_5 \\ q_4 & q_5 & -(q_1 + q_2) \end{pmatrix} = \sum_{i=1}^{5} u^i \mathbf{E}_i, \quad \text{where } u^i = \operatorname{tr}(\mathbf{Q}\mathbf{E}_i). \tag{2.2}$$

It easily follows that

$$u^1 = \frac{\sqrt{6}}{2}(q_1 + q_2)\,, \quad u^2 = \frac{\sqrt{2}}{2}(q_1 - q_2)\,, \quad u^i = \sqrt{2} q_i\,, \quad i = 3, 4, 5 \tag{2.3}$$

and then

$$q_1 = \frac{1}{\sqrt{6}}u^1 + \frac{1}{\sqrt{2}}u^2\,, \quad q_2 = \frac{1}{\sqrt{6}}u^1 - \frac{1}{\sqrt{2}}u^2\,, \quad q_i = \frac{1}{\sqrt{2}}u^i\,, \quad i = 3, 4, 5. \tag{2.4}$$

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

$$\mathbf{T}(\mathbf{Q}) = \mathbf{T}(u^1\mathbf{E}_1 + \cdots + u^5\mathbf{E}_5) := (u^1, \ldots, u^5) = \mathbf{u}, \tag{2.5}$$

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,

$$\mathrm{tr}(\mathbf{Q}^2) = 2\,(q_1^2 + q_2^2 + q_1 q_2 + q_3^2 + q_4^2 + q_5^2) = |\mathbf{T}(\mathbf{Q})|^2 = |\mathbf{u}|^2. \tag{2.6}$$

Following [10], 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 (2.5) establishes an isometric isomorphism between the Soboles classes $W^{1,2}(\Omega, \mathbb{R}^5)$ and $W^{1,2}(\Omega, \mathcal{S}_0)$ (cf. [10]). 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 2.1** Assume that the map $\Omega \ni x \mapsto \mathbf{Q}(x) \in \mathcal{S}_0$ is smooth. By the above identifications, using (2.2), (2.3) and (2.4), we compute

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

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

$$|\nabla \mathbf{Q}(x)| = |\nabla \mathbf{u}(x)|\,, \quad x \in \Omega\,. \tag{2.7}$$

**Remark 2.2** For $\mathbf{Q} \in \mathcal{S}_0$, with eigenvalues $\lambda_1, \lambda_2, \lambda_3$, $\mathrm{tr}(\mathbf{Q}^2) = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = -2(\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3)$, and then

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

From the Cayley–Hamilton theorem, it follows that

$$\mathbf{Q}^3 - \frac{\mathrm{tr}(\mathbf{Q}^2)}{2}\,\mathbf{Q} - (\det \mathbf{Q})\,\mathbf{I} = 0. \tag{2.8}$$

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

$$t^3 - \frac{\mathrm{tr}(\mathbf{Q}^2)}{2}\,t - \frac{\mathrm{tr}(\mathbf{Q}^3)}{3} = 0\,. \tag{2.9}$$

Using (2.8), 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 $\mathrm{tr}(\mathbf{Q}^3)$ [3, 16]. Moreover, it follows from (2.9) 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 (2.9) 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 if $(\mathrm{tr}(\mathbf{Q}^2))^3 = 6(\mathrm{tr}(\mathbf{Q}^3))^2$.

## 2.2 Plane representation of diagonal Q-tensors

Let $\mathbf{Q} = \mathbf{\Lambda}(\lambda_1, \lambda_2, \lambda_3) = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ 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

$$\mathbf{x} := \frac{\sqrt{6}}{2}\,(\lambda_1 + \lambda_2)\,, \quad \mathbf{y} := \frac{\sqrt{2}}{2}\,(\lambda_1 - \lambda_2). \tag{2.10}$$

By (2.4), we have the inverse formulas

$$\lambda_1 = \frac{\sqrt{2}}{2}\Big(\frac{\mathbf{x}}{\sqrt{3}} + \mathbf{y}\Big)\,, \quad \lambda_2 = \frac{\sqrt{2}}{2}\Big(\frac{\mathbf{x}}{\sqrt{3}} - \mathbf{y}\Big)\,, \quad \lambda_3 = -\frac{2}{\sqrt{6}}\,\mathbf{x}\,. \tag{2.11}$$

The physical constraints $-1/3 \leq \lambda_i \leq 2/3$ 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. [9, 28])

$$\triangleleft := \Big\{(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^2 \mid -(\mathbf{x}/\sqrt{3} + \sqrt{2}/3) \leq \mathbf{y} \leq (\mathbf{x}/\sqrt{3} + \sqrt{2}/3)\,, \quad -2/\sqrt{6} \leq \mathbf{x} \leq 1/\sqrt{6}\Big\}\,,$$

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

$$\lambda_1 = \lambda_2 \iff \mathbf{y} = 0\,, \quad \lambda_1 = \lambda_3 \iff \mathbf{y} = -\sqrt{3}\,\mathbf{x}\,, \quad \lambda_2 = \lambda_3 \iff \mathbf{y} = \sqrt{3}\,\mathbf{x} \tag{2.12}$$

and the so-called *maximally biaxial* phases are

$$\lambda_1 = 0 \iff \mathbf{y} = -\frac{\mathbf{x}}{\sqrt{3}}\,, \quad \lambda_2 = 0 \iff \mathbf{y} = \frac{\mathbf{x}}{\sqrt{3}}\,, \quad \lambda_3 = 0 \iff \mathbf{x} = 0\,. \tag{2.13}$$

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

$$\mathrm{tr}(\mathbf{Q}^2) = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = \mathbf{x}^2 + \mathbf{y}^2 \leq \frac{2}{3}. \tag{2.14}$$

As explained in Section 2.4 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, $\lambda_1 \geq \lambda_2 \geq \lambda_3$, the point $(\mathbf{x}, \mathbf{y})$ representing $\mathbf{Q}$ takes value in a subset $\triangleleft_f$ of $\triangleleft$,

$$\triangleleft_f := \Big\{(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^2 \mid 0 \leq \mathbf{x} \leq 1/\sqrt{6},\, 0 \leq \mathbf{y} \leq \sqrt{3}\mathbf{x}\Big\}$$

referred to as the *fundamental domain* (cf. for example [28]).

**Remark 2.3** In this representation, the diagonal $\mathbf{Q}$-tensors satisfying the condition $\mathrm{tr}(\mathbf{Q}^2) \equiv \rho^2$, for some positive constant $\rho$, correspond to the points of the intersection between $\triangleleft$ and the circle $\mathbb{S}^1_\rho$ of radius $\rho$ 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 $\triangleleft$;
- if $\rho^2 = 1/6$, the circle $\mathbb{S}^1_{1/\sqrt{6}}$ is tangent to the boundary of $\triangleleft$ 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 $\triangleleft$ in three points $(\mathbf{x}, \mathbf{y})$ whose first coordinates are, 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 $\triangleleft$ at the vertices $(\frac{-2}{\sqrt{6}}, 0)$, $(\frac{1}{\sqrt{6}}, \frac{\pm\sqrt{2}}{2})$;
- if $\rho^2 > 2/3$, the circle $\mathbb{S}^1_\rho$ does not intersect the triangle $\triangleleft$.

**Remark 2.4** Using the notation (2.10) and (2.11), we have

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

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

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

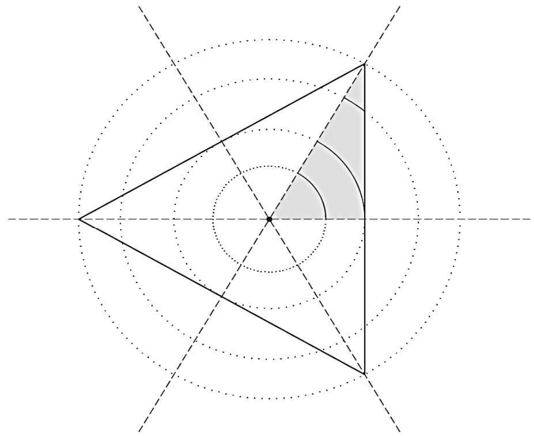

Figure 1: The *physical triangle* $\triangleleft$ and the *fundamental domain* $\triangleleft_f$ (shaded region) in the $\mathbf{xy}$-plane. The origin $(0,0)$ represents the isotropic phase. The dashed lines $U = \{(\mathbf{x},\mathbf{y}) \in \triangleleft \mid \mathbf{y} = 0 \text{ or } \mathbf{y}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

## 2.3 Soft biaxial nematic systems

According to the terminology introduced by Longa and Trebin [25] (cf. also the introduction), a biaxial nematic system is called *soft biaxial* if the corresponding tensor order parameter $\mathbf{Q}$ satisfies the additional constraint $\operatorname{tr}(\mathbf{Q}^2) = \text{const}$, independently of the position.

If $\operatorname{tr}(\mathbf{Q}^2) = \rho^2$, for some $\rho > 0$, by (2.6), the vector $\mathbf{u} = \mathbf{T}(\mathbf{Q})$ belongs to the four-sphere $\mathbb{S}^4_\rho$ of radius $\rho$ in $\mathbb{R}^5$. Let $\mathbb{S}^{(4)}_\rho$ be the space of matrices in $\mathcal{S}_0$ with matrix norm $\rho$, i.e.,

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

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 (2.5) 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 (2.14), we have that $0 < \operatorname{tr}(\mathbf{Q}^2) \leq 2/3$. Thus if $0 < \rho^2 \leq 2/3$, the tensor order parameter of a soft biaxial nematic system takes values in $\mathbb{S}^{(4)}_\rho$.

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 2.5** By Remark 2.3, 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 $0 < \rho^2 \leq 1/6$. This yields that for $0 < \rho^2 \leq 1/6$, the order parameter space of soft biaxial nematic liquid crystals agrees with the four-sphere $\mathbb{S}^4_\rho$.

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

In this section we describe the basic structure of the action of $SO(3)$ on the four-sphere $\mathbb{S}^4_\rho$. The rotation group $SO(3)$ acts on $\mathcal{S}_0$ by conjugation $\mathbf{G} \star \mathbf{Q} = \mathbf{G}\mathbf{Q}\mathbf{G}^T$ preserving the inner product $\langle \mathbf{Q}, \mathbf{P} \rangle = \operatorname{tr}(\mathbf{Q}\mathbf{P})$. It then induces an action on the four-sphere $\mathbb{S}^4_\rho \subset \mathcal{S}_0$ of radius $\rho$, for any fixed $\rho \leq \sqrt{2/3}$. The well known fact that every element of $\mathcal{S}_0$ can be diagonalized by an orthogonal matrix translates to the statement that 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 $SO(3) \star \Sigma_\rho = \mathbb{S}^4_\rho$. Therefore, every $SO(3)$-orbit passes through a diagonal matrix $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3) \in \Sigma_\rho$ and the *isotropy subgroup* $SO(3)_{\mathbf{\Lambda}} := \{\mathbf{G} \in SO(3) \mid \mathbf{G} \star \mathbf{\Lambda} = \mathbf{\Lambda}\}$ of $SO(3)$ at $\mathbf{\Lambda}$ 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 $\pm 1$ and with determinant one,

$$H = \{\mathrm{diag}(1, 1, 1),\, \mathrm{diag}(-1, -1, 1),\, \mathrm{diag}(-1, 1, -1),\, \mathrm{diag}(1, -1, -1)\}.$$

The isotropy subgroup $H$ is the dihedral group $D_2$ consisting of the identity and $180^o$-rotations about three mutually perpendicular axes. 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 $\mathcal{H} := \{\pm 1, \pm \mathsf{i}, \pm \mathsf{j}, \pm \mathsf{k}\}$ is the non-abelian eight-element quaternion group [37, 38]. This is achieved by lifting $SO(3)$ and $H$ to the unit sphere $\mathbb{S}^3$, viewed as the group $Sp(1)$ of unit quaternions, under the twofold cover $\mathbb{S}^3 \to SO(3)$ which sends $q \in Sp(1)$ into a rotation of angle $2\theta$ in the 2-plane $\mathrm{Im}(q)^\perp \subset \mathrm{Im}(\mathbb{H})$, where $\theta$ is the angle between $q$ and 1 in $\mathbb{S}^3$. 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 $D_\infty$ generated by the rotations around a fixed axis and $180^o$-rotations about an axis orthogonal to it. The group $D_\infty$ is actually isomorphic to $O(2)$, which implies that each (degenerate) orbit through $\mathbf{\Lambda}$ is diffeomorphic to the real projective plane $\mathbb{R}P^2$ (cf. [29]).

