ON THE LANDAU–DE GENNES ELASTIC ENERGY OF CONSTRAINED BIAXIAL NEMATICS*

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Abstract. In the Landau-de Gennes theory, a nematic liquid crystal is described by a tensor order parameter, $\mathbf{Q}$, which, at each point of the region Ω occupied by the system, is a symmetric, traceless 3×3 matrix. The free-energy density ψ of nematic liquid crystals is expanded into powers of the components $\mathbf{Q}_{ij}$ of $\mathbf{Q}$ and $\mathbf{Q}_{ij,k}$ of its gradient $\nabla\mathbf{Q}$, and can be decomposed in the sum $\psi = \psi_B + \psi_E$ of the bulk part $\psi_B(\mathbf{Q})$ and the elastic part $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$. A most common expression for ψ_E is given by the four-constant approximation $\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) = L_1\mathbf{Q}_{ij,j}\mathbf{Q}_{ik,k} + L_2\mathbf{Q}_{ik,j}\mathbf{Q}_{ij,k} + L_3\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k} + L_4\mathbf{Q}_{lk}\mathbf{Q}_{ij,l}\mathbf{Q}_{ij,k}$ [1, 26, 27]. For general $\mathbf{Q}$-tensors, it was shown that, if $L_4 \neq 0$, the corresponding free-energy functional is unbounded from below [1, 2]. On the other hand, if $L_4 = 0$ and L_1, L_2, and L_3 satisfy appropriate conditions, the elastic part of the energy functional is bounded and coercive [8, 21]. In the constrained theory in which $\mathbf{Q}$ has position independent eigenvalues, only the elastic energy has to be considered, since the bulk energy is constant. For constrained uniaxial systems, it is known that if $L_4 \neq 0$, the elastic density ψ_E reduces to the classical Oseen–Frank density and relations among L_1, L_2, L_3, and L_4 can be obtained so that the energy is coercive [3, 11, 21]. In this paper we address the question of coercivity for constrained biaxial systems. Conditions on L_1, L_2, L_3, and L_4 guaranteeing coercivity of the energy, and hence existence of minimizers, are established. In particular, we shall obtain the constrained biaxial counterpart of the classical Ericksen conditions for the constrained uniaxial case. For the proof, after deriving a Cartesian representation for ψ_E in terms of the three orthonormal eigenvector fields of $\mathbf{Q}$, we use the identification of the order parameter space with the eightfold quotient of $\mathbb{S}^3 \cong Sp(1)$ by the quaternion group $\mathcal{H}$ and the description, in this model, of the condition for the frame indifference of Landau–de Gennes energy densities as given in [29].

Key words. Landau–de Gennes energy, $\mathbf{Q}$-tensor theory, constrained biaxial nematics, liquid crystals

AMS subject classifications. 82D30, 76A15, 49J40

1. Introduction.

This paper continues our investigation on the properties of the Landau–de Gennes elastic free-energy for constrained biaxial nematic systems started in [29]. The principal aim of this paper is to discuss the question of coercivity for the most common four-elastic-constant form of the Landau–de Gennes elastic free-energy [1, 2, 18, 27] and the corresponding energy minimization problem.

Let us begin by recalling some facts about the Landau–de Gennes theory to better illustrate our results and put them in perspective. In the Landau–de Gennes theory [9, 17, 27], the orientational properties of a nematic liquid crystal occupying a region $\Omega \subset \mathbb{R}^3$ are described by a tensor order parameter $\mathbf{Q}$, the so-called $\mathbf{Q}$-*tensor*, which is a rank-two, symmetric, traceless tensor. This means that $\mathbf{Q}(x)$ defines a symmetric, traceless 3×3 matrix, at each point $x \in \Omega$. The tensor $\mathbf{Q}$ contains information about the degree of order and the deviation from isotropy of the liquid crystal at a point in Ω. More specifically, the eigenvectors of $\mathbf{Q}$ give the directions of preferred orientation of the molecules, while the eigenvalues give the degree of order about these directions. The state of a nematic liquid crystal is said to be (1) *isotropic* when $\mathbf{Q}$ has three equal eigenvalues (and hence, zero), i.e., when $\mathbf{Q}$ vanishes identically, (2) *uniaxial* when $\mathbf{Q}$ has two nonzero equal eigenvalues, and (3) *biaxial* when $\mathbf{Q}$ has

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three distinct eigenvalues. The terms uniaxial and biaxial refer to the shape and the symmetry of the molecules of the system. Either the molecules are uniaxial, in which case there is an axis of rotational symmetry, or biaxial, in which case there are no axis of complete rotational symmetry; in the latter case, however, two perpendicular axes can be defined for each of which there is a reflection symmetry. For an explanation of the molecular arrangement corresponding to a nematic system, we refer to [6, 27].

In a general biaxial state, the tensor order parameter $\mathbf{Q}$ can be written in the form

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

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

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

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. In the following, we may and do assume that $\lambda_1 \le \lambda_2 \le \lambda_3$ and $\lambda_1, \lambda_2, \lambda_3 \in (-\frac{1}{3}, \frac{2}{3})$ (cf. [2, 23]). 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

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

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 the angles needed to specify the principal directions.

The Landau–de Gennes free-energy functionals are nonlinear integral functionals of the components of $\mathbf{Q}$ and of its gradient $\nabla\mathbf{Q}$, subject to certain invariance and symmetry principles. In general, any density $\Psi = \Psi(\mathbf{Q}, \nabla\mathbf{Q})$ for the Landau–de Gennes integral functionals is required to satisfy the condition of *frame indifference* which amounts to

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

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 $\partial\mathbf{Q}_{ij}/\partial x_k =: \partial_k \mathbf{Q}_{ij}$ (cf. [1]). Here and below, the summation convention over repeated indices is assumed. Additional conditions expressing specific physical symmetries of the material can be required on densities, depending on the cases.

A commonly used expression for the Landau–de Gennes free energy of a nematic liquid crystal is [9, 27, 31]

$$\mathcal{F}[\mathbf{Q}] := \int_\Omega [\psi_B(\mathbf{Q}) + \psi_E(\mathbf{Q}, \nabla\mathbf{Q})]\, dx\,, \tag{1.5}$$

where $\psi_B(\mathbf{Q}) = f_B(\mathrm{tr}(\mathbf{Q}^2), \det(\mathbf{Q}))$ is a function of the principal invariants of $\mathbf{Q}$ that accounts for the bulk free-energy density and

$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) = L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4 \tag{1.6}$$

is the elastic free-energy density. The L_i are material constants and the elastic invariants I_i are given by

$$I_1 = \mathbf{Q}_{ij,j}\mathbf{Q}_{ik,k}\,, \quad I_2 = \mathbf{Q}_{ik,j}\mathbf{Q}_{ij,k}\,, \quad I_3 = \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}\,, \quad I_4 = \mathbf{Q}_{lk}\mathbf{Q}_{ij,l}\mathbf{Q}_{ij,k}\,. \tag{1.7}$$

Observe that $I_1 - I_2 = (\mathbf{Q}_{ij}\mathbf{Q}_{ik,k})_{,j} - (\mathbf{Q}_{ij}\mathbf{Q}_{ik,j})_{,k}$ 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 [1, 2]. On the other hand, it is known that, if $L_4 = 0$, the elastic part of the energy,

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

is bounded from below and coercive if the elastic constants L_1, L_2, and L_3 satisfy [8, 21]

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

In many applications, the scalar order parameters S_1, S_2 of $\mathbf{Q}$ can be regarded as independent of position, i.e., independent of $x \in \Omega$, and only the vectors $\mathbf{n}$ and $\mathbf{m}$ are allowed to vary in space [16, 21, 22]. It then suffices to consider the so-called *constrained Landau–de Gennes theory* of nematic liquid crystals in which $\mathbf{Q}$ has constant scalar order parameters, and hence constant eigenvalues [1, 3]. In the constrained theory, the bulk part of the energy is constant and so only the elastic free energy is to be considered. For the question of defects in the framework of the constrained theory, we refer to [1, 6, 7, 27] and the literature therein.

One motivation for considering the four-elastic-constant expression (1.6) is that, in the constrained uniaxial case in which $\mathbf{Q}$ has a constant scalar order parameter and the order parameter space identifies with the projective plane $\mathbb{R}P^2$, then $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ reduces to the classical Oseen-Frank density [13, 30, 35],

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

where the K_i are elastic constants. This is achieved (cf. [3, 5, 27]) by formally calculating the energy density (1.6) 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

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

In particular, relations among L_1, L_2, L_3, and L_4 can be determined so that the corresponding energy is coercive [3, 11, 21, 34]. Note that, although the elastic energies can be taken to be the same in the two theories, the result of the energy minimization might be different [3]. (See [3, 28] for the related problems of line field orientability and map lifting in the Sobolev setting.)

In the constrained theory of biaxial nematics, the order parameter space is the set $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ of all constrained biaxial $\mathbf{Q}$-tensors of the form (1.1) with distinct constant eigenvalues λ_1, λ_2, λ_3. Any element $\mathbf{Q} \in \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ can be written in the form $\mathbf{Q} = \mathbf{G}\mathbf{A}\mathbf{G}^T$, for some $\mathbf{G} \in SO(3)$, where $\mathbf{A} = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$ is the diagonal matrix of the eigenvalues. Thus, $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ coincides with the orbit of $\mathbf{A}$ with respect to the $SO(3)$-action by conjugation on the five-dimensional space of $\mathbf{Q}$-tensors, and can be identified with the homogeneous space $SO(3)/D_2$, where D_2 is the abelian four-element dihedral group (cf. [25, 27]). Using the identification of the unit 3-sphere

$\mathbb{S}^3$ with $Sp(1)$, the Lie group of unit quaternions, and the 2:1 universal covering map $\Phi : \mathbb{S}^3 \to SO(3)$, the order parameter space of constrained biaxial nematics is then diffeomorphic to the homogeneous manifold $\mathbb{S}^3/\mathcal{H}$, where $\mathcal{H} = \{\pm 1, \pm \mathsf{i}, \pm \mathsf{j}, \pm \mathsf{k}\}$ is the non-abelian eight-element quaternion group. In this model, a configuration of a biaxial nematic liquid crystal is described by a map from Ω to $\mathbb{S}^3/\mathcal{H}$.

2. Description of results. The purpose of this paper is to discuss the question of coercivity of $\mathcal{F}_E[\mathbf{Q}]$, subject to suitable boundary conditions, for the case of constrained biaxial systems (also called "hard biaxial" systems [22]). We will find explicit conditions on the elastic constant L_1, L_2, L_3, and L_4, under which the energy $\mathcal{F}_E[\mathbf{Q}]$, and hence $\mathcal{F}[\mathbf{Q}]$, is coercive. This is the content of Theorems 6.2, 6.3, 6.5, and 6.7.

The main points in our discussion are the following:

- Compute Cartesian expressions for the elastic invariants I_1, I_2, I_3, and I_4.
- Use the Cartesian expressions for I_1, I_2, I_3, and I_4 and the identification of $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ with $\mathbb{S}^3/\mathcal{H}$ to express the energy density $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ in terms of maps $q : \Omega \to \mathbb{S}^3$ and their derivatives, so that
$$\psi_E(\mathbf{Q}(q(x)), \nabla\mathbf{Q}(q(x))) = f_E(q(x), \nabla q(x)) \qquad \forall\, x \in \Omega\,,$$
for a suitably constructed energy density model $f_E(q, \nabla q)$ satisfying the required invariance conditions.
- Use the frame indifference to determine necessary and sufficient conditions on the elastic constants L_i for the (pointwise) expression of the energy density model $f_E(q, \nabla q)$ to be a positive definite quadratic function of ∇q.
- Apply the above results to the question of coercivity for the energy functional $\mathcal{F}_E[\mathbf{Q}]$.
- Apply the above results to the question of existence of minimizers for the energy functional $\mathcal{F}_E[\mathbf{Q}]$.