**Remark 2.6** 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 [7, 43]. For some physical applications of the theory, see also [31, 32].

Let $\mathbf{E}_1, \mathbf{E}_2$ be the first two vectors of the orthonormal basis $\{\mathbf{E}_i\}_{i=1}^5$ given in (2.1). Let $\mathbf{\Lambda} : \mathbb{R} \to \mathbb{S}^4_\rho \subset \mathcal{S}_0$ be the periodic parametrized 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 $\Sigma_\rho$ of all diagonal matrices in $\mathbb{S}^4_\rho$ and 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. [40, 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 rotation matrix

$$\mathbf{G}(\mathbf{e}_3, \pi/2) := \begin{pmatrix} \cos\frac{\pi}{2} & -\sin\frac{\pi}{2} & 0 \\ \sin\frac{\pi}{2} & \cos\frac{\pi}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

[1] Observe that this conditions holds on an open and dense subset.

which represents a rotation through $\pi/2$ about the $z$-axis (cf. (2.15)), 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] (Here and below, $\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3$ denote the standard orthonormal coordinate vectors of $\mathbb{R}^3$.) Next, consider the rotation matrix

$$\mathbf{G}(\mathbf{e},\theta):=\begin{pmatrix}\frac{1}{3}(2\cos\theta+1) & \frac{1}{3}(1-\cos\theta-\sqrt{3}\sin\theta) & \frac{1}{3}(1-\cos\theta+\sqrt{3}\sin\theta)\\ \frac{1}{3}(1-\cos\theta+\sqrt{3}\sin\theta) & \frac{1}{3}(2\cos\theta+1) & \frac{1}{3}(1-\cos\theta-\sqrt{3}\sin\theta)\\ \frac{1}{3}(1-\cos\theta-\sqrt{3}\sin\theta) & \frac{1}{3}(1-\cos\theta+\sqrt{3}\sin\theta) & \frac{1}{3}(2\cos\theta+1)\end{pmatrix},$$

representing the rotation though $\theta$ 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 rotation matrices $\mathbf{G}(\mathbf{e},\pm 2\pi/3)$, given by

$$\mathbf{G}(\mathbf{e},2\pi/3)=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}\quad\text{and}\quad\mathbf{G}(\mathbf{e},-2\pi/3)=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix},$$

the diagonal matrix $\mathbf{\Lambda}(t)$ is taken to $\mathbf{G}(\mathbf{e},\pm 2\pi/3)\star\mathbf{\Lambda}(t)=\mathbf{\Lambda}(t\mp\frac{2\pi}{3})$, 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 2.7** Observe that for $t\in[0,\frac{\pi}{3}\rho]$, $\mathbf{\Lambda}(t)=\operatorname{diag}(\lambda_1,\lambda_2,\lambda_3)$ 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 $\operatorname{diag}(\lambda_1,\lambda_2,\lambda_3)$ 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 $\mathbf{\Lambda}(\frac{\pi}{6}\rho)=\frac{\rho}{\sqrt{2}}\operatorname{diag}(1,0,-1)$, which corresponds to a maximally biaxial phase (cf. (2.13)). 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 $T_-=\operatorname{span}(\mathbf{E}_4,\mathbf{E}_5)$ and its orthogonal complement is $T_-^\perp=\operatorname{span}(\mathbf{E}_2,\mathbf{E}_3)$. Thus, $\mathbf{\Lambda}(t)$ is an arclength parametrized geodesic starting at $\mathbf{\Lambda}_-$ which is orthogonal to the orbit $B_-$ and hence to all orbits through $\mathbf{\Lambda}(t)$ (cf. [43]). Similarly, the isotropy group at $\mathbf{\Lambda}_+:=\mathbf{\Lambda}(\frac{\pi}{3}\rho)=\frac{\rho}{\sqrt{6}}\operatorname{diag}(2,-1,-1)$ 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. [18, 19]). 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, 7, 34]), 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 $\Sigma_\rho$ 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. [42, 43]).

**Remark 2.8** 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 $\Sigma_\rho$ 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 $\Delta_3$ is isomorphic to the subgroup of $SO(3)$ that takes $\Sigma_\rho$ into itself.

**Remark 2.9** From a differential geometric point of view, the principal orbits of the $SO(3)$-action on the four-sphere $\mathbb{S}^4_\rho$ are homogeneous hypersurfaces in $\mathbb{S}^4_\rho$. As such, they have constant principal curvatures and

[2]Note that $\mathbf{\Lambda}(-t)$ is obtained from $\mathbf{\Lambda}(t)$ by interchanging the first two eigenvalues.

are therefore examples of the so-called *isoparametric hypersurfaces* [8, 19, 42, 43]. 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. [18, 19, 22, 50]). 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 four-sphere $\mathbb{S}^4_\rho$ in $\mathbb{R}^5$ are provided in the next two sections via the isometric isomorphism $\mathbf{T}$ defined in (2.5).

**Remark 2.10** 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 2.2, Figure 1).

## 2.5 Principal orbits as order parameter spaces of constrained biaxial systems

Any 3-dimensional principal $SO(3)$-orbit in $\mathbb{S}^4_\rho$ can be interpreted as the order parameter space of a constrained (or hard) biaxial nematic system [29, 37, 38]. In this case, the *order parameter space* of the system is the set $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ of all $\mathbf{Q}$-tensors in $\mathcal{S}_0$ of the form (1.1) with three distinct eigenvalues $\lambda_1, \lambda_2, \lambda_3 \in (-1/3, 2/3)$ which are constant, independent of $x \in \Omega$. Any element $\mathbf{Q} \in \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ can be written in the form

$$\mathbf{Q} = \mathbf{G}\mathbf{\Lambda}\mathbf{G}^T \quad \text{for some} \quad \mathbf{G} \in SO(3),$$

where $\mathbf{\Lambda} = \mathbf{\Lambda}(\lambda_1, \lambda_2, \lambda_3) = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$ is the diagonal matrix of the eigenvalues of $\mathbf{Q}$ and thus $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ coincides with the orbit of $\mathbf{\Lambda}$ with respect to the $SO(3)$-action by conjugation on $\mathcal{S}_0$. If $\mathbf{Q} \in \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$, we have $\operatorname{tr}(\mathbf{Q}^2) = 2(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2)$.

Any element of $SO(3)$ represents a rotation through an angle $\theta$ about a fixed axis. The matrix of $SO(3)$ representing a rotation through $\theta$ with axis in direction of the unit vector $\mathbf{a} = a_1\mathbf{e}_1 + a_2\mathbf{e}_2 + a_3\mathbf{e}_3$ is

$$\mathbf{G}(\mathbf{a}, \theta) := \begin{pmatrix} a_1^2(1-\cos\theta)+\cos\theta & a_1a_2(1-\cos\theta)-a_3\sin\theta & a_1a_3(1-\cos\theta)+a_2\sin\theta \\ a_1a_2(1-\cos\theta)+a_3\sin\theta & a_2^2(1-\cos\theta)+\cos\theta & a_2a_3(1-\cos\theta)-a_1\sin\theta \\ a_1a_3(1-\cos\theta)-a_2\sin\theta & a_2a_3(1-\cos\theta)+a_1\sin\theta & a_3^2(1-\cos\theta)+\cos\theta \end{pmatrix}. \tag{2.15}$$

Therefore, using the expression (1.1), 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 matrix $\mathbf{G}(\mathbf{a}, \theta)$, respectively, and hence

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

with

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

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 four-sphere $\mathbb{S}^4_\rho$ of radius $\rho(\lambda_1, \lambda_2)$. This immersion is a homogeneous isoparametric hypersurface [8, 19, 42, 48].

## 2.6 Singular orbits as order parameter spaces of constrained uniaxial systems

In the constrained uniaxial case, the tensor field $\mathbf{Q}$ takes the form (1.3), 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 $\mathrm{tr}(\mathbf{Q}^2) = 2s^2/3$. 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 four-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. [22, 50] for more details).

# 3 Coercivity conditions

In this section, we study the coercivity properties of the elastic free-energy density (1.5) in the soft biaxial case, assuming that $L_4 = 0$. In the next section, we will deal with the case $L_4 \neq 0$. For this purpose, we shall exploit the constraint $\mathbf{Q} \in \mathbb{S}^4_\rho$, the existence of the section $\Sigma_\rho$ for $\mathbb{S}^4_\rho$ and the frame-indifference condition.

Since $\mathbb{S}^4_\rho = SO(3) \star \Sigma_\rho$ (cf. Section 2.4), 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 $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3) \in \Sigma_\rho$. 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 (1.4) yields that

$$\psi(\mathbf{Q}, \mathbf{D}) = \psi(\mathbf{\Lambda}, \mathbf{D}^*)\,, \quad \text{where} \quad \mathbf{D}^*_{ijk} = \mathbf{G}_i^l \mathbf{G}_j^m \mathbf{G}_k^p \mathbf{D}_{lmp}\,. \tag{3.1}$$

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 (3.1), we then may and do assume that $\mathbf{u}(x) = \mathbf{T}(\mathbf{\Lambda})$, where $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ 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 2.2)

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

and the orthogonality condition becomes

$$\sqrt{3}\,(\lambda_1 + \lambda_2)\partial_k u^1 + (\lambda_1 - \lambda_2)\partial_k u^2 = 0 \quad \forall\, k = 1, 2, 3\,. \tag{3.2}$$

In the case $\lambda_1 \neq \lambda_2$, the above condition (3.2) is equivalent to

$$\partial_k u^2 = \frac{\sqrt{3}}{3}\,\mathbf{t}\,\partial_k u^1\,, \quad \mathbf{t} := 3\,\frac{\lambda_1 + \lambda_2}{\lambda_2 - \lambda_1} = \frac{S_1 + S_2}{S_2 - S_1}\,. \tag{3.3}$$

The uniaxial phase $\lambda_1 = \lambda_2$ is treated separately at the end of the proof.

**Remark 3.1** By the expressions (2.10) and (2.11), we have

$$\mathbf{t} = -\sqrt{3}\,\frac{\mathbf{x}}{\mathbf{y}}\,, \tag{3.4}$$

which implies that $\mathbf{t} \in \mathbb{R}$. Actually, according to the observations on the fundamental domain given in Sections 2.2 and 2.4, the range of the parameter $\mathbf{t}$ can be restricted to $(-\infty, -1]$. However, this restriction does not help in simplifying computations.

We shall use that if $0 < \rho^2 \leq 1/6$, then the parameter $\mathbf{t}$ takes each real value. The case $1/6 < \rho^2 \leq 2/3$ will 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 $\mathrm{tr}(\mathbf{Q}^2) = 2/3$.