We will now address each of these issues in more detail.

2.1. Cartesian expressions. For a constrained biaxial $\mathbf{Q}$ of the form (1.1), with distinct constant eigenvalues $\lambda_1, \lambda_2, \lambda_3$, we derive Cartesian expressions for the elastic invariants I_1, I_2, I_3, and I_4 in terms of the gradient, the divergence, and the curl of the orthonormal eigenvector fields $(\mathbf{n},\ \mathbf{m},\ \boldsymbol{\ell})$ associated with $\mathbf{Q}$. More precisely, in Propositions 4.3, 4.5, and 4.2 we compute, respectively,

$$\begin{aligned} I_1(\mathbf{Q}, \nabla\mathbf{Q}) = {} & S_1(S_1 - S_2)\big((\operatorname{div}\mathbf{n})^2 + |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\big) \\ & + S_2(S_2 - S_1)\big((\operatorname{div}\mathbf{m})^2 + |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\big) \\ & + S_1 S_2\big((\operatorname{div}\boldsymbol{\ell})^2 + |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\big)\,, \end{aligned}$$

$$\begin{aligned} I_2(\mathbf{Q}, \nabla\mathbf{Q}) = {} & S_1(S_1 - S_2)\big(\operatorname{tr}[(\nabla\mathbf{n})^2] + |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\big) \\ & + S_2(S_2 - S_1)\big(\operatorname{tr}[(\nabla\mathbf{m})^2] + |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\big) \\ & + S_1 S_2\big(\operatorname{tr}[(\nabla\boldsymbol{\ell})^2] + |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\big)\,, \end{aligned}$$

$$I_3(\mathbf{Q}, \nabla\mathbf{Q}) = 2S_1(S_1 - S_2)|\nabla\mathbf{n}|^2 + 2S_2(S_2 - S_1)|\nabla\mathbf{m}|^2 + 2S_1 S_2|\nabla\boldsymbol{\ell}|^2\,,$$

and in Theorem 5.1, we compute

$$\begin{aligned}I_4(\mathbf{Q},\nabla\mathbf{Q}) &= 3^{-1}\, S_1(2S_1-S_2)(S_2-S_1)\left(\mathrm{tr}[(\nabla\mathbf{n})^2]+(\mathbf{n}\cdot\mathrm{curl}\,\mathbf{n})^2\right)\\ &+3^{-1}\, S_1(S_1-S_2)(4S_1-5S_2)\,|\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2\\ &+3^{-1}\, S_2(2S_2-S_1)(S_1-S_2)\left(\mathrm{tr}[(\nabla\mathbf{m})^2]+(\mathbf{m}\cdot\mathrm{curl}\,\mathbf{m})^2\right)\\ &+3^{-1}\, S_2(S_2-S_1)(S_1+4S_2)\,|\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2\\ &+3^{-1}\, S_1S_2(S_1+S_2)\,\left(\mathrm{tr}[(\nabla\boldsymbol{\ell})^2]+(\boldsymbol{\ell}\cdot\mathrm{curl}\,\boldsymbol{\ell})^2\right)\\ &+3^{-1}\, S_1S_2(S_2-5S_1)\,|\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2\\ &+2S_1S_2(S_1-S_2)\,[(\mathbf{m}\cdot\mathrm{curl}\,\mathbf{n})^2+(\boldsymbol{\ell}\cdot\mathrm{curl}\,\mathbf{m})^2+(\mathbf{n}\cdot\mathrm{curl}\,\boldsymbol{\ell})^2]\,,\end{aligned}$$

so that $\psi_E(\mathbf{Q},\nabla\mathbf{Q})=\tilde{f}(\mathbf{n},\mathbf{m},\mathbf{n},\nabla\mathbf{n},\nabla\mathbf{m},\nabla\boldsymbol{\ell})$. The important fact about these new Cartesian expressions for I_1,I_2,I_3,I_4 is that, unlike those computed for instance in [29], they are written, up to a divergence term (cf. (4.3)), using only the twelve independent quadratic first order invariants

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

which appear in the expansion up to second order of the elastic free-energy density of a constrained biaxial system [16, 22, 32]. Actually, the above expression for I_3 was already given in [29].

2.2. Energy density model. Using the identification of the order parameter space $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ of a constrained biaxial system with the homogeneous space $\mathbb{S}^3/\mathcal{H}$, to any unit quaternion $q\in\mathbb{S}^3$ there corresponds a tensor order parameter $\mathbf{Q}(q):=\mathbf{G}(q)\mathbf{A}\mathbf{G}(q)^T$, where $\mathbf{A}=\mathrm{diag}(\lambda_1,\lambda_2,\lambda_3)$ and $\mathbf{G}(q)=\Phi(q)$ is the orthogonal matrix having $\mathbf{n}(q)$, $\mathbf{m}(q)$, and $\boldsymbol{\ell}(q)$ as column vectors, being $\Phi:\mathbb{S}^3\to SO(3)$ the universal covering map of $SO(3)$ (cf. Section 3, Equation (3.1)). This, together with the Cartesian expressions above, allows us to express $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ in terms of maps $q:\Omega\to\mathbb{S}^3$ and their derivatives. Namely, there exists a function $f_E:\mathbb{S}^3\times\mathbb{M}_{4\times3}\to[0,+\infty]$, such that

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

In [29], we identified the conditions on f_E, so that: (1) f_E is independent of arbitrary superposed rigid rotations (frame indifference condition); (2) f_E is well defined on the class of configuration maps $\Omega\to\mathbb{S}^3/\mathcal{H}$ (residual symmetry condition). Condition (2) is a specific physical symmetry of the material that corresponds to the "head-to-tail" symmetry in the uniaxial case. As for condition (1), f_E is said to satisfy the *frame invariance condition* if, for any $q\in\mathbb{S}^3\cong Sp(1)$,

$$f_E(w,H)=f_E(qw,L(q)H\Phi(q)^T)\quad\forall\,(w,H)\in\mathbb{S}^3\times\mathbb{M}_{4\times3},\tag{2.1}$$

where $L(q)$ is the (orthogonal) matrix of the $\mathbb{R}$-linear map $w\mapsto qw$ on the algebra of quaternions $\mathbb{H}$, relative to $\{1,\mathsf{i},\mathsf{j},\mathsf{k}\}$. This invariance condition is indeed equivalent to the frame indifference condition (1.4) in the sense of $\mathbf{Q}$-tensors [29]. Therefore, the function $f_E(q,\nabla q)$ may be interpreted as the elastic energy density model for the configuration maps $q:\Omega\to\mathbb{S}^3/\mathcal{H}$ of a constrained biaxial nematic system, and the corresponding energy functional is well defined, for instance, on Sobolev maps $q:\Omega\to\mathbb{S}^3/\mathcal{H}$.

In principle, using the Cartesian expression for ψ_E and the above identifications, we could explicitly compute f_E arguing as in [29], where we computed f_3 such that $I_3(\mathbf{Q}(q),\nabla\mathbf{Q}(q))=f_3(q,\nabla q)$. However, for our purposes, such computations are not needed.

2.3. Coercivity conditions. In Theorems 6.2 and 6.5, for any given map $q:\Omega\to\mathbb{S}^3$, we determine necessary and sufficient conditions on the elastic constants L_i for the (pointwise) expression of the energy density model $f_E(q,\nabla q)$ to be a positive definite quadratic function of ∇q. Actually, we find necessary and sufficient conditions on the L_i under which the function f_E satisfies $f_E(q,H)>0$, for any given $q\in\mathbb{S}^3$ and all 4×3 matrices $H\neq 0$ such that $H^Tq=0$. This is achieved by first studying the positivity of the form $f_E(p_0,\cdot)$ at a fixed pole $p_0\in\mathbb{S}^3$ and by then exploiting the frame invariance condition (2.1) and Lemma 3.6 to prove the positivity for any $q\in\mathbb{S}^3$.

Note that the positivity of $f_E(q,\nabla q)$ holds true also for maps in $W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$ by the lifting result of Bethuel–Chiron [4, Theorem 1], which asserts that if Ω is bounded and simply connected, then for every $w\in W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$, there exists a $\widetilde{w}\in W^{1,2}(\Omega,\mathbb{S}^3)$, unique up to the action of an element of $\pi_1(\mathbb{S}^3/\mathcal{H})=\mathcal{H}$, such that $\Pi\circ\widetilde{w}=w$ a.e. in Ω, where $\Pi:\mathbb{S}^3\to\mathbb{S}^3/\mathcal{H}$ is the canonical projection, and $|\nabla w|=|\nabla\widetilde{w}|$ a.e. in Ω. In particular, for each Sobolev map $q\in W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$, the corresponding map $\Omega\ni x\mapsto\mathbf{Q}(q(x))$ belongs to the Sobolev class $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$.

Notice that the diffeomorphism $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)\cong\mathbb{S}^3/\mathcal{H}$ establishes a bijective correspondence between $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$ and $W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$; see, for example, [29] for details. Moreover, using the Nash–Moser isometric embedding of the Riemannian homogeneous manifold $\mathbb{S}^3/\mathcal{H}\cong\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ into some Euclidean space $\mathbb{R}^N$, the elements $\mathbf{Q}$ of $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$ are identified with the Sobolev functions w in $W^{1,2}(\Omega,\mathbb{R}^N)$, such that $w(x)\in\mathbb{S}^3/\mathcal{H}$, for a.e. $x\in\Omega$.

2.4. Coercivity of the energy functional. As a consequence of the previous discussion, we have the following.

Theorem A. *For a constrained biaxial nematic system, let $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ be of the form (1.6), for constants $L_1,L_2,L_3,L_4\in\mathbb{R}$. Then, there exists $\nu>0$ such that*

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

if and only if the constants L_1,L_2,L_3, and L_4 satisfy the conditions established in Theorem 6.5.

The necessary and sufficient conditions of Theorem 6.5 can be interpreted as the constrained biaxial counterpart of the classical *Ericksen inequalities* [11, 34] for the constrained uniaxial case, see (6.2) below, which can be rewritten in terms of the coefficients L_i as

$$2L_1+L_2+2L_3>\frac{2}{3}L_4s\,,\quad L_1+L_2+2L_3+\frac{4}{3}L_4s>0\,,\quad 2L_3-\frac{2}{3}L_4s>|L_2|\,.$$

Assume now that the admissible $\mathbf{Q}$ for the functional $\mathcal{F}[\mathbf{Q}]$ satisfy Dirichlet boundary conditions given as follows [9, 12, 20]. Let $\Omega\subset\mathbb{R}^3$ be a bounded and simply connected domain with smooth boundary $\partial\Omega$. For a smooth function $\varphi:\Omega\cup\partial\Omega\to\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$, we define the class $W^{1,2}_\varphi$ of admissible tensor fields by

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

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

In Theorems 6.3 and 6.7, we find sufficient conditions on the L_i under which there exists a positive constant $\nu > 0$, such that

$$\psi_E(\mathbf{Q}(q), \nabla\mathbf{Q}(q)) = f_E(q, \nabla q) \geq \nu\,|\nabla q|^2 + \text{divergence term.} \tag{2.2}$$

As a consequence, we have the following.

THEOREM B. *For a constrained biaxial nematic system, let $\mathcal{F}[\mathbf{Q}]$ be of the form (1.5), and let $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ be of the form (1.6), for some constants $L_1, L_2, L_3, L_4 \in \mathbb{R}$. Then, there exists $\nu > 0$ such that*

$$\mathcal{F}_E[\mathbf{Q}] \geq \nu \int_{\Omega} |\nabla\mathbf{Q}|^2\, dx + c_{\varphi}\,, \quad \textit{for all} \quad \mathbf{Q} \in W^{1,2}_{\varphi}\,,$$

provided that L_1, L_2, L_3, L_4 satisfy the conditions established in Theorem 6.7.

The sufficient conditions of Theorem 6.7 for the constrained biaxial case, can be seen as the counterpart of the analogous conditions for the constrained uniaxial case; cf., e.g., [15, Section 5.1], which in terms of the coefficients L_i read

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

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

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

if the L_i satisfy the inequalities established in Theorem 6.5, there exist constants $K > \nu > 0$ such that for all $\mathbf{Q} \in W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))$

$$c_B + \nu \int_{\Omega} |\nabla\mathbf{Q}|^2\, dx \leq \mathcal{F}[\mathbf{Q}] \leq c_B + K \int_{\Omega} |\nabla\mathbf{Q}|^2\, dx\,.$$

In a similar way, if the L_i satisfy the inequalities established in Theorem 6.7, there exist constants $K > \nu > 0$ such that

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

Next, arguing as in [8, Section 4], it follows that the functional $\mathcal{F}[\mathbf{Q}]$ is convex in $\nabla\mathbf{Q}$ (and continuous in the strong $W^{1,2}$-topology) and hence weakly sequentially lower semicontinuous in $W^{1,2}$. Moreover, both classes $W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))$ and $W^{1,2}_{\varphi}$ are nonempty and closed under sequential weak convergence. Therefore, by compactness of the target manifold $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$, existence of minimizers for $\mathcal{F}[\mathbf{Q}]$ is guaranteed by the direct method of the calculus of variations (see, for instance, [14, Chapter I]). We can thus state the following existence results.

THEOREM I. *Let $\Omega \subset \mathbb{R}^3$ be a bounded, simply connected domain with smooth boundary $\partial\Omega$. Let the elastic constants L_1, L_2, L_3, and L_4 satisfy the inequalities established in Theorem 6.5. Then, the functional $\mathcal{F}[\mathbf{Q}]$ attains a minimum on the class $W^{1,2}(\Omega, \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3))$.*

THEOREM II. *Let $\Omega \subset \mathbb{R}^3$ be a bounded, simply connected domain with smooth boundary $\partial\Omega$. Let the elastic constants L_1, L_2, L_3, and L_4 satisfy the inequalities established in Theorem 6.7. Let $\varphi : \Omega \cup \partial\Omega \to \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ be smooth. Then, the functional $\mathcal{F}[\mathbf{Q}]$ attains a minimum on the class $W^{1,2}_\varphi$.*

There are several interesting open questions still to be investigated. A first problem would be that of finding the necessary and sufficient conditions in Theorem B. Another interesting question would be that of determining the precise inequalities which guarantee coercivity under the so-called *partial* Dirichlet boundary conditions or the physically relevant *conical anchoring* conditions proposed in [1].

This paper is organized as follows. Section 3 fixes notation and recalls some background material, mainly taken from [29]. Section 4 computes explicit Cartesian representations for I_1, I_2, I_3. Section 5 does the same for I_4. Section 6 obtains conditions on L_1, L_2, L_3, and L_4, under which the energy $\mathcal{F}[\mathbf{Q}]$ is coercive.

3. Preliminaries and notation. In this section, we fix the notation and briefly recall some background material and results to be used in the sections that follow. The reader is referred to [29] for additional details.

3.1. Quaternions and rotations. Let $\mathbb{H}$ be the real noncommutative algebra of quaternions, with the standard basis $\{1, \mathsf{i}, \mathsf{j}, \mathsf{k}\}$, where multiplication is determined by the rules $\mathsf{i}^2 = \mathsf{j}^2 = \mathsf{k}^2 = \mathsf{ijk} = -1$. If $q \in \mathbb{H}$, we write

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

The real and imaginary parts of q are q_0 and $q_1\mathsf{i}+q_2\mathsf{j}+q_3\mathsf{k}$, respectively. The conjugate of q is $\bar{q} = q_0-q_1\mathsf{i}-q_2\mathsf{j}-q_3\mathsf{k}$ and the norm $|q|$ is defined by $|q|^2 = q\bar{q} = \bar{q}q = q_0^2+q_1^2+q_2^2+q_3^2$. The multiplicative inverse of any nonzero quaternion is $q^{-1} = \bar{q}/|q|^2$. As a vector space, $\mathbb{H}$ is identified with $\mathbb{R}^4$ via the usual isomorphism, $q = q_0 + q_1\mathsf{i} + q_2\mathsf{j} + q_3\mathsf{k} \longleftrightarrow (q_0, q_1, q_2, q_3)^T$, which in turn induces an isomorphism between the subspace of pure quaternions $\operatorname{span}\{\mathsf{i}, \mathsf{j}, \mathsf{k}\}$ and $\mathbb{R}^3$. In view of this isomorphism, the elements $1, \mathsf{i}, \mathsf{j}, \mathsf{k}$ of $\mathbb{H}$ will be identified with the elements of the canonical basis $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ of $\mathbb{R}^4$, respectively. We will also use the decomposition $\mathbb{H} = \mathbb{R} \oplus \mathbb{R}^3 = \operatorname{span}\{1\} \oplus \operatorname{span}\{\mathsf{i}, \mathsf{j}, \mathsf{k}\}$ into the real and imaginary parts, and write $(q_0, \mathbf{q})$ for $q = (q_0, q_1, q_2, q_3)^T$.

There is a diffeomorphism between the unit 3-sphere $\mathbb{S}^3 \subset \mathbb{R}^4$ and the group $Sp(1) = \{q \in \mathbb{H} \mid |q| = 1\}$ of unit quaternions. Let $q \in Sp(1)$ and let $C_q : \mathbb{H} \to \mathbb{H}$ be the $\mathbb{R}$-linear transformation defined by $C_q(w) = qw\bar{q}$, for all $w \in \mathbb{H}$. The map C_q is an isometry, $|C_q(w)| = |w|$, and preserves the decomposition $\mathbb{H} = \mathbb{R} \oplus \mathbb{R}^3$ into real and imaginary parts. It can then be interpreted as a rotation of $\mathbb{R}^3$.

Let $M(q)$ be the 4×4 matrix that represents the linear transformation $C_q : \mathbb{H} \to \mathbb{H}$ with respect to the standard basis $\{1, \mathsf{i}, \mathsf{j}, \mathsf{k}\}$. Since $|C_q(w)| = |w|$, for all $w \in \mathbb{H}$, $M(q)$ must be an orthogonal matrix, that is, $M(q) \in O(4)$. The continuity of the determinant and the connectedness of $\mathbb{S}^3$ imply that the determinant of $M(q)$ is positive, so that $M(q) \in SO(4)$. The first column of $M(q)$ is the vector representing the quaternion $q1\bar{q} = q\bar{q} = 1$, that is, $\mathbf{e}_0$. The fact that $M(q)$ belongs to $SO(4)$ now forces $M(q)$ to be of the form $M(q) = \left(\begin{smallmatrix} 1 & 0 \\ 0 & \Phi(q) \end{smallmatrix}\right)$, where $\Phi(q)$ is an element of the special orthogonal group $SO(3)$. The map $\Phi : \mathbb{S}^3 \cong Sp(1) \to SO(3)$, $q \mapsto \Phi(q)$, is a homomorphism of groups which is surjective and has kernel $\{\pm 1\}$ (see [10] for more details). In particular, two matrices $\Phi(p)$ and $\Phi(q)$ represent the same rotation if and only if $p = \pm q$. The rotation matrix corresponding to the unit quaternion

$q = q_0 + q_1\mathsf{i} + q_2\mathsf{j} + q_3\mathsf{k}$ is given explicitly by

$$\Phi(q) = \mathbf{G}(q_0, \mathbf{q}) := \begin{pmatrix} q_0^2 + q_1^2 - (q_2^2 + q_3^2) & 2(q_1q_2 - q_0q_3) & 2(q_1q_3 + q_0q_2) \\ 2(q_1q_2 + q_0q_3) & q_0^2 + q_2^2 - (q_1^2 + q_3^2) & 2(q_2q_3 - q_0q_1) \\ 2(q_1q_3 - q_0q_2) & 2(q_2q_3 + q_0q_1) & q_0^2 + q_3^2 - (q_1^2 + q_2^2) \end{pmatrix}. \tag{3.1}$$

REMARK 3.1. In this paper, we think of vectors as column vectors. If $\mathbf{n}, \mathbf{m} \in \mathbb{R}^3$, the tensor product $\mathbf{n} \otimes \mathbf{m}$ is the matrix $\mathbf{n}\mathbf{m}^T$, so that if $\mathbf{n} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)^T$ and $\mathbf{m} = (\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)^T$, then $(\mathbf{n} \otimes \mathbf{m})^i_j = \mathbf{n}_i\mathbf{m}_j$. We denote by $\mathbf{n} \cdot \mathbf{m}$ the scalar product and by $\mathbf{n} \times \mathbf{m}$ the vector product of $\mathbf{n}, \mathbf{m}$.

3.2. Models for constrained biaxial systems. In the *constrained Landau–de Gennes theory* [3, 24, 25, 22], the scalar order parameters S_1 and S_2 are required to be constant, so that the structure of the liquid crystal at each point $x \in \Omega$ only depends on the value of the orthonormal vectors $\mathbf{n}$, $\mathbf{m}$ at x. In particular, the eigenvalues in (1.2) are constant. In the constrained uniaxial case, according to (1.3), any tensor order parameter $\mathbf{Q}$ has two degrees of freedom given by $\mathbf{r} \in \mathbb{S}^2$. Actually, if $\mathbf{r}$ is replaced by $-\mathbf{r}$ in (1.3), $\mathbf{Q}$ remains the same, and can then be identified with the pair $\{\mathbf{r}, -\mathbf{r}\}$, $\mathbf{r} \in \mathbb{S}^2$, which in turn determines a point in the projective plane $\mathbb{R}P^2$. In the constrained biaxial case, $\mathbf{Q}$ has instead three degrees of freedom.