**Remark 3.2** Equivalently to (3.2), by conditions

$$\partial_k(q_1^2 + q_2^2 + q_1 q_2 + q_3^2 + q_4^2 + q_5^2) = 0\,, \quad \mathbf{Q} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$$

we obtain

$$(2\lambda_2+\lambda_1)\partial_k q_1 + (2\lambda_1+\lambda_2)\partial_k q_2 = 0 \quad \forall\, k=1,2,3$$

that in terms of the scalar order parameters $S_1, S_2$ reads as

$$S_2\,\partial_k q_1 + S_1\,\partial_k q_2 = 0 \quad \forall\, k=1,2,3\,.$$

Notice also that in the uniaxial phases, if $\lambda_1=\lambda_3$ we have $S_1=0$ and $\mathbf{t}=1$, whereas if $\lambda_2=\lambda_3$ then $S_2=0$ and $\mathbf{t}=-1$.

We are now in a position to prove our first coercivity result for the elastic energy of a soft biaxial nematic system. If $L_4=0$ and if $0<\rho^2\le 1/6$, the conditions (1.8) of Longa–Monselesan–Trebin [24] and Davis–Gartland [10] are necessary and sufficient for coercivity. More precisely, we have the following.

**Theorem 3.3** *Assume that $0<\rho^2\le 1/6$. The elastic energy density* (1.5) *with $L_4=0$ is positive definite in the soft biaxial class $\mathbb{S}^4_\rho$ if and only if the following conditions hold:*

$$2L_3 > L_2\,, \quad L_3+L_2>0\,, \quad 10L_1+L_2+6L_3>0\,. \tag{3.5}$$

Proof: We impose (3.3) in the computation of the elastic invariants $I_i$. As for the third elastic invariant, by (2.7) we have

$$I_3 = |\nabla u|^2 = \Big(1+\frac{\mathbf{t}^2}{3}\Big)|\nabla u^1|^2 + |\nabla u^3|^2 + |\nabla u^4|^2 + |\nabla u^5|^2\,. \tag{3.6}$$

We now compute the term $I_1=\mathbf{Q}_{ij,j}\mathbf{Q}_{ik,k}$ as

$$I_1 = (\partial_1 q_1 + \partial_2 q_3 + \partial_3 q_4)^2 + (\partial_1 q_3 + \partial_2 q_2 + \partial_3 q_5)^2 + (\partial_1 q_4 + \partial_2 q_5 - \partial_3(q_1+q_2))^2\,. \tag{3.7}$$

By the inverse formulas (2.4) we get

$$\partial_k q_1 = \frac{\sqrt2}{2}\Big(\frac{\sqrt3}{3}\,\partial_k u^1 + \partial_k u^2\Big)\,, \quad \partial_k q_2 = \frac{\sqrt2}{2}\Big(\frac{\sqrt3}{3}\,\partial_k u^1 - \partial_k u^2\Big)\,, \quad \partial_k q_j = \frac{\sqrt2}{2}\,\partial_k u^j\,, \quad j=3,4,5$$

and hence, by the relation (3.3), we have

$$\partial_k q_1 = \frac{\sqrt2}{2}\,\frac{1}{\sqrt3}\,(1+\mathbf{t})\,\partial_k u^1, \quad \partial_k q_2 = \frac{\sqrt2}{2}\,\frac{1}{\sqrt3}\,(1-\mathbf{t})\,\partial_k u^1, \quad \partial_k(q_1+q_2) = \frac{\sqrt2}{2}\,\frac{2}{\sqrt3}\,\partial_k u^1\,.$$

This yields that at the point $\mathbf{Q}=\mathbf{\Lambda}$

$$\begin{aligned}
2\,I_1 = {} & \Big(\frac{1}{\sqrt3}\,(1+\mathbf{t})\,\partial_1 u^1 + \partial_2 u^3 + \partial_3 u^4\Big)^2 \\
& + \Big(\partial_1 u^3 + \frac{1}{\sqrt3}\,(1-\mathbf{t})\,\partial_2 u^1 + \partial_3 u^5\Big)^2 \\
& + \Big(\partial_1 u^4 + \partial_2 u^5 - \frac{2}{\sqrt3}\,\partial_3 u^1\Big)^2 \\
= {} & \frac13\,(1+\mathbf{t})^2(\partial_1 u^1)^2 + \frac13\,(1-\mathbf{t})^2(\partial_2 u^1)^2 + \frac43\,(\partial_3 u^1)^2 \\
& + (\partial_1 u^3)^2 + (\partial_2 u^3)^2 + (\partial_1 u^4)^2 + (\partial_3 u^4)^2 + (\partial_2 u^5)^2 + (\partial_3 u^5)^2 \\
& + \frac{2}{\sqrt3}\,(1+\mathbf{t})\,\partial_1 u^1\,(\partial_2 u^3 + \partial_3 u^4) + \frac{2}{\sqrt3}\,(1-\mathbf{t})\,\partial_2 u^1\,(\partial_1 u^3 + \partial_3 u^5) \\
& - \frac{4}{\sqrt3}\,\partial_3 u^1\,(\partial_1 u^4 + \partial_2 u^5) + 2\left(\partial_2 u^3 \partial_3 u^4 + \partial_1 u^3 \partial_3 u^5 + \partial_1 u^4 \partial_2 u^5\right).
\end{aligned}$$

Similarly, we compute the term $I_2=\mathbf{Q}_{ik,j}\mathbf{Q}_{ij,k}$ as

$$\begin{aligned}
I_2 = {} & (\partial_1 q_1)^2 + (\partial_2 q_3)^2 + (\partial_3 q_4)^2 + (\partial_1 q_3)^2 + (\partial_2 q_2)^2 + (\partial_3 q_5)^2 + (\partial_1 q_4)^2 + (\partial_2 q_5)^2 + (\partial_3(q_1+q_2))^2 \\
& + 2\left(\partial_2 q_1 \partial_1 q_3 + \partial_3 q_1 \partial_1 q_4 + \partial_3 q_3 \partial_2 q_4 + \partial_2 q_3 \partial_1 q_2 + \partial_3 q_3 \partial_1 q_5 + \partial_3 q_2 \partial_2 q_5 + \partial_2 q_4 \partial_1 q_5\right) \\
& - 2\left(\partial_3 q_4 \partial_1(q_1+q_2) + \partial_3 q_5 \partial_2(q_1+q_2)\right).
\end{aligned} \tag{3.8}$$

Arguing as before, at the point $\mathbf{Q} = \mathbf{\Lambda}$ we get

$$\begin{aligned} 2\, I_2 = \; & \frac{1}{3}\,(1+\mathbf{t})^2(\partial_1 u^1)^2 + \frac{1}{3}\,(1-\mathbf{t})^2(\partial_2 u^1)^2 + \frac{4}{3}\,(\partial_3 u^1)^2 \\ & +(\partial_1 u^3)^2 + (\partial_2 u^3)^2 + (\partial_1 u^4)^2 + (\partial_3 u^4)^2 + (\partial_2 u^5)^2 + (\partial_3 u^5)^2 \\ & + \frac{2}{\sqrt{3}}\,(1+\mathbf{t})\left(\partial_2 u^1 \partial_1 u^3 + \partial_3 u^1 \partial_1 u^4\right) + \frac{2}{\sqrt{3}}\,(1-\mathbf{t})\left(\partial_1 u^1 \partial_2 u^3 + \partial_3 u^1 \partial_2 u^5\right) \\ & - \frac{4}{\sqrt{3}}\left(\partial_1 u^1 \partial_3 u^4 + \partial_2 u^1 \partial_3 u^5\right) + 2\left(\partial_3 u^3 \partial_2 u^4 + \partial_3 u^3 \partial_1 u^5 + \partial_2 u^4 \partial_1 u^5\right). \end{aligned}$$

For any choice of the real coefficients $L_i$, we may thus decompose the elastic energy density into a sum of four quadratic forms:

$$L_1 I_1 + L_2 I_2 + L_3 I_3 = \mathcal{F}_1(\mathbf{t}) + \mathcal{F}_2(\mathbf{t}) + \mathcal{F}_3(\mathbf{t}) + \mathcal{F}_4(\mathbf{t})\,,$$

where we have set:

$$\mathcal{F}_1(\mathbf{t}) := a_1(\mathbf{t})\,(\partial_1 u^1)^2 + b_1\,(\partial_2 u^3)^2 + c_1\,(\partial_3 u^4)^2 + 2d_1(\mathbf{t})\,\partial_1 u^1 \partial_2 u^3 + 2e_1(\mathbf{t})\,\partial_1 u^1 \partial_3 u^4 + 2f_1\,\partial_2 u^3 \partial_3 u^4$$

with

$$\begin{gathered} a_1(\mathbf{t}) := L_3\Big(1 + \frac{\mathbf{t}^2}{3}\Big) + (L_1+L_2)\frac{(1+\mathbf{t})^2}{6}\,, \quad b_1 = c_1 := L_3 + \frac{L_1+L_2}{2}\,, \\ d_1(\mathbf{t}) := \frac{1}{2\sqrt{3}}\left((L_1-L_2)\,\mathbf{t} + (L_1+L_2)\right), \quad e_1(\mathbf{t}) := \frac{1}{2\sqrt{3}}\left(L_1\,\mathbf{t} + (L_1-2L_2)\right), \quad f_1 := \frac{1}{2}\,L_1\,; \end{gathered}$$

$$\mathcal{F}_2(\mathbf{t}) := a_2(\mathbf{t})\,(\partial_2 u^1)^2 + b_2\,(\partial_1 u^3)^2 + c_2\,(\partial_3 u^5)^2 + 2d_2(\mathbf{t})\,\partial_2 u^1 \partial_1 u^3 + 2e_2(\mathbf{t})\,\partial_2 u^1 \partial_3 u^5 + 2f_2\,\partial_1 u^3 \partial_3 u^5$$

with

$$\begin{gathered} a_2(\mathbf{t}) := L_3\Big(1 + \frac{\mathbf{t}^2}{3}\Big) + (L_1+L_2)\frac{(1-\mathbf{t})^2}{6}\,, \quad b_2 = c_2 := L_3 + \frac{L_1+L_2}{2}\,, \\ d_2(\mathbf{t}) := \frac{1}{2\sqrt{3}}\left((L_2-L_1)\,\mathbf{t} + (L_1+L_2)\right), \quad e_2(\mathbf{t}) := \frac{1}{2\sqrt{3}}\left(-L_1\,\mathbf{t} + (L_1-2L_2)\right), \quad f_2 := \frac{1}{2}\,L_1\,; \end{gathered}$$

$$\mathcal{F}_3(\mathbf{t}) := a_3(\mathbf{t})\,(\partial_3 u^1)^2 + b_3\,(\partial_1 u^4)^2 + c_3\,(\partial_2 u^5)^2 + 2d_3(\mathbf{t})\,\partial_3 u^1 \partial_1 u^4 + 2e_3(\mathbf{t})\,\partial_3 u^1 \partial_2 u^5 + 2f_3\,\partial_1 u^4 \partial_2 u^5$$

with

$$\begin{gathered} a_3(\mathbf{t}) := L_3\Big(1 + \frac{\mathbf{t}^2}{3}\Big) + \frac{2}{3}\,(L_1+L_2)\,, \quad b_3 = c_3 := L_3 + \frac{L_1+L_2}{2}\,, \\ d_3(\mathbf{t}) := \frac{1}{2\sqrt{3}}\left(L_2\,\mathbf{t} + (L_2-2L_1)\right), \quad e_3(\mathbf{t}) := \frac{1}{2\sqrt{3}}\left(-L_2\,\mathbf{t} + (L_2-2L_1)\right), \quad f_3 := \frac{1}{2}\,L_1\,; \end{gathered}$$

and

$$\mathcal{F}_4(\mathbf{t}) := a_4\,(\partial_3 u^3)^2 + b_4\,(\partial_2 u^4)^2 + c_4\,(\partial_1 u^5)^2 + 2d_4\,\partial_3 u^3 \partial_2 u^4 + 2e_4\,\partial_3 u^3 \partial_1 u^5 + 2f_4\,\partial_2 u^4 \partial_1 u^5$$

with

$$a_4 = b_4 = c_4 := L_3\,, \quad d_4 = e_4 = f_4 := \frac{1}{2}\,L_2\,.$$

We now compute the positivity of the previous quadratic forms independently of the parameter $\mathbf{t} \in \mathbb{R}$. We shall denote by $\Phi_i(\mathbf{t})$ the determinant of the matrix corresponding to $\mathcal{F}_i$, for $i = 1, 2, 3, 4$.