Let $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ be the set of all constrained biaxial $\mathbf{Q}$-tensors of the form (1.1) with distinct constant eigenvalues $\lambda_1, \lambda_2, \lambda_3$. Any element $\mathbf{Q} \in \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ can be written in the form $\mathbf{Q} = \mathbf{G}\mathbf{A}\mathbf{G}^T$, for some $\mathbf{G} \in SO(3)$, where $\mathbf{A} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ is the diagonal matrix of the eigenvalues. Therefore, $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ coincides with the orbit of $\mathbf{A}$ with respect to the $SO(3)$-action by conjugation on the space of $\mathbf{Q}$-tensors, and can be identified with the homogeneous space $SO(3)/D_2$, where D_2 is the abelian four-element dihedral group [7, 25, 29]. Using the identification of $\mathbb{S}^3$ with the Lie group of unit quaternions, $Sp(1)$, and the 2:1 covering map $\Phi : \mathbb{S}^3 \to SO(3)$, the order parameter space $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ of constrained biaxial nematics is then diffeomorphic to the homogeneous manifold $\mathbb{S}^3/\mathcal{H}$, where $\mathcal{H} = \{\pm 1, \pm\mathsf{i}, \pm\mathsf{j}, \pm\mathsf{k}\}$ is the non-abelian eight-element quaternion group [29]. To each $\mathbf{Q} \in \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ there corresponds a set of eight elements $q \in \mathbb{S}^3$, a right coset of $\mathcal{H}$ in $\mathbb{S}^3 \cong Sp(1)$. In this model, a configuration of a biaxial nematic liquid crystal is described by a map from Ω to $\mathbb{S}^3/\mathcal{H}$, as opposed to the constrained uniaxial case where the order parameter space is $\mathbb{RP}^2$.

REMARK 3.2. From (1.2) and the specific ordering $\lambda_1 < \lambda_2 < \lambda_3$ of the eigenvalues in the representation (1.1), it follows that $S_1 < S_2 < 0$. Moreover, according to the analysis in the proof of Proposition 1 in [24], one can indeed conclude that either

$$\frac{S_1}{2} \leq S_2 < 0, \quad \text{or} \quad S_2 \leq \frac{S_1}{2} < 0\,. \tag{3.2}$$

In fact, using the notation from [24], condition $\lambda_1 < \lambda_2 < \lambda_3$ yields that R_2^- and R_3^+ are the only admissible regions.

3.3. Frame indifference. In the framework of $\mathbf{Q}$-tensor theory, two observers see the same free-energy density $\psi(\mathbf{Q}, \nabla\mathbf{Q})$. This amounts to the requirement that

$$\psi(\mathbf{Q}, \nabla\mathbf{Q}) = \psi(M\mathbf{Q}M^T, \mathbf{D}^*) \qquad \forall M \in SO(3)\,, \tag{3.3}$$

where $\mathbf{D}^*_{ijk} := M^i_l M^j_m M^k_p \mathbf{Q}_{lm,p}$; cf., e.g., [1]. Here and in the following, the symbol "${}_{,k}$" denotes the partial derivative "$\frac{\partial}{\partial x_k} =: \partial_k$" in the kth canonical direction w.r.t. $x \in \Omega$, so that $\mathbf{Q}_{ij,k} = \frac{\partial}{\partial x_k}\mathbf{Q}_{ij} = \partial_k \mathbf{Q}_{ij}$.

In the constrained uniaxial case, condition (3.3) is equivalent to the well known frame invariance

$$w(\mathbf{r}, H) = w(R\mathbf{r}, RHR^T) \qquad \forall\, \mathbf{r} \in \mathbb{S}^2\,, \quad H \in \mathbb{M}_{3\times 3}\,, \quad R \in SO(3) \tag{3.4}$$

that is satisfied by an energy density in the Oseen-Frank theory of uniaxial nematic liquid crystals [15, 19].

Remark 3.3. The elastic free-energy densities I_1, I_2, I_3, I_4 as given in (1.7) satisfy condition (3.3) for the full orthogonal group $O(3)$. This is a material symmetry reflecting the lack of chirality of the molecules constituting nematic liquid crystals (cf. [1]).

In the above model for constrained biaxial systems, the Landau–de Gennes elastic free-energy density $\psi_E(\mathbf{Q}, \nabla\mathbf{Q})$ is expressed as a density on maps $q : \Omega \to \mathbb{S}^3$, depending on q and its first derivatives. In [29], we identified the conditions on a generic energy density $f : \mathbb{S}^3 \times \mathbb{M}_{4\times 3} \to [0, +\infty)$, in order that:

(1) f is independent of arbitrary superposed rigid rotations (frame indifference condition);
(2) f is well defined on the class of configuration maps $\Omega \to \mathbb{S}^3/\mathcal{H}$ (residual symmetry condition).

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

Definition 3.4. An energy density $f : \mathbb{S}^3 \times \mathbb{M}_{4\times 3} \to [0, +\infty)$ satisfies the *frame invariance condition* if, for any $q \in \mathbb{S}^3$,

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

where $L(q)$ denotes the orthogonal matrix representing the real linear map on $\mathbb{H}$ defined by $w \mapsto q\, w$, with respect to the standard basis $\{1, \mathsf{i}, \mathsf{j}, \mathsf{k}\}$, and $\Phi : \mathbb{S}^3 \to SO(3)$ is the 2:1 group homomorphism given in (3.1).

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

Theorem 3.5 (see [29]). *For constrained biaxial nematics, the frame invariance condition* (3.5) *is equivalent to the frame invariance* (3.3) *in the sense of* $\mathbf{Q}$*-tensors.*

As a consequence, we have the following useful result.

Lemma 3.6. *If the condition* (3.5) *holds and if* $f(q_0, H) \geq 0$ *for a given* $q_0 \in \mathbb{S}^3$ *and all* $H \in \mathbb{M}_{4\times 3}$ *such that* $H^T q_0 = 0$, *then* $f(q, H) \geq 0$ *for any* $q \in \mathbb{S}^3$ *and all* $H \in \mathbb{M}_{4\times 3}$ *such that* $H^T q = 0$.

Proof. For any $q \in \mathbb{S}^3$, there exists $p \in \mathbb{S}^3 \cong Sp(1)$ such that $q = pq_0$. Let $H \in \mathbb{M}_{4\times 3}$ such that $H^T q = 0$. Since the conjugate $\bar{p} = p^{-1} \in Sp(1)$, by (3.5), we have

$$f(q, H) = f(\bar{p}q, L(\bar{p})H\Phi(\bar{p})^T) = f(q_0, L(\bar{p})H\Phi(\bar{p})^T),$$

where $L(\bar{p})H\Phi(\bar{p})^T$ satisfies $\big(L(\bar{p})H\Phi(\bar{p})^T\big)^T q_0 = 0$. In fact,

$$\begin{aligned} \big(L(\bar{p})H\Phi(\bar{p})^T\big)^T q_0 &= \big(L(p)^T H\Phi(\bar{p})^T\big)^T q_0 = \Phi(\bar{p})H^T L(p) q_0 \\ &= \Phi(\bar{p})H^T p q_0 = \Phi(\bar{p})H^T q = 0. \end{aligned}$$

Therefore, $f(q,H) = f(q_0, L(\bar{p})H\Phi(\bar{p})^T) \geq 0$, as claimed. □

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

DEFINITION 3.7. An energy density $f : \mathbb{S}^3 \times \mathbb{M}_{4\times 3} \to [0,+\infty)$ is said to satisfy the *residual symmetry property* if, for any $q \in \mathcal{H}$, one has

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

The above symmetry property is the counterpart of the property

$$w(\mathbf{r},H) = w(-\mathbf{r},-H) \qquad \forall\, \mathbf{r} \in \mathbb{S}^2\,, \quad H \in \mathbb{M}_{3\times 3}\,,$$

satisfied by the energy density of uniaxial nematic liquid crystals in the sense of Oseen–Frank [15, 19].

REMARK 3.8. Conditions (3.5) and (3.6) are necessary for a map $f : \mathbb{S}^3 \times \mathbb{M}_{4\times 3} \to [0,+\infty)$ representing an energy density for constrained biaxial nematic states.

4. Cartesian representations for the first three invariants. We first collect collect some useful formulas.

For a smooth unit vector field $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)^T : \mathbb{R}^3 \to \mathbb{S}^2$, let the 3×3 matrix $\nabla\mathbf{r} = (\mathbf{r}_{i,j})$, $i,j = 1,2,3$, denote the gradient of $\mathbf{r}$, $\operatorname{div}\mathbf{r} = \operatorname{tr}(\nabla\mathbf{r}) = \mathbf{r}_{i,i}$ the divergence of $\mathbf{r}$, and $\operatorname{curl}\mathbf{r} = (\mathbf{r}_{3,2} - \mathbf{r}_{2,3}, \mathbf{r}_{1,3} - \mathbf{r}_{3,1}, \mathbf{r}_{2,1} - \mathbf{r}_{1,2})^T$ the curl of $\mathbf{r}$. Using $\mathbf{r}_i\mathbf{r}_{i,j} = 0$, it follows that

$$\begin{aligned} |\operatorname{curl}\mathbf{r}|^2 &= (\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 + |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2\,,\\ |\nabla\mathbf{r}|^2 &= \operatorname{tr}[(\nabla\mathbf{r})^2] + |\operatorname{curl}\mathbf{r}|^2\,,\\ |\nabla\mathbf{r}|^2 &= \operatorname{tr}[(\nabla\mathbf{r})^2] + (\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 + |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2\,, \end{aligned} \tag{4.1}$$

where $|\nabla\mathbf{r}|^2 = \mathbf{r}_{i,j}\mathbf{r}_{i,j}$, $\operatorname{tr}[(\nabla\mathbf{r})^2] = \mathbf{r}_{k,j}\mathbf{r}_{j,k}$, $\mathbf{r}\times\operatorname{curl}\mathbf{r} = -(\nabla\mathbf{r})\mathbf{r}$, and

$$|\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2 = \mathbf{r}_{i,k}\mathbf{r}_k\mathbf{r}_{i,l}\mathbf{r}_l\,. \tag{4.2}$$

REMARK 4.1. We recall that the term

$$\left[\operatorname{tr}[(\nabla\mathbf{r})^2] - (\operatorname{div}\mathbf{r})^2\right] = \operatorname{div}[(\nabla\mathbf{r})\mathbf{r} - (\operatorname{div}\mathbf{r})\mathbf{r}] \tag{4.3}$$

is a divergence term.