As for $\mathcal{F}_4$, since $\Phi_4(\mathbf{t}) \equiv (L_3 - L_2/2)^2(L_3 + L_2)$, we readily obtain the conditions

$$L_3 > 0\,, \quad 2L_3 > |L_2|\,, \quad L_3 + L_2 > 0,$$

which reduce to the system

$$L_3 > 0\,, \quad 2L_3 > L_2\,, \quad L_3 + L_2 > 0\,. \tag{3.9}$$

As for $\mathcal{F}_3$, the first two conditions are $L_1 + L_2 + 2L_3 > 0$ and $L_1 + L_2 + 2L_3 > |L_1|$, that combined with (3.9) imply a fourth condition:

$$2L_1 + L_2 + 2L_3 > 0\,. \tag{3.10}$$

In order to prove the positivity of the determinant, we first observe that $\Phi_3(\mathbf{t}) = A_3\mathbf{t}^2 + B_3\mathbf{t} + C_3$ and hence $\dot\Phi_3(\mathbf{t}) = 2A_3\mathbf{t} + B_3$ for some constants $A_3, B_3, C_3 \in \mathbb{R}$ depending on the coefficients $L_i$. We actually have

$$\dot\Phi_3(\mathbf{t}) = \dot a_3(\mathbf{t})\,(b_3^2 - f_3^2) + 2f_3\,\big(d_3(\mathbf{t})\,\dot e_3(\mathbf{t}) + e_3(\mathbf{t})\,\dot d_3(\mathbf{t})\big) - 2b_3\,\big(d_3(\mathbf{t})\,\dot d_3(\mathbf{t}) + e_3(\mathbf{t})\,\dot e_3(\mathbf{t})\big),$$

where we compute

$$\dot a_3(\mathbf{t}) = \frac{2}{3}\,L_3\,\mathbf{t}\,, \quad \dot d_3(\mathbf{t}) = \frac{1}{2\sqrt{3}}\,L_2\,, \quad \dot e_3(\mathbf{t}) = -\frac{1}{2\sqrt{3}}\,L_2$$

and hence

$$d_3(\mathbf{t})\,\dot d_3(\mathbf{t}) + e_3(\mathbf{t})\,\dot e_3(\mathbf{t}) = \frac{1}{6}\,L_2^2\,\mathbf{t}\,, \quad d_3(\mathbf{t})\,\dot e_3(\mathbf{t}) + e_3(\mathbf{t})\,\dot d_3(\mathbf{t}) = -\frac{1}{6}\,L_2^2\,\mathbf{t}\,.$$

Denoting $K := L_1 + L_2 + 2L_3$, these formulas yield to

$$\dot\Phi_3(\mathbf{t}) = \frac{2}{3}\,L_3\,\mathbf{t}\,\frac{1}{4}\,(K^2 - L_1^2) - \frac{1}{6}L_2^2\,(L_1 + K)\,\mathbf{t}$$

so that we obtain $B_3 = 0$ and

$$\begin{aligned} 6\,A_3 &= (K + L_1)\,\big[L_3(K - L_1) - L_2^2\big] \\ &= (2L_1 + L_2 + 2L_3)\,(2L_3 - L_2)\,(L_3 + L_2) \end{aligned}$$

and hence $A_3$ is positive by the assumptions (3.9) and (3.10).

We thus have to check that $C_3 > 0$. We have $C_3 = \Phi_3(0)$, where

$$a_3(0) := L_3 + \frac{2}{3}\,(L_1 + L_2)\,, \quad d_3(0) = e_3(0) = \frac{1}{2\sqrt{3}}\,(L_2 - 2L_1)$$

so that we compute

$$C_3 = a_3(0)\cdot(b_3^2 - f_3^2) - 2d_3^2(0)\cdot(b_3 - f_3) = (b_3 - f_3)\,[a_3(0)\cdot(b_3 + f_3) - 2d_3^2(0)]$$

from which we easily deduce that:

$$\begin{aligned} 12C_3 &= (L_2 + 2L_3)\,[6L_3^2 + (10L_1 + 7L_2)L_3 + 10L_1L_2 + L_2^2] \\ &= (L_2 + 2L_3)\,(L_2 + L_3)\,(6L_3 + 10L_1 + L_2)\,. \end{aligned}$$

In conclusion, on account of (3.9) and (3.10), the positivity of $\mathcal{F}_3(\mathbf{t})$ holds true for every $\mathbf{t} \in \mathbb{R}$ by imposing in addition that

$$10L_1 + L_2 + 6L_3 > 0\,. \tag{3.11}$$

We now wish to study in a similar way the positivity of $\mathcal{F}_1(\mathbf{t})$. First, notice that the coefficients of $\mathcal{F}_2(\mathbf{t})$ are equal to the corresponding ones in $\mathcal{F}_1(\mathbf{t})$ provided that one replaces the parameter $\mathbf{t}$ with $-\mathbf{t}$. This yields that it suffices to analyze $\mathcal{F}_1(\mathbf{t})$, as no other conditions are obtained from $\mathcal{F}_2(\mathbf{t})$.

Since $b_1 = c_1 = b_3 = c_3$ and $f_1 = f_3$, it suffices to check the positivity of the determinant, i.e.

$$\Phi_1(\mathbf{t}) > 0 \qquad \forall\,\mathbf{t} \in \mathbb{R}\,.$$

To this purpose, as before, we write $\Phi_3(\mathbf{t}) = A_1\mathbf{t}^2 + B_1\mathbf{t} + C_1$ for some constants $A_1, B_1, C_1 \in \mathbb{R}$ depending on the coefficients $L_i$. We thus impose the conditions:

$$A_1 > 0\,, \quad 4A_1C_1 > B_1^2\,.$$

We compute:

$$\dot\Phi_1(\mathbf{t}) = \dot a_1(\mathbf{t})\,(b_1^2 - f_1^2) + 2f_1\,\big(d_1(\mathbf{t})\,\dot e_1(\mathbf{t}) + e_1(\mathbf{t})\,\dot d_1(\mathbf{t})\big) - 2b_1\,\big(d_1(\mathbf{t})\,\dot d_1(\mathbf{t}) + e_1(\mathbf{t})\,\dot e_1(\mathbf{t})\big)$$

where this time we have

$$\dot a_1(\mathbf{t}) = \frac{1}{3}\,(L_1 + L_2 + 2L_3)\,\mathbf{t} + \frac{1}{3}\,(L_1 + L_2)\,, \quad \dot d_1(\mathbf{t}) = \frac{1}{2\sqrt{3}}\,(L_1 - L_2)\,, \quad \dot e_1(\mathbf{t}) = \frac{1}{2\sqrt{3}}\,L_1$$

and hence

$$d_1(\mathbf{t})\,\dot d_1(\mathbf{t}) + e_1(\mathbf{t})\,\dot e_1(\mathbf{t}) = \frac{1}{12}\left[(2L_1^2+L_2^2-2L_1L_2)\,\mathbf{t} + (2L_1^2-L_2^2-2L_1L_2)\right],$$

$$d_1(\mathbf{t})\,\dot e_1(\mathbf{t}) + e_1(\mathbf{t})\,\dot d_1(\mathbf{t}) = \frac{1}{12}\left[(2L_1^2-2L_1L_2)\,\mathbf{t} + (2L_1^2+2L_2^2-2L_1L_2)\right].$$

Denoting as before $K := L_1 + L_2 + 2L_3$, we also have

$$b_1^2 - f_1^2 = \frac{1}{4}\,(K^2 - L_1^2) = L_2^2 + 4L_3^2 + 2L_1L_2 + 4(L_1+L_2)L_3\,.$$

In conclusion, we get:

$$\begin{array}{rl} 12\,\dot\Phi_1(\mathbf{t}) = & (K\mathbf{t}+L_1+L_2)\left[L_2^2+4L_3^2+2L_1L_2+4(L_1+L_2)L_3\right] \\ & +L_1\left[(2L_1^2-2L_1L_2)\,\mathbf{t}+(2L_1^2+2L_2^2-2L_1L_2)\right] \\ & -K\left[(2L_1^2+L_2^2-2L_1L_2)\,\mathbf{t}+(2L_1^2-L_2^2-2L_1L_2)\right]. \end{array}$$

By plugging into the formula $\dot\Phi_1(\mathbf{t}) = 2A_1\mathbf{t} + B_1$, we obtain:

$$\begin{array}{rl} 24\,A_1 = & (L_1+L_2+2L_3)\left[4L_3^2+4L_1L_2+4(L_1+L_2)L_3-2L_1^2\right]+2L_1^2(L_1-L_2) \\ = & 8L_3^3+12(L_1+L_2)L_3^2+(4L_2^2+16L_1L_2)L_3+4L_1L_2^2 \end{array}$$

so that

$$12A_1 = 2(L_2+L_3)\left(2L_3^2+(3L_1+L_2)L_3+L_1L_2\right)$$

and also

$$\begin{array}{rl} 12\,B_1 = & (L_1+L_2)\left[L_2^2+4L_3^2+2L_1L_2+4(L_1+L_2)L_3\right] \\ & +L_1\left[2L_1^2+2L_2^2-2L_1L_2\right] \\ & -(L_1+L_2+2L_3)\left[2L_1^2-L_2^2-2L_1L_2\right] \\ = & 4(L_1+L_2)L_3^2+6(L_2^2+2L_1L_2)L_3+2(L_2^3+4L_1L_2^2) \\ = & 2(L_2+L_3)\left(2(L_1+L_2)L_3+(L_2^2+4L_1L_2)\right). \end{array}$$

Therefore, on account of (3.9), the necessary condition $A_1 > 0$ holds true if in addition

$$2L_3^2 + (3L_1+L_2)L_3 + L_1L_2 > 0\,. \tag{3.12}$$

As before, we now compute

$$C_1 = \Phi_1(0) = a_1(0)\cdot(b_1^2-f_1^2) + 2f_1\,d_1(0)\,e_1(0) - b_1\left(d_1^2(0)+e_2^2(0)\right)$$

where this time

$$a_1(0) = \frac{1}{6}\,(L_1+L_2+6L_3)\,,\quad b_1 = c_1 = \frac{K}{2}\,,\quad d_1(0) = \frac{1}{2\sqrt3}\,(L_1+L_2)\,,\quad e_1(0) = \frac{1}{2\sqrt3}\,(L_1-2L_2)\,,\quad f_1 = \frac{L_1}{2}\,.$$