In the constrained biaxial case, we have (1.1), where $S_1 \neq S_2$ are nonzero constants and $\mathbf{n}$, $\mathbf{m} \in \mathbb{S}^2$ satisfy $\mathbf{n}\cdot\mathbf{m} = 0$ and depend on the position $x \in \Omega$. Using the completeness property of the eigenvectors,

$$\mathbf{n}\otimes\mathbf{n} + \mathbf{m}\otimes\mathbf{m} + \boldsymbol{\ell}\otimes\boldsymbol{\ell} = \mathbf{I}\,, \qquad \boldsymbol{\ell} := \mathbf{n}\times\mathbf{m} \in \mathbb{S}^2\,, \tag{4.4}$$

we have that

$$\mathbf{Q} = \lambda_1\mathbf{n}\otimes\mathbf{n} + \lambda_2\mathbf{m}\otimes\mathbf{m} + \lambda_3\boldsymbol{\ell}\otimes\boldsymbol{\ell}\,, \tag{4.5}$$

with $\lambda_1, \lambda_2, \lambda_3$ as in (1.2), and hence

$$\begin{aligned} \mathbf{Q}_{ij} &= \lambda_1\mathbf{n}_i\mathbf{n}_j + \lambda_2\mathbf{m}_i\mathbf{m}_j + \lambda_3\boldsymbol{\ell}_i\boldsymbol{\ell}_j\,,\\ \mathbf{Q}_{ij,k} &= \lambda_1(\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_{i,k}\mathbf{n}_j) + \lambda_2(\mathbf{m}_i\mathbf{m}_{j,k} + \mathbf{m}_{i,k}\mathbf{m}_j) + \lambda_3(\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_j)\,. \end{aligned}$$

Property (4.4) yields that, for each i, j, k,

$$\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_j\mathbf{n}_{i,k} + \mathbf{m}_i\mathbf{m}_{j,k} + \mathbf{m}_j\mathbf{m}_{i,k} + \boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k} = 0\,. \tag{4.6}$$

Moreover, for $\mathbf{r}, \mathbf{s} \in \{\mathbf{n}, \mathbf{m}, \boldsymbol{\ell}\}$, it follows from the orthonormality of $\mathbf{n}$, $\mathbf{m}$, and $\boldsymbol{\ell}$ that

$$\mathbf{r}_i\mathbf{s}_{i,j} = (\mathbf{r}_i\mathbf{s}_i)_{,j} - \mathbf{s}_i\mathbf{r}_{i,j} = -\mathbf{s}_i\mathbf{r}_{i,j}. \tag{4.7}$$

4.1. The term I_3. In [29], we explicitly computed the third elastic invariant

$$I_3(\mathbf{Q}, \nabla\mathbf{Q}) := \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}\,.$$

For our purposes, in what follows we shall denote

$$\Lambda_1 := (2\lambda_1^2 + \lambda_2\lambda_3)\,, \quad \Lambda_2 := (2\lambda_2^2 + \lambda_3\lambda_1)\,, \quad \Lambda_3 := (2\lambda_3^2 + \lambda_1\lambda_2)\,. \tag{4.8}$$

The invariant I_3 has the following expression.

Proposition 4.2 (see [29]). *Under the previous hypotheses, we have*

$$I_3(\mathbf{Q}, \nabla\mathbf{Q}) = 2\Lambda_1|\nabla\mathbf{n}|^2 + 2\Lambda_2|\nabla\mathbf{m}|^2 + 2\Lambda_3|\nabla\boldsymbol{\ell}|^2\,.$$

4.2. The term I_1. We now focus our attention on the first elastic invariant

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

Proposition 4.3. *Under the previous hypotheses, we have*

$$\begin{aligned} I_1(\mathbf{Q}, \nabla\mathbf{Q}) \;&= \Lambda_1\big((\operatorname{div}\mathbf{n})^2 + |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\big) \\ &\quad +\Lambda_2\big((\operatorname{div}\mathbf{m})^2 + |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\big) \\ &\quad +\Lambda_3\big((\operatorname{div}\boldsymbol{\ell})^2 + |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\big)\,. \end{aligned}$$

Proof. We first decompose $I_1 = I_{11} + I_{12} + I_{13} + I_{14} + I_{15} + I_{16}$ according to the coefficients $\lambda_i\lambda_j$. Using $\mathbf{r}_{\alpha,\alpha} = \operatorname{div}\mathbf{r}$, we have

$$\begin{aligned} I_{11} &= \lambda_1^2((\operatorname{div}\mathbf{n})\mathbf{n}_i + \mathbf{n}_{i,j}\mathbf{n}_j)((\operatorname{div}\mathbf{n})\mathbf{n}_i + \mathbf{n}_{i,k}\mathbf{n}_k) \\ I_{12} &= \lambda_2^2((\operatorname{div}\mathbf{m})\mathbf{m}_i + \mathbf{m}_{i,j}\mathbf{m}_j)((\operatorname{div}\mathbf{m})\mathbf{m}_i + \mathbf{m}_{i,k}\mathbf{m}_k) \\ I_{13} &= \lambda_3^2((\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i + \boldsymbol{\ell}_{i,j}\boldsymbol{\ell}_j)((\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_k) \\ I_{14} &= \lambda_1\lambda_2[((\operatorname{div}\mathbf{n})\mathbf{n}_i + \mathbf{n}_{i,j}\mathbf{n}_j)((\operatorname{div}\mathbf{m})\mathbf{m}_i + \mathbf{m}_{i,k}\mathbf{m}_k) \\ &\qquad +((\operatorname{div}\mathbf{n})\mathbf{n}_i + \mathbf{n}_{i,k}\mathbf{n}_k)((\operatorname{div}\mathbf{m})\mathbf{m}_i + \mathbf{m}_{i,j}\mathbf{m}_j)] \\ I_{15} &= \lambda_2\lambda_3[((\operatorname{div}\mathbf{m})\mathbf{m}_i + \mathbf{m}_{i,j}\mathbf{m}_j)((\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_k) \\ &\qquad +((\operatorname{div}\mathbf{m})\mathbf{m}_i + \mathbf{m}_{i,k}\mathbf{m}_k)((\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i + \boldsymbol{\ell}_{i,j}\boldsymbol{\ell}_j)] \\ I_{16} &= \lambda_3\lambda_1[((\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i + \boldsymbol{\ell}_{i,j}\boldsymbol{\ell}_j)((\operatorname{div}\mathbf{n})\mathbf{n}_i + \mathbf{n}_{i,k}\mathbf{n}_k) \\ &\qquad +((\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_k)((\operatorname{div}\mathbf{n})\mathbf{n}_i + \mathbf{n}_{i,j}\mathbf{n}_j)]\,. \end{aligned}$$

Since $\mathbf{r}_\beta\mathbf{r}_{\beta,\alpha} = 0$, by (4.2), we get

$$I_{11} = \lambda_1^2((\operatorname{div}\mathbf{n})^2 + \mathbf{n}_j\mathbf{n}_k\mathbf{n}_{i,j}\mathbf{n}_{i,k}) = \lambda_1^2((\operatorname{div}\mathbf{n})^2 + |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2)$$

and similarly

$$I_{12} = \lambda_2^2((\operatorname{div}\mathbf{m})^2 + |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2)\,, \qquad I_{13} = \lambda_3^2((\operatorname{div}\boldsymbol{\ell})^2 + |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2)\,.$$

The other three terms read

$$\begin{aligned} I_{14} &= 2\lambda_1\lambda_2[(\operatorname{div}\mathbf{n})\mathbf{n}_i\mathbf{m}_{i,k}\mathbf{m}_k + (\operatorname{div}\mathbf{m})\mathbf{m}_i\mathbf{n}_{i,j}\mathbf{n}_j + \mathbf{n}_j\mathbf{n}_{i,j}\mathbf{m}_k\mathbf{m}_{i,k}] \\ I_{15} &= 2\lambda_2\lambda_3[(\operatorname{div}\mathbf{m})\mathbf{m}_i\boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_k + (\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i\mathbf{m}_{i,j}\mathbf{m}_j + \mathbf{m}_j\mathbf{m}_{i,j}\boldsymbol{\ell}_k\boldsymbol{\ell}_{i,k}] \\ I_{16} &= 2\lambda_3\lambda_1[(\operatorname{div}\boldsymbol{\ell})\boldsymbol{\ell}_i\mathbf{n}_{i,k}\mathbf{n}_k + (\operatorname{div}\mathbf{n})\mathbf{n}_i\boldsymbol{\ell}_{i,j}\boldsymbol{\ell}_j + \boldsymbol{\ell}_j\boldsymbol{\ell}_{i,j}\mathbf{n}_k\mathbf{n}_{i,k}]\,. \end{aligned}$$

Now denote

$$\begin{array}{ll} a^n_m := \mathbf{n}_i\mathbf{m}_{i,k}\mathbf{m}_k & a^m_n := \mathbf{m}_i\mathbf{n}_{i,j}\mathbf{n}_j \\ a^m_l := \mathbf{m}_i\boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_k & a^l_m := \boldsymbol{\ell}_i\mathbf{m}_{i,j}\mathbf{m}_j \\ a^l_n := \boldsymbol{\ell}_i\mathbf{n}_{i,k}\mathbf{n}_k & a^n_l := \mathbf{n}_i\boldsymbol{\ell}_{i,j}\boldsymbol{\ell}_j \end{array}$$

and

$$\begin{array}{l} b^n_m := \mathbf{n}_j\mathbf{n}_{i,j}\mathbf{m}_k\mathbf{m}_{i,k} = \mathbf{m}_j\mathbf{m}_{i,j}\mathbf{n}_k\mathbf{n}_{i,k} =: b^m_n \\ b^m_l := \mathbf{m}_j\mathbf{m}_{i,j}\boldsymbol{\ell}_k\boldsymbol{\ell}_{i,k} = \boldsymbol{\ell}_j\boldsymbol{\ell}_{i,j}\mathbf{m}_k\mathbf{m}_{i,k} =: b^l_m \\ b^l_n := \boldsymbol{\ell}_j\boldsymbol{\ell}_{i,j}\mathbf{n}_k\mathbf{n}_{i,k} = \mathbf{n}_j\mathbf{n}_{i,j}\boldsymbol{\ell}_k\boldsymbol{\ell}_{i,k} =: b^n_l \end{array}$$

so that the above terms become

$$\begin{aligned} I_{14} &= 2\lambda_1\lambda_2[(\operatorname{div}\mathbf{n})\,a^n_m + (\operatorname{div}\mathbf{m})\,a^m_n + b^n_m] \\ I_{15} &= 2\lambda_2\lambda_3[(\operatorname{div}\mathbf{m})\,a^m_l + (\operatorname{div}\boldsymbol{\ell})\,a^l_m + b^m_l] \\ I_{16} &= 2\lambda_3\lambda_1[(\operatorname{div}\boldsymbol{\ell})\,a^l_n + (\operatorname{div}\mathbf{n})\,a^n_l + b^l_n]\,. \end{aligned}$$

Using (4.6), with $k = j$ in the term $\mathbf{m}_j\mathbf{m}_{i,k}$, we compute, for example, $a^n_m = -\operatorname{div}\mathbf{n} - a^n_l$, so that

$$a^n_m + a^n_l = -\operatorname{div}\mathbf{n}\,, \quad a^m_l + a^m_n = -\operatorname{div}\mathbf{m}\,, \quad a^l_n + a^l_m = -\operatorname{div}\boldsymbol{\ell}\,. \tag{4.9}$$

With the same strategy, we compute

$$\begin{aligned} b^n_m &= \mathbf{n}_j\mathbf{n}_{i,j}\mathbf{m}_k\mathbf{m}_{i,k} \\ &= -\mathbf{n}_j\mathbf{n}_{i,j}\mathbf{n}_k\mathbf{n}_{i,k} - (\operatorname{div}\mathbf{m})\,\mathbf{m}_i\,\mathbf{n}_j\mathbf{n}_{i,j} - (\operatorname{div}\boldsymbol{\ell})\,\boldsymbol{\ell}_i\,\mathbf{n}_j\mathbf{n}_{i,j} - \mathbf{n}_j\mathbf{n}_{i,j}\boldsymbol{\ell}_k\boldsymbol{\ell}_{i,k}, \end{aligned}$$

which, on account of (4.2), reads

$$b^n_m = -|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 - (\operatorname{div}\mathbf{m})\,a^m_n - (\operatorname{div}\boldsymbol{\ell})\,a^l_n - b^n_l.$$

In a similar way, we get

$$\begin{array}{l} b^m_l = -|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2 - (\operatorname{div}\boldsymbol{\ell})\,a^l_m - (\operatorname{div}\mathbf{n})\,a^n_m - b^m_n, \\ b^l_n = -|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2 - (\operatorname{div}\mathbf{n})\,a^n_l - (\operatorname{div}\mathbf{m})\,a^m_l - b^l_m\,. \end{array}$$

Therefore, denoting

$$X := b^n_m = b^m_n\,, \quad Y := b^m_l = b^l_m\,, \quad Z := b^l_n = b^n_l,$$

we obtain the system

$$\begin{cases} X + Z = \alpha \\ X + Y = \beta \\ Y + Z = \gamma \end{cases} \tag{4.10}$$

where

$$\begin{aligned} \alpha :=&\ -|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 - (\operatorname{div}\mathbf{m})\,a^m_n - (\operatorname{div}\boldsymbol{\ell})\,a^l_n \\ \beta :=&\ -|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2 - (\operatorname{div}\boldsymbol{\ell})\,a^l_m - (\operatorname{div}\mathbf{n})\,a^n_m \\ \gamma :=&\ -|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2 - (\operatorname{div}\mathbf{n})\,a^n_l - (\operatorname{div}\mathbf{m})\,a^m_l \end{aligned}$$

which has the solution

$$X=\frac{1}{2}(\alpha+\beta-\gamma)\,,\quad Y=\frac{1}{2}(\beta+\gamma-\alpha)\,,\quad Z=\frac{1}{2}(\gamma+\alpha-\beta)\,. \tag{4.11}$$

By replacing the expressions for α,β,γ, and using the third formula from (4.9), we obtain

$$\begin{aligned} b^n_m = \ & \tfrac{1}{2}\big[-|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2-|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2+|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2 \\ & +(\operatorname{div}\boldsymbol{\ell})^2+(\operatorname{div}\mathbf{n})(a^n_l-a^n_m)+(\operatorname{div}\mathbf{m})(a^m_l-a^m_n)\big] \end{aligned}$$

and hence, by the first two formulas in (4.9), we get

$$\begin{aligned} (\operatorname{div}\mathbf{n})\,a^n_m+(\operatorname{div}\mathbf{m})\,a^m_n+b^n_m = \ & \frac{1}{2}\big(-|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2-|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2 \\ & +|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2+(\operatorname{div}\boldsymbol{\ell})^2-(\operatorname{div}\mathbf{n})^2-(\operatorname{div}\mathbf{m})^2\big), \end{aligned}$$

that gives

$$I_{14}=\lambda_1\lambda_2\left(|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2+(\operatorname{div}\boldsymbol{\ell})^2-|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2-(\operatorname{div}\mathbf{n})^2-|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2-(\operatorname{div}\mathbf{m})^2\right).$$

In a similar way, we obtain

$$\begin{aligned} I_{15}=\lambda_2\lambda_3\,\big(&|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2+(\operatorname{div}\mathbf{n})^2-|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2 \\ &-(\operatorname{div}\mathbf{m})^2-|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2-(\operatorname{div}\boldsymbol{\ell})^2\big), \\ I_{16}=\lambda_3\lambda_1\,\big(&|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2+(\operatorname{div}\mathbf{m})^2-|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2 \\ &-(\operatorname{div}\boldsymbol{\ell})^2-|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2-(\operatorname{div}\mathbf{n})^2\big)\,. \end{aligned}$$

Adding the six terms I_{1h}, and using that $\lambda_1+\lambda_2+\lambda_3=0$, the formula for I_1 is readily proved. □

REMARK 4.4. The above invariants $a^n_m, a^m_n, a^m_l, a^l_m, a^l_n, a^n_l$ are related to the linear first order invariants D_{ij}, $i,j=1,2,3$, introduced in [32]. According to [32], where the oriented frame is $(\boldsymbol{\ell},\mathbf{m},\mathbf{n})$ instead of $(\mathbf{n},\mathbf{m},\boldsymbol{\ell})$, so that the role of $\boldsymbol{\ell}$ and $\mathbf{n}$ is interchanged, we obtain the following vector expressions for the invariants,

$$\begin{aligned} a^n_m &= D_{23}:=\mathbf{m}_\alpha\mathbf{n}_\beta\mathbf{m}_{\beta,\alpha}=-\boldsymbol{\ell}\cdot\operatorname{curl}\mathbf{m} \\ a^m_l &= D_{31}:=\boldsymbol{\ell}_\alpha\mathbf{m}_\beta\boldsymbol{\ell}_{\beta,\alpha}=-\mathbf{n}\cdot\operatorname{curl}\boldsymbol{\ell} \\ a^l_n &= D_{12}:=\mathbf{n}_\alpha\boldsymbol{\ell}_\beta\mathbf{n}_{\beta,\alpha}=-\mathbf{m}\cdot\operatorname{curl}\mathbf{n} \\ a^m_n &= -D_{13}:=-\mathbf{n}_\alpha\mathbf{n}_\beta\mathbf{m}_{\beta,\alpha}=\boldsymbol{\ell}\cdot\operatorname{curl}\mathbf{n} \\ a^l_m &= -D_{21}:=-\mathbf{m}_\alpha\mathbf{m}_\beta\boldsymbol{\ell}_{\beta,\alpha}=\mathbf{n}\cdot\operatorname{curl}\mathbf{m} \\ a^n_l &= -D_{32}:=-\boldsymbol{\ell}_\alpha\boldsymbol{\ell}_\beta\mathbf{n}_{\beta,\alpha}=\mathbf{m}\cdot\operatorname{curl}\boldsymbol{\ell}. \end{aligned} \tag{4.12}$$

In particular, the first of (4.9) reduces to the well-known identity $\operatorname{div}\mathbf{n}=\operatorname{div}(\mathbf{m}\times\boldsymbol{\ell})$ $=\boldsymbol{\ell}\cdot\operatorname{curl}\mathbf{m}-\mathbf{m}\cdot\operatorname{curl}\boldsymbol{\ell}$.

4.3. The term I_2. Similarly, we now deal with the second elastic invariant

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

PROPOSITION 4.5. *Under the previous hypotheses, we have*

$$\begin{aligned} I_2(\mathbf{Q},\nabla\mathbf{Q}) \ &= \Lambda_1\left(\operatorname{tr}[(\nabla\mathbf{n})^2]+|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\right) \\ &\quad +\Lambda_2\left(\operatorname{tr}[(\nabla\mathbf{m})^2]+|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\right) \\ &\quad +\Lambda_3\left(\operatorname{tr}[(\nabla\boldsymbol{\ell})^2]+|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\right). \end{aligned}$$

Proof. As before, we decompose $I_2 = I_{21} + I_{22} + I_{23} + I_{24} + I_{25} + I_{26}$. Using that $(\mathbf{n}, \mathbf{m}, \boldsymbol{\ell})$ is an orthonormal frame, so that $\mathbf{r}_\beta \mathbf{r}_{\beta,\alpha} = 0$, for $\mathbf{r} \in \{\mathbf{n}, \mathbf{m}, \boldsymbol{\ell}\}$, and recalling the formulas

$$\mathbf{r}_{k,j}\mathbf{r}_{j,k} = \mathrm{tr}[(\nabla \mathbf{r})^2]\,, \qquad \mathbf{r}_l \mathbf{r}_k \mathbf{r}_{i,l} \mathbf{r}_{i,k} = |\mathbf{r} \times \mathrm{curl}\,\mathbf{r}|^2,$$

we get

$$\begin{aligned}
I_{21} &= \lambda_1^2(\mathrm{tr}[(\nabla \mathbf{n})^2] + |\mathbf{n} \times \mathrm{curl}\,\mathbf{n}|^2) \\
I_{22} &= \lambda_2^2(\mathrm{tr}[(\nabla \mathbf{m})^2] + |\mathbf{m} \times \mathrm{curl}\,\mathbf{m}|^2) \\
I_{23} &= \lambda_3^2(\mathrm{tr}[(\nabla \boldsymbol{\ell})^2] + |\boldsymbol{\ell} \times \mathrm{curl}\,\boldsymbol{\ell}|^2) \\
I_{24} &= 2\lambda_1\lambda_2[\mathbf{n}_i\mathbf{m}_j\mathbf{n}_{k,j}\mathbf{m}_{i,k} + \mathbf{n}_k\mathbf{m}_i\mathbf{n}_{i,j}\mathbf{m}_{j,k} + \mathbf{n}_k\mathbf{m}_j\mathbf{n}_{i,j}\mathbf{m}_{i,k}] \\
I_{25} &= 2\lambda_2\lambda_3[\mathbf{m}_i\boldsymbol{\ell}_j\mathbf{m}_{k,j}\boldsymbol{\ell}_{i,k} + \mathbf{m}_k\boldsymbol{\ell}_i\mathbf{m}_{i,j}\boldsymbol{\ell}_{j,k} + \mathbf{m}_k\boldsymbol{\ell}_j\mathbf{m}_{i,j}\boldsymbol{\ell}_{i,k}] \\
I_{26} &= 2\lambda_3\lambda_1[\boldsymbol{\ell}_i\mathbf{n}_j\boldsymbol{\ell}_{k,j}\mathbf{n}_{i,k} + \boldsymbol{\ell}_k\mathbf{n}_i\boldsymbol{\ell}_{i,j}\mathbf{n}_{j,k} + \boldsymbol{\ell}_k\mathbf{n}_j\boldsymbol{\ell}_{i,j}\mathbf{n}_{i,k}]\,.
\end{aligned}$$

We now denote

$$\begin{aligned}
c_m^n &:= \mathbf{n}_i\mathbf{m}_j\mathbf{n}_{k,j}\mathbf{m}_{i,k} & c_n^m &:= \mathbf{n}_k\mathbf{m}_i\mathbf{n}_{i,j}\mathbf{m}_{j,k} \\
c_l^m &:= \mathbf{m}_i\boldsymbol{\ell}_j\mathbf{m}_{k,j}\boldsymbol{\ell}_{i,k} & c_m^l &:= \mathbf{m}_k\boldsymbol{\ell}_i\mathbf{m}_{i,j}\boldsymbol{\ell}_{j,k} \\
c_n^l &:= \boldsymbol{\ell}_i\mathbf{n}_j\boldsymbol{\ell}_{k,j}\mathbf{n}_{i,k} & c_l^n &:= \boldsymbol{\ell}_k\mathbf{n}_i\boldsymbol{\ell}_{i,j}\mathbf{n}_{j,k}
\end{aligned}$$

and also

$$\begin{aligned}
d_m^n &:= \mathbf{n}_k\mathbf{m}_j\mathbf{n}_{i,j}\mathbf{m}_{i,k} = \mathbf{m}_k\mathbf{n}_j\mathbf{m}_{i,j}\mathbf{n}_{i,k} =: d_n^m \\
d_l^m &:= \mathbf{m}_k\boldsymbol{\ell}_j\mathbf{m}_{i,j}\boldsymbol{\ell}_{i,k} = \boldsymbol{\ell}_k\mathbf{m}_j\boldsymbol{\ell}_{i,j}\mathbf{m}_{i,k} =: d_m^l \\
d_n^l &:= \boldsymbol{\ell}_k\mathbf{n}_j\boldsymbol{\ell}_{i,j}\mathbf{n}_{i,k} = \mathbf{n}_k\boldsymbol{\ell}_j\mathbf{n}_{i,j}\boldsymbol{\ell}_{i,k} =: d_l^n,
\end{aligned}$$

so that the above terms become

$$\begin{aligned}
I_{24} &= 2\lambda_1\lambda_2[c_m^n + c_n^m + d_m^n] \\
I_{25} &= 2\lambda_1\lambda_2[c_l^m + c_m^l + d_l^m] \\
I_{26} &= 2\lambda_1\lambda_2[c_n^l + c_l^n + d_n^l]\,.
\end{aligned}$$