Therefore, we have

$$\begin{array}{rl} 24\,C_1 = & (6L_3+L_1+L_2)\,(K^2-L_1^2)+2L_1\,[L_1^2-L_1L_2-2L_2^2]-K\,[2L_1^2+5L_2^2-2L_1L_2] \\ = & 24L_3^3+28(L_1+L_2)L_3^2+24L_1L_2L_3-4L_1L_2^2-4L_2^3 \\ = & 4\left[6L_3^3+7(L_1+L_2)L_3^2+6L_1L_2L_3-(L_1L_2^2+L_2^3)\right] \end{array}$$

and hence

$$12\,C_1 = 2(L_2+L_3)\left(6L_3^2+(7L_1+L_2)L_3-L_2(L_1+L_2)\right).$$

On account of condition $A_1 > 0$, inequality $\Phi_1(\mathbf{t}) > 0$ holds true for each $\mathbf{t} \in \mathbb{R}$ provided that the discriminant $B_1^2 - 4A_1C_1$ is negative. By the expressions of $A_1, B_1, C_1$, and using that $(L_2+L_3)^2 > 0$, this property is equivalent to:

$$4\left(2L_3^2+(3L_1+L_2)L_3+L_1L_2\right)\left(6L_3^2+(7L_1+L_2)L_3-L_2(L_1+L_2)\right) > \left(2(L_1+L_2)L_3+(L_2^2+4L_1L_2)\right)^2.$$

This inequality becomes

$$48L_3^4+32(4L_1+L_2)L_3^3+8(10L_1^2+6L_1L_2-L_2^2)L_3^2-8(4L_1L_2^2+L_2^3)-(20L_1^2L_2^2+12L_1L_2^3+L_1^4) > 0$$

and hence

$$(2L_3+L_2)\,(2L_3-L_2)\,(2L_1+L_2+2L_3)\,(10L_1+L_2+6L_3) > 0\,.$$

By (3.9), (3.10), (3.11), and (3.12) we thus deduce the positivity of the determinant $\Phi_1(\mathbf{t})$ for each $\mathbf{t} \in \mathbb{R}$.

**Remark 3.4** The necessary and sufficient conditions obtained are therefore given by the following system of five strict inequalities, that clearly also imply $L_3 > 0$:

$$2L_3 > L_2\,, \quad L_3 + L_2 > 0\,, \quad 2L_1 + L_2 + 2L_3 > 0\,,$$
$$2L_3^2 + (3L_1 + L_2)L_3 + L_1L_2 > 0\,, \quad 10L_1 + L_2 + 6L_3 > 0\,.$$

We now see that it can be reduced to the system (3.5).

In fact, denoting $\alpha := L_2/L_3$ and $\beta := L_1/L_3$, and using that $L_3 > 0$, the above inequalities become:

$$-1 < \alpha < 2\,, \quad 2\beta + \alpha + 2 > 0\,, \quad 2 + 3\beta + \alpha + \alpha\beta > 0\,, \quad 10\beta + \alpha + 6 > 0\,.$$

If $\beta > 0$, condition $2\beta + \alpha + 2 > 0$ follows from $\alpha > -1$, whereas if $\beta < 0$, the equivalent condition $10\beta + 5\alpha + 10 > 0$ follows from $10\beta + \alpha + 6 > 0$, since $5\alpha + 10 > \alpha + 6$ when $\alpha > -1$. As for the inequality $2 + 3\beta + \alpha + \alpha\beta > 0$, using that $\alpha + 3 > 0$, it is equivalent to $\beta > -(\alpha + 2)/(\alpha + 3)$, whereas $10\beta + \alpha + 6 > 0$ is equivalent to $\beta > -(\alpha + 6)/10$. Therefore, it suffices to check that for $\alpha > -3$,

$$-\frac{\alpha + 2}{\alpha + 3} < -\frac{\alpha + 6}{10} \iff \alpha^2 - \alpha + 2 < 0 \iff -1 < \alpha < 2\,.$$

Finally, the uniaxial phase $\lambda_1 = \lambda_2$ corresponds, up to the action by conjugation of an element of $SO(3)$, to the values of $\mathbf{t} = \pm 1$. The corresponding system reduces to the following one:

$$L_3 > |L_2|\,, \quad 2L_2 + L_2 + L_3 > 0 \tag{3.13}$$

that actually gives the well-known Ericksen conditions when $L_4 = 0$. □

**Remark 3.5 (Coercivity for larger $\rho$)** In Theorem 3.3, we assumed $\rho^2 := \mathrm{tr}(\mathbf{Q}^2)$ sufficiently small, i.e., $0 < \rho^2 \leq 1/6$. When $1/6 < \rho^2 \leq 2/3$, the range of $\mathbf{t}$ is smaller than $\mathbb{R}$ (cf. also Remark 3.1) and different conditions are obtained.

More precisely, when $1/6 < \rho^2 \leq 2/3$, in polar coordinates $\mathbf{x} = \rho\cos\theta$, $\mathbf{y} = \rho\sin\theta$, by (3.4) we have

$$\mathbf{t} = -\sqrt{3}\,(\tan\theta)^{-1}\,, \quad \theta \in \Omega_\rho,$$

where

$$\Omega_\rho := I_\rho \cup \left(\frac{2\pi}{3} + I_\rho\right) \cup \left(\frac{4\pi}{3} + I_\rho\right), \quad I_\rho := \left[\arctan\sqrt{6\rho^2 - 1}, \frac{2\pi}{3} - \arctan\sqrt{6\rho^2 - 1}\right].$$

Working on the fundamental domain $\lhd_f$ (cf. Section 2.2), we infer that it suffices to minimize the above quadratic forms $\mathcal{F}_i(\mathbf{t})$ on smaller ranges depending on $\rho$, i.e.,

$$\begin{cases} |\mathbf{t}| \leq \dfrac{\sqrt{3}}{R(\rho^2)} & \text{if} \quad 1/6 < \rho^2 \leq 2/9 \\ \dfrac{3R(\rho^2) - \sqrt{3}}{R(\rho^2) + \sqrt{3}} \leq |\mathbf{t}| \leq \dfrac{\sqrt{3}}{R(\rho^2)} & \text{if} \quad 2/9 < \rho^2 \leq 2/3 \end{cases} \tag{3.14}$$

where we have denoted $R(\rho^2) := \sqrt{6\rho^2 - 1}$. Notice that $R(1/6) = 0$, $R(2/9) = 1/\sqrt{3}$, and $R(2/3) = \sqrt{3}$, so that in the limiting case $\rho^2 = 2/3$ corresponding to the limiting uniaxial phases, condition (3.14) reduces to $|\mathbf{t}| = 1$, and we obtain again the Ericksen system (3.13).

In the following proposition, we shall denote for brevity:

$$\begin{aligned} \widetilde{A}_3 :=&\quad (2L_1 + L_2 + 2L_3)\,(2L_3 - L_2) \\ \widetilde{C}_3 :=&\quad (L_2 + 2L_3)\,(6L_3 + 10L_1 + L_2) \\ \widetilde{A}_1 :=&\quad 2L_3^2 + (3L_1 + L_2)L_3 + L_1L_2 \\ \widetilde{B}_1 :=&\quad 2(L_1 + L_2)L_3 + (L_2^2 + 4L_1L_2) \\ \widetilde{C}_1 :=&\quad 6L_3^2 + (7L_1 + L_2)L_3 - L_2(L_1 + L_2) \end{aligned}$$

and we shall correspondingly consider, in addition to (3.9), (3.10), (3.11), the following three inequalities:

$$6\,(9\rho^2 - 1 - \sqrt{18\rho^2 - 3})\,\widetilde{A}_3 + (3\rho^2 + 1 + \sqrt{18\rho^2 - 3})\,\widetilde{C}_3 > 0 \tag{3.15}$$

$$(6\rho^2-1)\,\widetilde{C}_1 > -3\widetilde{A}_1 + \sqrt{18\rho^2-3}\,|\widetilde{B}_1| \tag{3.16}$$

$$3\,(9\rho^2-1-\sqrt{18\rho^2-1})\,\widetilde{A}_1 - (9\rho^2-3+\sqrt{18\rho^2-1})\,|\widetilde{B}_1| + (3\rho^2+1+\sqrt{18\rho^2-3})\,\widetilde{C}_1 > 0\,. \tag{3.17}$$

In fact, due to the ranges (3.14), we do not need to assume $A_1 > 0$, that is the inequality (3.12), and we shall obtain different conditions depending on the sign of $\widetilde{A}_1$ and the possible validity of the inequalities:

$$\sqrt{6\rho^2-1}\,|\widetilde{B}_1| \geq 2\sqrt{3}\,\widetilde{A}_1 \tag{3.18}$$

$$(\sqrt{6\rho^2-1}+\sqrt{3})\,|\widetilde{B}_1| \leq 2\,(3\sqrt{6\rho^2-1}-\sqrt{3})\,\widetilde{A}_1\,. \tag{3.19}$$

**Proposition 3.6** *Assume that $1/6 < \rho^2 < 2/3$. The following are necessary and sufficient conditions for the positivity of the elastic energy density* (1.5) *with $L_4 = 0$ in the soft biaxial class $\mathbb{S}^4_\rho$:*

1. (3.9), (3.10), (3.11), *and* (3.16) $\iff$ $1/6 < \rho^2 \leq 2/9$ *and either* $\widetilde{A}_1 \leq 0$ *or* (3.18) *holds;*
2. (3.9), (3.10), *and* (3.11) $\iff$ $1/6 < \rho^2 \leq 2/9$ *and* $\widetilde{A}_1 > 0$ *but* (3.18) *fails to hold;*
3. (3.9), (3.10), (3.15), *and* (3.16) $\iff$ $2/9 < \rho^2 < 2/3$ *and either* $\widetilde{A}_1 \leq 0$ *or* (3.18) *holds;*
4. (3.9), (3.10), (3.15), *and* (3.17) $\iff$ $2/9 < \rho^2 < 2/3$ *and* $\widetilde{A}_1 > 0$ *and* (3.19) *holds;*
5. (3.9), (3.10), (3.11), *and* (3.15) $\iff$ $2/9 < \rho^2 < 2/3$ *and* $\widetilde{A}_1 > 0$ *but both the conditions* (3.18) *and* (3.19) *fail to hold.*

Proof: Following the proof of Theorem 3.3, we first obtain the conditions (3.9) and (3.10), as they are given by the positivity of matrices which do not depend on $\mathbf{t}$. We have to check the positivity of the determinant $\Phi_3(\mathbf{t})$ or, equivalently, of the quadratic function $\widetilde{\Phi}_3(\mathbf{t}) := 2\widetilde{A}_3\mathbf{t}^2 + \widetilde{C}_3$, where $\widetilde{A}_3 > 0$ by (3.9) and (3.10). When $1/6 < \rho^2 \leq 2/9$ the minimum is $\widetilde{\Phi}_3(0) = \widetilde{C}_3$, yielding again (3.11). Instead, when $2/9 < \rho^2 < 2/3$, the minimum of the quadratic function $\widetilde{\Phi}_3(\mathbf{t})$ is given by (3.15), as it is attained when $|\mathbf{t}| = (3R(\rho^2)-\sqrt{3})/(R(\rho^2)+\sqrt{3})$, according to the ranges (3.14).