Using (4.6) to replace the term $\mathbf{m}_j\mathbf{m}_{i,k}$, we compute, for example, $c_m^n = -\mathbf{n}_{k,j}\mathbf{n}_{j,k} - c_l^n$, and readily obtain

$$c_m^n + c_l^n = -\mathrm{tr}[(\nabla \mathbf{n})^2]\,, \quad c_l^m + c_n^m = -\mathrm{tr}[(\nabla \mathbf{m})^2]\,, \quad c_n^l + c_m^l = -\mathrm{tr}[(\nabla \boldsymbol{\ell})^2]\,. \tag{4.13}$$

With the same strategy, we compute

$$d_m^n = \mathbf{n}_k\mathbf{m}_j\mathbf{n}_{i,j}\mathbf{m}_{i,k} = -\mathbf{n}_k\mathbf{n}_j\mathbf{n}_{i,j}\mathbf{n}_{i,k} - \mathbf{n}_k\mathbf{n}_{i,j}\mathbf{m}_i\mathbf{m}_{j,k} - \mathbf{n}_k\boldsymbol{\ell}_i\mathbf{n}_{i,j}\boldsymbol{\ell}_{j,k} - \mathbf{n}_k\mathbf{n}_{i,j}\boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k}$$

that reads

$$d_m^n = -|\mathbf{n} \times \mathrm{curl}\,\mathbf{n}|^2 - c_n^m - c_n^l - d_l^n\,.$$

In a similar way, we compute

$$d_l^m = -|\mathbf{m} \times \mathrm{curl}\,\mathbf{m}|^2 - c_m^l - c_m^n - d_n^m\,, \qquad d_n^l = -|\boldsymbol{\ell} \times \mathrm{curl}\,\boldsymbol{\ell}|^2 - c_l^n - c_l^m - d_m^l\,.$$

Therefore, denoting

$$X := d_m^n = d_n^m\,, \quad Y := d_l^m = d_m^l\,, \quad Z := d_n^l = d_l^n,$$

we find again the system (4.10), where this time

$$\begin{aligned}
\alpha &:= -|\mathbf{n} \times \mathrm{curl}\,\mathbf{n}|^2 - c_n^m - c_n^l\,, \\
\beta &:= -|\mathbf{m} \times \mathrm{curl}\,\mathbf{m}|^2 - c_m^l - c_m^n\,, \\
\gamma &:= -|\boldsymbol{\ell} \times \mathrm{curl}\,\boldsymbol{\ell}|^2 - c_l^n - c_l^m\,.
\end{aligned}$$

By replacing the above expressions for α, β, γ in the solution (4.11) of the system, we obtain, for example,

$$d^n_m = \frac{1}{2}\big[\mathrm{tr}[(\nabla\boldsymbol{\ell})^2] + (c^n_l - c^n_m) + (c^m_l - c^m_n) - |\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2 - |\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2 + |\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2\big]$$

and hence, by the first two formulas in (4.13),

$$\begin{aligned}[c^n_m + c^m_n + d^n_m] = \frac{1}{2}\big((\mathrm{tr}[(\nabla\boldsymbol{\ell})^2] + |\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2) - (\mathrm{tr}[(\nabla\mathbf{n})^2] + |\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2)\\ -(\mathrm{tr}[(\nabla\mathbf{m})^2] + |\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2)\big),\end{aligned}$$

which gives

$$\begin{aligned}I_{24} = \lambda_1\lambda_2\,\big((\mathrm{tr}[(\nabla\boldsymbol{\ell})^2] + |\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2) - (\mathrm{tr}[(\nabla\mathbf{n})^2] + |\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2)\\ -(\mathrm{tr}[(\nabla\mathbf{m})^2] + |\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2)\big)\,.\end{aligned}$$

In a similar way, we get

$$\begin{aligned}I_{25} &= \lambda_2\lambda_3\,\big((\mathrm{tr}[(\nabla\mathbf{n})^2] + |\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2) - (\mathrm{tr}[(\nabla\mathbf{m})^2] + |\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2)\\ &\qquad -(\mathrm{tr}[(\nabla\boldsymbol{\ell})^2] + |\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2)\big),\\ I_{26} &= \lambda_3\lambda_1\,\big((\mathrm{tr}[(\nabla\mathbf{m})^2] + |\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2) - (\mathrm{tr}[(\nabla\boldsymbol{\ell})^2] + |\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2)\\ &\qquad -(\mathrm{tr}[(\nabla\mathbf{n})^2] + |\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2)\big)\,.\end{aligned}$$

Adding the six terms I_{2h} and using that $\lambda_1 + \lambda_2 + \lambda_3 = 0$, we obtain the required formula for I_2. □

Remark 4.6. In the uniaxial case, taking for example $\lambda_1 = \lambda_2$, by (1.2) we get $S_1 = S_2$ and hence the representation (1.3) holds with $s := -S_1$ and $\mathbf{r} = \boldsymbol{\ell}$, where $\boldsymbol{\ell}$ is the eigenvector corresponding to λ_3. In this case we have $\lambda_1 = \lambda_2 = -s/3$ and $\lambda_3 = 2s/3$. Moreover, the coefficients Λ_i defined in (4.8) satisfy $\Lambda_1 = 0$, $\Lambda_2 = 0$, and $\Lambda_3 = s^2$. By Propositions 4.3, 4.5, and 4.2 we thus recover the well-known formulas for the first three elastic invariants in the uniaxial case:

$$\begin{aligned}&I_1 = s^2\big((\mathrm{div}\,\mathbf{r})^2 + |\mathbf{r}\times\mathrm{curl}\,\mathbf{r}|^2\big)\,, \quad I_2 = s^2\big(\mathrm{tr}[(\nabla\mathbf{r})^2] + |\mathbf{r}\times\mathrm{curl}\,\mathbf{r}|^2\big)\,,\\ &I_3 = 2s^2\big(\mathrm{tr}[(\nabla\mathbf{r})^2] + (\mathbf{r}\cdot\mathrm{curl}\,\mathbf{r})^2 + |\mathbf{r}\times\mathrm{curl}\,\mathbf{r}|^2\big)\,.\end{aligned}$$

In the biaxial case, recalling the formulas (1.2) we deduce that the coefficients Λ_i in (4.8) satisfy

$$\Lambda_1 = S_1(S_1 - S_2)\,, \quad \Lambda_2 = S_2(S_2 - S_1)\,, \quad \Lambda_3 = S_1S_2\,. \tag{4.14}$$

Therefore, the formulas from Propositions 4.3, 4.5, and 4.2 read, equivalently,

$$\begin{aligned}I_1(\mathbf{Q},\nabla\mathbf{Q}) &= S_1(S_1 - S_2)\big((\mathrm{div}\,\mathbf{n})^2 + |\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2\big)\\ &\quad + S_2(S_2 - S_1)\big((\mathrm{div}\,\mathbf{m})^2 + |\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2\big)\\ &\quad + S_1S_2\big((\mathrm{div}\,\boldsymbol{\ell})^2 + |\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2\big),\\ I_2(\mathbf{Q},\nabla\mathbf{Q}) &= S_1(S_1 - S_2)\big(\mathrm{tr}[(\nabla\mathbf{n})^2] + |\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2\big)\\ &\quad + S_2(S_2 - S_1)\big(\mathrm{tr}[(\nabla\mathbf{m})^2] + |\mathbf{m}\times\mathrm{curl}\,\mathbf{m}|^2\big)\\ &\quad + S_1S_2\big(\mathrm{tr}[(\nabla\boldsymbol{\ell})^2] + |\boldsymbol{\ell}\times\mathrm{curl}\,\boldsymbol{\ell}|^2\big),\\ I_3(\mathbf{Q},\nabla\mathbf{Q}) &= 2S_1(S_1 - S_2)|\nabla\mathbf{n}|^2 + 2S_2(S_2 - S_1)|\nabla\mathbf{m}|^2 + 2S_1S_2|\nabla\boldsymbol{\ell}|^2\,.\end{aligned}$$

5. Cartesian representation for the fourth invariant. In this section we focus on the fourth elastic invariant

$$I_4 = \mathbf{Q}_{lk}\mathbf{Q}_{ij,l}\mathbf{Q}_{ij,k}\,.$$

According to [16, 32, 33], the following twelve independent quadratic first order invariants,

$$\mathbf{N} := |\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\,,\quad \mathbf{M} := |\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\,,\quad \mathbf{L} := |\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2,$$

$$\begin{array}{ccc} (\operatorname{div}\mathbf{n})^2\,, & (\operatorname{div}\mathbf{m})^2\,, & (\operatorname{div}\boldsymbol{\ell})^2\,,\\ (\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2\,, & (\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2\,, & (\boldsymbol{\ell}\cdot\operatorname{curl}\boldsymbol{\ell})^2\,,\\ (\mathbf{m}\cdot\operatorname{curl}\mathbf{n})^2\,, & (\boldsymbol{\ell}\cdot\operatorname{curl}\mathbf{m})^2\,, & (\mathbf{n}\cdot\operatorname{curl}\boldsymbol{\ell})^2\,, \end{array}\tag{5.1}$$

are needed to describe, up to a divergence term, the expansion to second order of the elastic free energy density of a constrained biaxial nematic system.

For simplicity, let us denote $\Lambda^{\mathbf{r}}_{\mathbf{s}} := (\mathbf{s}\cdot\operatorname{curl}\mathbf{r})^2$. From Equations (4.12), we get

$$\begin{array}{ll} \Lambda^{\mathbf{n}}_{\mathbf{m}} = \mathbf{n}_\alpha\mathbf{n}_\gamma\boldsymbol{\ell}_\beta\boldsymbol{\ell}_\delta\mathbf{n}_{\beta,\alpha}\mathbf{n}_{\delta,\gamma} & \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} = \mathbf{n}_\alpha\mathbf{n}_\beta\mathbf{n}_\gamma\mathbf{n}_\delta\mathbf{m}_{\beta,\alpha}\mathbf{m}_{\delta,\gamma}\\ \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} = \mathbf{m}_\alpha\mathbf{m}_\gamma\mathbf{n}_\beta\mathbf{n}_\delta\mathbf{m}_{\beta,\alpha}\mathbf{m}_{\delta,\gamma} & \Lambda^{\mathbf{m}}_{\mathbf{n}} = \mathbf{m}_\alpha\mathbf{m}_\beta\mathbf{m}_\gamma\mathbf{m}_\delta\boldsymbol{\ell}_{\beta,\alpha}\boldsymbol{\ell}_{\delta,\gamma}\\ \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} = \boldsymbol{\ell}_\alpha\boldsymbol{\ell}_\gamma\mathbf{m}_\beta\mathbf{m}_\delta\boldsymbol{\ell}_{\beta,\alpha}\boldsymbol{\ell}_{\delta,\gamma} & \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} = \boldsymbol{\ell}_\alpha\boldsymbol{\ell}_\beta\boldsymbol{\ell}_\gamma\boldsymbol{\ell}_\delta\mathbf{n}_{\beta,\alpha}\mathbf{n}_{\delta,\gamma}\,. \end{array}\tag{5.2}$$

From the above formulas, one recovers, in particular, the following relations (see, for instance, [32]):

$$\mathbf{N} = \Lambda^{\mathbf{n}}_{\mathbf{m}} + \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}}\,,\quad \mathbf{M} = \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} + \Lambda^{\mathbf{m}}_{\mathbf{n}}\,,\quad \mathbf{L} = \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} + \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}}\,.\tag{5.3}$$

We have the following.