We now deal with the positivity of the determinant $\Phi_1(\mathbf{t})$ or, equivalently, of the quadratic function $\widetilde{\Phi}_1(\mathbf{t}) := \widetilde{A}_1\mathbf{t}^2 + \widetilde{B}_1\mathbf{t} + \widetilde{C}_1$. If $\widetilde{A}_1 \leq 0$, this follows from condition (3.16). In this case, in fact, the minimum of $\widetilde{\Phi}_1(\mathbf{t})$ is attained for $\mathbf{t} = \pm\sqrt{3}/R(\rho^2)$, according to the sign of $\widetilde{B}_1$. When $\widetilde{A}_1 > 0$, the same condition (3.16) is obtained if the distance from the origin of the critical point of $\widetilde{\Phi}_1(\mathbf{t})$ is more than $\sqrt{3}/R(\rho^2)$, i.e., if (3.18) holds. If the distance from the origin of the critical point of $\widetilde{\Phi}_1(\mathbf{t})$ is less than $(3R(\rho^2)-\sqrt{3})/(R(\rho^2)+\sqrt{3})$, i.e., if (3.19) holds (which implies $2/9 < \rho^2 \leq 2/3$), then one obtains condition (3.17). In the remaining cases, the minimum of $\Phi_1(\mathbf{t})$ in the ranges (3.14) is equal to $\min_{\mathbb{R}} \Phi_1$, which yields the additional condition (3.11). We omit the other details of the proof. □

Dirichlet boundary conditions. Assume now that any admissible $\mathbf{Q}$ for the functional $\mathcal{F}[\mathbf{Q}]$ satisfy Dirichlet boundary conditions given as follows [11, 13, 23]. 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 $W^{1,2}_\varphi$ of admissible tensor fields by

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

where equality is understood in the sense of traces.

**Corollary 3.7** *If $0 < \rho^2 \leq 1/6$ and $L_4 = 0$, then the elastic energy functional* (1.7) *is coercive on the admissible set $W^{1,2}_\varphi$ if and only if*

$$\begin{cases} L_3 > 0 & \textit{in case} \quad L_1 + L_2 \geq 0 \\ 2L_1 + 2L_2 + 3L_3 > 0 & \textit{in case} \quad L_1 + L_2 < 0\,. \end{cases} \tag{3.20}$$

Proof: We exploit the property that the difference $I_1 - I_2$ is a null-Lagrangian, namely

$$I_1 - I_2 = (\mathbf{Q}_{ij}\mathbf{Q}_{ik,k})_{,j} - (\mathbf{Q}_{ij}\mathbf{Q}_{ik,j})_{,k} .$$

Using that for any $\lambda, \mu \in \mathbb{R}$

$$I_1 = \lambda I_2 + (1-\lambda)I_1 + \lambda(I_1 - I_2) , \quad I_2 = \mu I_1 + (1-\mu)I_2 - \mu(I_1 - I_2)$$

we have

$$L_1 I_1 + L_2 I_2 + L_3 I_3 = \widetilde{L}_1 I_1 + \widetilde{L}_2 I_2 + L_3 I_3 + (\lambda L_1 - \mu L_2)(I_1 - I_2)$$

where we have set

$$\widetilde{L}_1 := \nu , \quad \widetilde{L}_2 := L - \nu , \quad \nu := (1-\lambda)L_1 + \mu L_2 , \quad L := L_1 + L_2 .$$

On account of the trace condition $\mathbf{Q}_{|\partial\Omega} = \varphi_{|\partial\Omega}$, the coercivity assumptions (3.5) reduce to

$$2L_3 > \widetilde{L}_2 , \quad L_3 + \widetilde{L}_2 > 0 , \quad 10\widetilde{L}_1 + \widetilde{L}_2 + 6L_3 > 0$$

which can be re-written as the system

$$\nu > L - 2L_3 , \quad L_3 + L > \nu , \quad 9\nu > -6L_3 - L$$

for some choice of the parameter $\nu \in \mathbb{R}$. This yields to the equivalent system $L_3 > 0$ and $3L_3 + 2L > 0$. Formula (3.20) readily follows. □

# 4 The fourth elastic invariant

In this section we consider the elastic energy (1.5) 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. For the sake of simplicity, we shall assume that $L_1 = L_2 = 0$. In the more general case, sufficient conditions are readily obtained, whereas necessary conditions involve nontrivial computations.

**Theorem 4.1** *Assume that* $0 < \rho^2 \leq 1/6$ *and* $L_1 = L_2 = 0$. *Then the elastic energy density* (1.5) *is positive definite in the soft biaxial class* $\mathbb{S}^4_\rho$ *if and only if the following condition holds:*

$$\sqrt{6}\, L_3 > 2\rho\, |L_4| . \tag{4.1}$$

Proof: Recalling that

$$I_4(\mathbf{Q}, \nabla\mathbf{Q}) := \mathbf{Q}_{lk}\mathbf{Q}_{ij,l}\mathbf{Q}_{ij,k} ,$$

at the point $\mathbf{Q} = \mathbf{\Lambda}$ we have $\mathbf{Q}_{lk} = \delta_{lk}\,\lambda_k$ and hence

$$I_4(\mathbf{\Lambda}, \nabla\mathbf{Q}) = \sum_{k=1}^{3} \lambda_k\, |\partial_k \mathbf{Q}|^2 . \tag{4.2}$$

Using (2.2) and (2.4), similarly to (2.7) we get

$$|\partial_k\mathbf{Q}|^2 = 2((\partial_k \nabla q_1)^2 + (\partial_k q_2)^2 + \partial_k q_1\, \partial_k q_2 + (\partial_k q_3)^2 + (\partial_k q_4)^2 + (\partial_k q_5)^2\big) = |\partial_k \mathbf{u}|^2$$

for $k = 1, 2, 3$. Therefore, by imposing (3.3), similarly to the computation of $I_3$, by (2.7) we have

$$I_4 = \sum_{k=1}^{3} \lambda_k \left( \left(1 + \frac{\mathbf{t}^2}{3}\right)(\partial_k u^2)^2 + (\partial_k u^3)^2 + (\partial_k u^4)^2 + (\partial_k u^5)^2 \right) . \tag{4.3}$$

On account of (3.6), and using that $L_1 = L_2 = 0$, we are reduced to check the positivity of four diagonal $3\times 3$-matrices $M_i$, $i = 1,\dots,4$, whose eigenvalues $a_i$, $b_i$, $c_i$ are respectively

$$\begin{array}{lll}
a_1(\mathbf{t}) := \Big(1+\dfrac{\mathbf{t}^2}{3}\Big)\, L_3 + \lambda_1\, L_4 & b_1 := L_3 + \lambda_2\, L_4 & c_1 := L_3 + \lambda_1\, L_4 \\
a_2(\mathbf{t}) := \Big(1+\dfrac{\mathbf{t}^2}{3}\Big)\, L_3 + \lambda_2\, L_4 & b_2 := L_3 + \lambda_1\, L_4 & c_2 := L_3 + \lambda_3\, L_4 \\
a_3(\mathbf{t}) := \Big(1+\dfrac{\mathbf{t}^2}{3}\Big)\, L_3 + \lambda_3\, L_4 & b_3 := L_3 + \lambda_1\, L_4 & c_3 := L_3 + \lambda_2\, L_4 \\
a_4 := L_3 + \lambda_3\, L_4 & b_4 := L_3 + \lambda_2\, L_4 & c_4 := L_3 + \lambda_1\, L_4\,.
\end{array}$$

For this reason, we use the representation (2.10) and (2.11), so that by (3.3) we have (3.4) where, we recall, condition $\mathbf{y}\neq 0$ excludes the uniaxial case $\lambda_1=\lambda_2$ that will be treated separately. We set

$$\mathbf{s} := \frac{\mathbf{t}}{\sqrt{3+\mathbf{t}^2}} \iff \mathbf{t} = \frac{\sqrt{3}\,\mathbf{s}}{\sqrt{1-\mathbf{s}^2}}\,.$$

Using (2.11) and (3.4), and imposing condition $\mathbf{x}^2+\mathbf{y}^2=\rho^2$ and $\mathbf{y}\geq 0$, where $0<\rho^2\leq 1/6$, we get

$$\mathbf{x} = -\rho\,\mathbf{s}\,, \quad \mathbf{y} = \rho\sqrt{1-\mathbf{s}^2}\,, \quad \mathbf{t}\,\mathbf{y} = \sqrt{3}\,\rho\,\mathbf{s}\,.$$

In terms of the new variable $\mathbf{s}\in(-1,1)$, we get:

$$\Big(1+\frac{\mathbf{t}^3}{3}\Big) = \frac{1}{1-\mathbf{s}^2}\,, \quad \lambda_1 = \frac{1}{\sqrt{6}}\,\rho\,(\sqrt{3}\sqrt{1-\mathbf{s}^2}-\mathbf{s})\,, \quad \lambda_2 = -\frac{1}{\sqrt{6}}\,\rho\,(\sqrt{3}\sqrt{1-\mathbf{s}^2}+\mathbf{s})\,, \quad \lambda_3 = \frac{2}{\sqrt{6}}\,\rho\,\mathbf{s}\,,$$

so that in particular

$$-\frac{2}{\sqrt{6}}\,\rho \leq \lambda_i \leq \frac{2}{\sqrt{6}}\,\rho\,, \quad i = 1,\,2,\,3\,.$$

Therefore, the first positivity condition $L_3+\lambda_i\,L_4>0$ is satisfied if and only if (4.1) holds.

As for the second one, $\Big(1+\dfrac{\mathbf{t}^2}{3}\Big)\, L_3 + \lambda_i\, L_4 > 0$, it clearly suffices to check the case $i=3$, that in terms of the variable $\mathbf{s}$ becomes

$$\frac{L_3}{1-\mathbf{s}^2} + \frac{2}{\sqrt{6}}\,\rho\,\mathbf{s}\,L_4 > 0\,.$$

This inequality is satisfied for each $\mathbf{s}\in(-1,1)$ provided that (4.1) holds.

In the remaining uniaxial case $\lambda_1=\lambda_2$, by condition (3.2) we again have $\nabla u^1 = 0$, so that we obtain:

$$I_3 = |\nabla u^2|^2 + |\nabla u^3|^2 + |\nabla u^4|^2 + |\nabla u^5|^2\,,$$

$$I_4 = \sum_{k=1}^{3} \lambda_k\,\Big((\partial_k u^2)^2 + (\partial_k u^3)^2 + (\partial_k u^4)^2 + (\partial_k u^5)^2\Big)$$

yielding to the positivity condition $L_3+\lambda_i\,L_4>0$, and hence the inequality (4.1). □

**Remark 4.2** When $1/6<\rho\leq 2/3$, sharper conditions (that we shall not describe) can be obtained (cf. Remark 3.5). Notice that if $\mathbf{t}\in(-\infty,-1]$, then one has $-1<\mathbf{s}\leq-\frac{1}{2}$, which implies

$$\lambda_1 \in \Big(\frac{\rho}{\sqrt{6}},\frac{2\rho}{\sqrt{6}}\Big), \quad \lambda_2 \in \Big(-\frac{\rho}{\sqrt{6}},\frac{\rho}{\sqrt{6}}\Big), \quad \lambda_3 \in \Big(-\frac{2\rho}{\sqrt{6}},-\frac{\rho}{\sqrt{6}}\Big).$$

Therefore, restriction to the fundamental domain does not simplify the computations.

General sufficient conditions. Obtaining necessary and sufficient conditions for the elastic energy density (1.5), 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 3.3, Corollary 3.7, and Theorem 4.1, we readily obtain a range of sufficient conditions for positivity in the soft biaxial regime.

**Corollary 4.3** *Assume that* $0 < \rho^2 \le 1/6$*. Then the elastic energy density* (1.5) *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* (1.7) *is coercive on the admissible set* $W^{1,2}_\varphi(\Omega,\mathbb{S}^4_\rho)$ *if (and only if)* $L_3 > 0$*, in case* $L_1 + L_2 \ge 0$*, and provided that:*

$$2L_1 + 2L_2 + 3(1-\alpha)\,L_3 > 0\,, \quad \alpha\sqrt{6}\,L_3 > 2\rho\,|L_4|$$

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

Proof: The first assertion is obtained by decomposing

$$\psi_E(\mathbf{Q},\nabla\mathbf{Q}) = (L_1 I_1 + L_2 I_2 + (1-\alpha)\,L_3) + (\alpha\,I_3 + L_4 I_4)$$

and writing separately the inequalities in (3.5) and (4.1). Under Dirichlet-type boundary conditions, using this time the inequalities (3.20) and (4.1), we similarly get

$$\begin{cases} (1-\alpha)\,L_3 > 0\,, \quad \alpha\sqrt{6}\,L_3 > 2\rho\,|L_4| & \text{in case} \quad L_1 + L_2 \ge 0 \\ 2L_1 + 2L_2 + 3(1-\alpha)\,L_3 > 0\,, \quad \alpha\sqrt{6}\,L_3 > 2\rho\,|L_4| & \text{in case} \quad L_1 + L_2 < 0\,. \end{cases}$$

The claim readily follows. □

# Appendix A The Longa–Monselesan–Trebin conditions

In this appendix, using the scalar coordinates corresponding to the representation of **Q**-tensors described in Section 2.1, we compute the Longa–Monselesan–Trebin positivity conditions

$$2L_3 > L_2\,, \quad L_3 + L_2 > 0\,, \quad 10L_1 + L_2 + 6L_3 > 0 \tag{A.1}$$

for the three-elastic-constant form $L_1I_1 + L_2I_2 + L_3I_3$ of the elastic energy density $\psi_E$ in the general biaxial case (cf. (1.8)).

These conditions were originally obtained by Longa–Monselesan–Trebin [24] (cf. also [10]) by writing the elastic energy density $L_1I_1 + L_2I_2 + L_3I_3$ 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 [30].

In general, by (2.7) we have $I_3 = |\nabla\mathbf{u}|^2$. Also, by (3.7), in terms of $\mathbf{u}$ we have

$$2I_1 = \Big(\frac{1}{\sqrt{3}}\partial_1 u^1 + \partial_1 u^2 + \partial_2 u^3 + \partial_3 u_4\Big)^2 + \Big(\frac{1}{\sqrt{3}}\partial_2 u^1 - \partial_2 u^2 + \partial_3 u^5 + \partial_1 u^3\Big)^2 + \Big(-\frac{2}{\sqrt{3}}\partial_3 u^1 + \partial_1 u^4 + \partial_2 u^5\Big)^2.$$

Similarly, by (3.8) we find the formula

$$\begin{aligned} 2I_2 = \;& \Big(\frac{1}{\sqrt{3}}\partial_1 u^1 + \partial_1 u^2\Big)^2 + (\partial_2 u^3)^2 + (\partial_3 u^4)^2 + 2\Big(-\frac{2}{\sqrt{3}}\partial_1 u^1 \partial_3 u^4 + \frac{1}{\sqrt{3}}\partial_1 u^1 \partial_2 u^3 - \partial_1 u^2 \partial_2 u^3\Big) \\ & + \Big(\frac{1}{\sqrt{3}}\partial_2 u^1 - \partial_2 u^2\Big)^2 + (\partial_3 u^5)^2 + (\partial_1 u^3)^2 + 2\Big(-\frac{2}{\sqrt{3}}\partial_2 u^1 \partial_3 u^5 + \frac{1}{\sqrt{3}}\partial_2 u^1 \partial_1 u^3 - \partial_2 u^2 \partial_1 u^3\Big) \\ & + \Big(-\frac{2}{\sqrt{3}}\partial_3 u^1\Big)^2 + (\partial_1 u^4)^2 + (\partial_2 u^5)^2 + 2\Big(\frac{1}{\sqrt{3}}\partial_3 u^1 \partial_1 u^4 + \partial_3 u^2 \partial_1 u^4 + \frac{1}{\sqrt{3}}\partial_3 u^1 \partial_2 u^5 - \partial_3 u^2 \partial_2 u^5\Big) \\ & + 2\left(\partial_3 u^3 \partial_2 u^4 + \partial_3 u^3 \partial_1 u^5 + \partial_2 u^4 \partial_1 u^5\right). \end{aligned}$$

For any choice of the real coefficients $L_i$ we thus may decompose into four quadratic forms:

$$L_1I_1 + L_2I_2 + L_3I_3 = \mathcal{F}_1 + \mathcal{F}_2 + \mathcal{F}_3 + \mathcal{F}_4\,.$$

The quadratic form $\mathcal{F}_1$ depends on the four variables $\partial_1 u^1$, $\partial_1 u^2$, $\partial_2 u^3$, $\partial_3 u_4$ and its related matrix is:

$$M_1 := \begin{pmatrix} L_3 + \dfrac{L_1+L_2}{6} & \dfrac{1}{2\sqrt{3}}(L_1+L_2) & \dfrac{1}{2\sqrt{3}}(L_1+L_2) & \dfrac{1}{2\sqrt{3}}(L_1-2L_2) \\ \dfrac{1}{2\sqrt{3}}(L_1+L_2) & \dfrac{K}{2} & \dfrac{1}{2}(L_1-L_2) & \dfrac{L_1}{2} \\ \dfrac{1}{2\sqrt{3}}(L_1+L_2) & \dfrac{1}{2}(L_1-L_2) & \dfrac{K}{2} & \dfrac{L_1}{2} \\ \dfrac{1}{2\sqrt{3}}(L_1-2L_2) & \dfrac{L_1}{2} & \dfrac{L_1}{2} & \dfrac{K}{2} \end{pmatrix}$$

where we have denoted $K := L_1 + L_2 + 2L_3$. The second one, $\mathcal{F}_2$, depends on the four variables $\partial_2 u^1$, $\partial_2 u^2$, $\partial_3 u^5$, $\partial_1 u^3$ and its corresponding matrix is:

$$M_2 := \begin{pmatrix} L_3 + \dfrac{L_1+L_2}{6} & -\dfrac{1}{2\sqrt{3}}(L_1+L_2) & \dfrac{1}{2\sqrt{3}}(L_1-2L_2) & \dfrac{1}{2\sqrt{3}}(L_1+L_2) \\ -\dfrac{1}{2\sqrt{3}}(L_1+L_2) & \dfrac{K}{2} & -\dfrac{L_1}{2} & -\dfrac{1}{2}(L_1-L_2) \\ \dfrac{1}{2\sqrt{3}}(L_1-2L_2) & -\dfrac{L_1}{2} & \dfrac{K}{2} & \dfrac{L_1}{2} \\ \dfrac{1}{2\sqrt{3}}(L_1+L_2) & -\dfrac{1}{2}(L_1-L_2) & \dfrac{L_1}{2} & \dfrac{K}{2} \end{pmatrix}.$$

The third one, $\mathcal{F}_3$, depends on the four variables $\partial_3 u^1$, $\partial_3 u^2$, $\partial_1 u^4$, $\partial_2 u^5$ and its corresponding matrix is:

$$M_3 := \begin{pmatrix} L_3 + \dfrac{2}{3}(L_1+L_2) & 0 & \dfrac{1}{2\sqrt{3}}(-2L_1+L_2) & \dfrac{1}{2\sqrt{3}}(-2L_1+L_2) \\ 0 & L_3 & \dfrac{L_2}{2} & -\dfrac{L_2}{2} \\ \dfrac{1}{2\sqrt{3}}(-2L_1+L_2) & \dfrac{L_2}{2} & \dfrac{K}{2} & \dfrac{L_1}{2} \\ \dfrac{1}{2\sqrt{3}}(-2L_1+L_2) & -\dfrac{L_2}{2} & \dfrac{L_1}{2} & \dfrac{K}{2} \end{pmatrix}.$$

Finally, the fourth one, $\mathcal{F}_4$, depends on the three remaining variables $\partial_3 u^3$, $\partial_2 u^4$, $\partial_1 u^5$ and its corresponding matrix is:

$$M_4 := \begin{pmatrix} L_3 & \dfrac{L_2}{2} & \dfrac{L_2}{2} \\ \dfrac{L_2}{2} & L_3 & \dfrac{L_2}{2} \\ \dfrac{L_2}{2} & \dfrac{L_2}{2} & L_3 \end{pmatrix}.$$

The matrix $M_4$ has determinant $(L_3 - L_2/2)^2(L_3 + L_2)$, whence $\mathcal{F}_4$ is positive definite if and only if the conditions $L_3 > 0$, $2L_3 > |L_2|$, $L_3 + L_2 > 0$ hold, which clearly reduce to the system

$$L_3 > 0\,, \quad 2L_3 > L_2\,, \quad L_3 + L_2 > 0\,. \tag{A.2}$$

Dealing with $M_3$, and starting from the right-bottom corner, we obtain the first two conditions $K > 0$ and $K > |L_1|$, which reduce to

$$L_2 + 2L_3 > 0\,, \quad 2L_1 + L_2 + 2L_3 > 0\,, \tag{A.3}$$

where the first inequality follows from (A.2). The determinant of the $3 \times 3$ right-bottom minor is

$$\frac{1}{4}\,(2L_1 + L_2 + 2L_3)(2L_3^2 + L_2L_3 - L_2^2) = \frac{1}{4}\,(2L_1 + L_2 + 2L_3)(2L_3 - L_2)(L_3 + L_2)$$

and hence it is positive under the assumptions (A.2) and (A.3). Finally, we compute $\det M_3$ by applying Laplace's formula w.r.t. the first column, and we write

$$\det M_3 = A_3^1 - A_3^2 + A_3^3 - A_3^4$$

where $A_3^2 = 0$ and we respectively compute:

$$A_3^1 = \Big(L_3 + \frac{2}{3}\,(L_1 + L_2)\Big) \cdot \frac{1}{4}\,(2L_1 + L_2 + 2L_3)(2L_3 - L_2)(L_3 + L_2)\,,$$

$$A_3^3 - A_3^4 = -\frac{1}{12}\,(-2L_1 + L_2)^2\,(2L_3 - L_2)(L_3 + L_2)$$

and hence

$$\begin{aligned} 12\det M_3 = \quad & (2L_3 - L_2)(L_3 + L_2)\,[(3L_3 + 2L_1 + 2L_2)(2L_1 + L_2 + 2L_3) - (-2L_1 + L_2)^2] \\ & = (2L_3 - L_2)(L_3 + L_2)^2(6L_3 + L_1 + 10L_2)\,. \end{aligned}$$

Therefore, under the conditions (A.2) and (A.3), the determinant of $M_3$ is positive if and only if we also have

$$6L_3 + L_1 + 10L_2 > 0\,. \tag{A.4}$$

We now consider the matrix $M_2$. Starting from the right-bottom corner, we again obtain the first two conditions $K > 0$ and $K > |L_1|$. This time, the determinant $D$ of the $3 \times 3$ right-bottom minor is

$$D = \frac{1}{8}\left[K(K^2 - 2L_1^2 - (L_2 - L_1)^2) - 2L_1^2(L_2 - L_1)\right] = \frac{1}{2}\,(L_3 + L_2)(2L_3^2 + (3L_1 + L_2)L_3 + L_1L_2) \tag{A.5}$$

and hence it is positive under the additional assumption

$$2L_3^2 + (3L_1 + L_2)L_3 + L_1L_2 > 0\,. \tag{A.6}$$

As before, we now compute $\det M_2$ by applying Laplace's formula w.r.t. the first column, and we write

$$\det M_2 = A_2^1 - A_2^2 + A_2^3 - A_2^4\,.$$

We have:

$$A_2^1 = \frac{6L_3 + L_1 + L_2}{6} \cdot \frac{1}{2}\,(L_3 + L_2)(2L_3^2 + (3L_1 + L_2)L_3 + L_1L_2)\,,$$

$$-A_2^2 = -\frac{1}{24}\,(L_3 + L_2)(L_1 + L_2)(4L_1L_2 + L_2^2 + 2L_1L_3 + 2L_2L_3)\,,$$

$$A_2^3 = \frac{1}{24}\,(L_3 + L_2)(L_1 - 2L_2)(3L_1L_2 - L_1L_3 + 2L_2L_3)\,,$$

$$-A_2^4 = -\frac{1}{24}\,(L_3 + L_2)(L_1 + L_2)(4L_1L_2 + L_2^2 + 2L_1L_3 + 2L_2L_3) = -A_2^2\,,$$

and hence we obtain:

$$\begin{aligned} 12\det M_2 = (L_2 + L_3)\,\big[\quad & (6L_3 + L_1 + L_2)(2L_3^2 + (3L_1 + L_2)L_3 + L_1L_2) \\ & -(L_1 + L_2)(4L_1L_2 + L_2^2 + 2L_1L_3 + 2L_2L_3) \\ & +(L_1 - 2L_2)(3L_1L_2 - L_1L_3 + 2L_2L_3)\ \big] \\ = \ (L_2 + L_3)\,\big[\quad & 12L_3^3 + 4(5L_1 + 2L_2)L_3^2 + (10L_1L_2 - 5L_2^2)L_3 - (10L_1L_2^2 + L_2^3)\ \big] \\ = \ (L_2 + L_3)\,\big[\quad & (L_2 + L_2)(2L_3 - L_2)(6L_3 + 10L_1 + L_2)\ \big]\,. \end{aligned}$$

Therefore, condition $\det M_3 > 0$ follows from (A.2), (A.3), and (A.4).

We finally deal with the matrix $M_1$, obtaining exactly the same positivity conditions as for $M_2$. In fact, starting from the right-bottom corner, the first two conditions are again $K > 0$ and $K > |L_1|$, whereas the determinant $D$ of the $3 \times 3$ right-bottom minor is equal to the expression from (A.5). Computing as before the determinant of $M_1$ by means of Laplace's formula w.r.t. the first column, and writing

$$\det M_1 = A_1^1 - A_1^2 + A_1^3 - A_1^4\,,$$

it is not difficult to check that we have:

$$A_1^1 = A_1^2\,, \quad -A_1^2 = -A_2^2\,, \quad A_1^3 = -A_2^4\,, \quad -A_1^4 = A_2^3$$

and hence we get $\det M_1 = \det M_2$.

In conclusion, arguing as in Remark 3.4 we deduce that the system (A.2), (A.3), (A.4), and (A.6) is equivalent to the one in (A.1).

# References


[1] A. V. Alekseevsky and D. V. Alekseevsky, *Riemannian G-manifold with one-dimensional orbit space*, Ann. Global Anal. Geom., 11 (1993), no. 3, pp. 197–211.

[2] D. Allender and L. Longa, *Landau–de Gennes theory of biaxial nematics reexamined*, Phys. Rev. E, 78 (2008), pp. 011704–011714.

[3] J. M. Ball, *The Mathematics of Liquid Crystals*, Cambridge Centre for Analysis short course, 13-17 February, 2012, https://people.maths.ox.ac.uk/ball/teaching.shtml.

[4] J. M. Ball and A. Majumdar, *Nematic liquid crystals: from Maier–Saupe to a continuum theory*, Mol. Cryst. Liq. Cryst., 525 (2010), pp. 1–11.

[5] J. M. Ball and A. Zarnescu, *Orientability and energy minimization in liquid cristal models*, Arch. Ration. Mech. Anal., 202 (2011), pp. 493–535.

[6] D. W. Berreman and S. Meiboom, *Tensor representation of Oseen–Frank strain energy in uniaxial cholesterics*, Phys. Rev. A, 30 (1984), pp. 1955–1959.

[7] G. E. Bredon, *Introduction to Compact Transformation Groups*, Pure and Applied Mathematics, 46, Academic Press, New York, 1972.

[8] E. Cartan, *Sur des families remarquables d'hypersurfaces isoparamétriques dans les espaces sphériques*, Math. Z., 45 (1939), pp. 335–367.

[9] D. Chillingworth, *Perturbed hedgehogs: continuous deformation of point defects in biaxial nematic liquid crystals*, IMA J. Appl. Math., 81 (2016), n. 4, pp. 647–661.

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

[11] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals*, 2nd ed., International Series of Monographs on Physics, 83, Oxford University Press, Oxford, 1993.

[12] J. L. Ericksen, *Inequalities in liquid crystal theory*, Phys. Fluids, 9 (1966), pp. 1205–1207.

[13] J. L. Ericksen and D. Kinderlehrer, eds., *Theory and Applications of Liquid Crystals*, IMA Volumes in Mathematics and Its Applications, 5, Springer-Verlag, New York, 1987.

[14] F. C. Frank, *I. Liquid crystals. On the theory of liquid crystals*, Discuss. Faraday Soc., 25 (1958), pp. 19–28.

[15] E. Govers and G. Vertogen, *Elastic continuum theory of biaxial nematics*, Phys. Rev. A, 30 (1984), pp. 1998–2000; Phys. Rev. A, 31 (1985), p. 1957.

[16] E. F. Gramsbergen, L. Longa, and W. H. de Jeu, *Landau theory of the nematic-isotropic phase transition*, Phys. Rep., 135 (1986), pp. 195–257.

[17] R. Hardt and D. Kinderlehrer, *Mathematical questions of liquid crystal theory*, in Theory and Applications of Liquid Crystals, J. L. Ericksen and D. Kinderlehrer, eds., IMA Volumes in Mathematics and Its Applications, 5, Springer-Verlag, New York, 1987, pp. 151–184.

[18] W.-Y. Hsiang, *On the compact homogeneous minimal submanifolds*, Proc. Nat. Acad. Sci. U.S.A., 56 (1966), pp. 5–6.

[19] W.-Y. Hsiang and H. B. Lawson, Jr., *Minimal submanifolds of low cohomogeneity*, J. Differential Geometry, 5 (1971), pp. 1–38.

[20] G. Iyer, X. Xu, and A. Zarnescu, *Dynamic cubic instability in a 2D Q-tensor model for liquid crystals*, Math. Models Methods Appl. Sci., 25 (2015), pp. 1477–1517.

[21] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, 2nd ed., Pergamon, Oxford, 1969.

[22] H. B. Lawson, Jr., *Lectures on Minimal Submanifolds*, vol. I, 2nd ed., Mathematics Lecture Series, 9, Publish or Perish, Inc., Wilmington, Del., 1980.

[23] F. H. Lin and C. Liu, *Static and dynamic theories of liquid crystals*, J. Partial Differential Equations, 14 (2001), pp. 289–330.

[24] L. Longa, D. Monselesan, and H.-R. Trebin, *An extension of the Landau–Ginzburg–de Gennes theory for liquid crystals*, Liquid Crystals, 2 (1987), pp. 769–796.

[25] L. Longa and H.-R. Trebin, *Structure of the elastic free energy for chiral nematic liquid crystals*, Phys. Rev. A, 39 (1989), pp. 2160–2168.

[26] L. Longa, G. Pajak, and T. Wydro, *Stability of biaxial nematic phase for systems with variable molecular shape anisotropy*, Phys. Rev. E, 76 (2007), pp. 011703–011709.

[27] L. Longa, Private communication, March, 2016.

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

[29] N. D. Mermin, *The topological theory of defects in ordered media*, Rev. Modern Phys., 51 (1979), pp. 591–648.

[30] A. Messiah, *Quantum Mechanics*, Dover Publications, Inc., Mineola, NY, 2003.

[31] L. Michel, *Points critiques des fonctions invariantes sur une G-variété*, C. R. Acad. Sci. Paris Sér. A-B, 272 (1971), pp. A433–A436.

[32] L. Michel, *Symmetry defects and broken symmetry. Configurations. Hidden symmetry*, Rev. Modern Phys., 52 (1980), n. 3, pp. 617–651.

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

[34] P. Mostert, *On a compact Lie group acting on a manifold*, Ann. of Math., 65 (1957), pp. 447–455; Errata, Ann. of Math., 66 (1957), 589.

[35] N. J. Mottram and C. Newton, *Introduction to Q-tensor theory*, Technical report, University of Strathclyde, Department of Mathematics (2004), arXiv:1409.3542 [cond-mat.soft], 2014.

[36] D. Mucci, *Maps into projective spaces: liquid crystals and conformal energies*, Discrete Contin. Dyn. Syst. Ser. B, 17 (2012), pp. 597–635.

[37] D. Mucci and L. Nicolodi, *On the elastic energy density of constrained Q-tensor models for biaxial nematics*, Arch. Ration. Mech. Anal., 206 (2012), pp. 853–884.

[38] D. Mucci and L. Nicolodi, *On the Landau–de Gennes elastic energy of constrained biaxial nematics*, SIAM J. Math. Anal., 48 (2016), no. 3, pp. 1954–1987.

[39] L. Nicolodi, *Models for biaxial nematic liquid crystals*, Journal of Physics: Conference Series, 410 (2013), pp. 012043–012046.

[40] B. O'Neill, *Semi-Riemannian Geometry. With application to relativity*, Pure and Applied Mathematics, 103, Academic Press, Inc., New York, 1983.

[41] C. W. Oseen, *The theory of liquid crystals*, Trans. Faraday Soc., 29 (1933), pp. 883–899.

[42] R. S. Palais and C.-L. Terng, *A general theory of canonical forms*, Trans. Amer. Math. Soc., 300 (1987), pp. 771–789.

[43] R. S. Palais and C.-L. Terng, *Critical Point Theory and Submanifold Geometry*, Lecture Notes in Mathematics, 1353, Springer-Verlag, Berlin, 1988.

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

[45] R. Rosso and E. G. Virga, *Metastable Nematic Hedgehogs*, J. Phys. A, 29 (1996), pp. 4247–4264.

[46] N. Schopohl and T. J. Sluckin, *Defect core structure in nematic liquid crystals*, Phys. Rev. Lett., 59 (1987), pp. 2582–2584.

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

[48] R. Takagi and T. Takahashi, *On the principal curvatures of homogeneous hypersurfaces in a sphere*, in Differential geometry in honor of Kentaro Yano, pp. 469–481, Kinokuniya, Tokyo, 1972.

[49] E. Virga, *Variational Theories for Liquid Crystals*, Applied Mathematics and Mathematical Computation, 8, Chapman & Hall, London, 1994.

[50] T. J. Willmore, *Total Curvature in Riemannian Geometry*, Hellis Horwood Series in Mathematics and its Applications, Hellis Horwood, Chichester, 1982.

[51] H. Zocher, *The effect of a magnetic field on the nematic state*, Trans. Faraday Soc., 29 (1933), pp. 945–957.

Dipartimento di Scienze Matematiche, Fisiche e Informatiche,
Università di Parma,
Parco Area delle Scienze 53/A, I-43124 Parma, Italy
E-Mail: `domenico.mucci@unipr.it`, `lorenzo.nicolodi@unipr.it`