THEOREM 5.1. *According to the previous notation, we have:*

$$\begin{aligned} I_4 \;&= 3^{-1}\,S_1(2S_1-S_2)(S_2-S_1)\,|\nabla\mathbf{n}|^2 + 2S_1(S_2-S_1)^2\,\mathbf{N}\\ &+3^{-1}\,S_2(2S_2-S_1)(S_1-S_2)\,|\nabla\mathbf{m}|^2 + 2S_2^2(S_2-S_1)\,\mathbf{M}\\ &+3^{-1}\,S_1S_2(S_1+S_2)\,|\nabla\boldsymbol{\ell}|^2 - 2S_1^2S_2\,\mathbf{L}\\ &+2S_1S_2(S_1-S_2)\,[\Lambda^{\mathbf{n}}_{\mathbf{m}}+\Lambda^{\mathbf{m}}_{\boldsymbol{\ell}}+\Lambda^{\boldsymbol{\ell}}_{\mathbf{n}}]\,. \end{aligned}$$

REMARK 5.2. In the uniaxial case, taking for instance $\lambda_1=\lambda_2$ as in Remark 4.6, we get

$$I_4 = 2s^3\Big(|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2 - \frac{1}{3}|\nabla\boldsymbol{\ell}|^2\Big),\tag{5.4}$$

and hence, by using the third equation in (4.1), we recover the known formula for the uniaxial case:

$$I_4 = 2s^3\Big(\frac{2}{3}|\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2 - \frac{1}{3}\operatorname{tr}[(\nabla\mathbf{r})^2] - \frac{1}{3}(\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2\Big)\,.$$

In the biaxial case, by applying the third identity in (4.1) to $\mathbf{r}\in\{\mathbf{n},\mathbf{m},\boldsymbol{\ell}\}$, I_4 takes the equivalent form

$$\begin{aligned} I_4 = 3^{-1}&\,S_1(2S_1-S_2)(S_2-S_1)\,\big(\operatorname{tr}[(\nabla\mathbf{n})^2]+(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2\big)\\ &+3^{-1}\,S_1(S_1-S_2)(4S_1-5S_2)\,|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\\ &+3^{-1}\,S_2(2S_2-S_1)(S_1-S_2)\,\big(\operatorname{tr}[(\nabla\mathbf{m})^2]+(\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2\big)\\ &+3^{-1}\,S_2(S_2-S_1)(S_1+4S_2)\,|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\\ &+3^{-1}\,S_1S_2(S_1+S_2)\,\big(\operatorname{tr}[(\nabla\boldsymbol{\ell})^2]+(\boldsymbol{\ell}\cdot\operatorname{curl}\boldsymbol{\ell})^2\big)\\ &+3^{-1}\,S_1S_2(S_2-5S_1)\,|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\\ &+2S_1S_2(S_1-S_2)\,[\Lambda^{\mathbf{n}}_{\mathbf{m}}+\Lambda^{\mathbf{m}}_{\boldsymbol{\ell}}+\Lambda^{\boldsymbol{\ell}}_{\mathbf{n}}]\,. \end{aligned}\tag{5.5}$$

Proof of Theorem 5.1. Using that

$$\begin{aligned}\mathbf{Q}_{lk} &= \lambda_1 \mathbf{n}_l \mathbf{n}_k + \lambda_2 \mathbf{m}_l \mathbf{m}_k + \lambda_3 \boldsymbol{\ell}_l \boldsymbol{\ell}_k \,, \\ \mathbf{Q}_{ij,l} &= \lambda_1(\mathbf{n}_i \mathbf{n}_{j,l} + \mathbf{n}_{i,l} \mathbf{n}_j) + \lambda_2(\mathbf{m}_i \mathbf{m}_{j,l} + \mathbf{m}_{i,l} \mathbf{m}_j) + \lambda_3(\boldsymbol{\ell}_i \boldsymbol{\ell}_{j,l} + \boldsymbol{\ell}_{i,l} \boldsymbol{\ell}_j) \,, \\ \mathbf{Q}_{ij,k} &= \lambda_1(\mathbf{n}_i \mathbf{n}_{j,k} + \mathbf{n}_{i,k} \mathbf{n}_j) + \lambda_2(\mathbf{m}_i \mathbf{m}_{j,k} + \mathbf{m}_{i,k} \mathbf{m}_j) + \lambda_3(\boldsymbol{\ell}_i \boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_{i,k} \boldsymbol{\ell}_j) \,,\end{aligned}$$

we first write as before the formula

$$\begin{aligned}I_4 = {}& \alpha_1 \lambda_1^3 + \alpha_2 \lambda_2^3 + \alpha_3 \lambda_3^3 + \alpha_{123} \lambda_1 \lambda_2 \lambda_3 + \alpha_{12} \lambda_1^2 \lambda_2 \\ & + \alpha_{23} \lambda_2^2 \lambda_3 + \alpha_{31} \lambda_3^2 \lambda_1 + \alpha_{21} \lambda_2^2 \lambda_1 + \alpha_{32} \lambda_3^2 \lambda_2 + \alpha_{13} \lambda_1^2 \lambda_3 \,.\end{aligned} \tag{5.6}$$

The first coefficients are

$$\alpha_1 = 2\mathbf{N} \,, \qquad \alpha_2 = 2\mathbf{M} \,, \qquad \alpha_3 = 2\mathbf{L} \,. \tag{5.7}$$

In fact, we have, for example,

$$\alpha_1 = \mathbf{n}_l \mathbf{n}_k \, (\mathbf{n}_i \mathbf{n}_{j,l} + \mathbf{n}_{i,l} \mathbf{n}_j)(\mathbf{n}_i \mathbf{n}_{j,k} + \mathbf{n}_{i,k} \mathbf{n}_j) = 2 \mathbf{n}_l \mathbf{n}_k \mathbf{n}_{j,l} \mathbf{n}_{j,k} = 2\mathbf{N},$$

where the last identity follows from (4.2), with $\mathbf{r} = \mathbf{n}$. Next, we write the fourth term as

$$\alpha_{123} = 4(B_n + B_m + B_l), \tag{5.8}$$

where we have set

$$\begin{aligned} B_n &:= \mathbf{n}_l \mathbf{n}_k \mathbf{m}_i \mathbf{m}_{j,l} \boldsymbol{\ell}_j \boldsymbol{\ell}_{i,k} \,, \\ B_m &:= \mathbf{m}_l \mathbf{m}_k \boldsymbol{\ell}_i \boldsymbol{\ell}_{j,l} \mathbf{n}_j \mathbf{n}_{i,k} \,, \\ B_l &:= \boldsymbol{\ell}_l \boldsymbol{\ell}_k \mathbf{n}_i \mathbf{n}_{j,l} \mathbf{m}_j \mathbf{m}_{i,k} \,. \end{aligned} \tag{5.9}$$

The other terms can be written as follows:

LEMMA 5.3. *According to the notation (5.2), we have*

$$\begin{array}{ll} \alpha_{12} = 2\Omega^n_m - 4\Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} & \alpha_{21} = 2\Omega^m_n - 4\Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} \\ \alpha_{23} = 2\Omega^m_l - 4\Lambda^{\mathbf{m}}_{\mathbf{n}} & \alpha_{32} = 2\Omega^l_m - 4\Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} \\ \alpha_{31} = 2\Omega^l_n - 4\Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} & \alpha_{13} = 2\Omega^n_l - 4\Lambda^{\mathbf{n}}_{\mathbf{m}} \end{array}$$

where the coefficients Ω^r_s *are*

$$\begin{array}{ll} \Omega^n_m := \mathbf{m}_l \mathbf{m}_k \mathbf{n}_{j,l} \mathbf{n}_{j,k} & \Omega^m_n := \mathbf{n}_l \mathbf{n}_k \mathbf{m}_{j,l} \mathbf{m}_{j,k} \\ \Omega^m_l := \boldsymbol{\ell}_l \boldsymbol{\ell}_k \mathbf{m}_{j,l} \mathbf{m}_{j,k} & \Omega^l_m := \mathbf{m}_l \mathbf{m}_k \boldsymbol{\ell}_{j,l} \boldsymbol{\ell}_{j,k} \\ \Omega^l_n := \mathbf{n}_l \mathbf{n}_k \boldsymbol{\ell}_{j,l} \boldsymbol{\ell}_{j,k} & \Omega^n_l := \boldsymbol{\ell}_l \boldsymbol{\ell}_k \mathbf{n}_{j,l} \mathbf{n}_{j,k} \,. \end{array} \tag{5.10}$$

Moreover, on account of (5.9), we have

$$\begin{array}{ll} \Omega^n_m = \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} - B_m & \Omega^m_n = \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} - B_n \\ \Omega^m_l = \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} - B_l & \Omega^l_m = \Lambda^{\mathbf{m}}_{\mathbf{n}} - B_m \\ \Omega^l_n = \Lambda^{\mathbf{n}}_{\mathbf{m}} - B_n & \Omega^n_l = \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} - B_l \,. \end{array}$$

Proof. We first write

$$\begin{array}{ll} \alpha_{12} = 4A^n_m + 2\Omega^n_m & \alpha_{21} = 4A^m_n + 2\Omega^m_n \\ \alpha_{23} = 4A^m_l + 2\Omega^m_l & \alpha_{32} = 4A^l_m + 2\Omega^l_m \\ \alpha_{31} = 4A^l_n + 2\Omega^l_n & \alpha_{13} = 4A^n_l + 2\Omega^n_l \end{array}$$

where we have set

$$\begin{array}{ll} A^n_m := \mathbf{n}_l\mathbf{n}_k\mathbf{n}_i\mathbf{n}_{j,l}\mathbf{m}_j\mathbf{m}_{i,k}\,, & A^m_n := \mathbf{m}_l\mathbf{m}_k\mathbf{m}_i\mathbf{m}_{j,l}\mathbf{n}_j\mathbf{n}_{i,k} \\ A^m_l := \mathbf{m}_l\mathbf{m}_k\mathbf{m}_i\mathbf{m}_{j,l}\boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k} & A^l_m := \boldsymbol{\ell}_l\boldsymbol{\ell}_k\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,l}\mathbf{m}_j\mathbf{m}_{i,k} \\ A^l_n := \boldsymbol{\ell}_l\boldsymbol{\ell}_k\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,l}\mathbf{n}_j\mathbf{n}_{i,k} & A^n_l := \mathbf{n}_l\mathbf{n}_k\mathbf{n}_i\mathbf{n}_{j,l}\boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k}\,. \end{array}$$

Using that $\mathbf{m}_j\mathbf{n}_{j,l} = -\mathbf{m}_{j,l}\mathbf{n}_j$, we have

$$A^n_m = -\mathbf{n}_l\mathbf{n}_k\mathbf{n}_i\mathbf{n}_j\mathbf{m}_{j,l}\mathbf{m}_{i,k} = -\Lambda^{\mathbf{n}}_{\boldsymbol{\ell}}$$

on account of (5.2). By cyclic permutations of the letters n, m, and l, we also obtain

$$A^m_l = -\Lambda^{\mathbf{m}}_{\mathbf{n}}\,, \quad A^l_n = -\Lambda^{\boldsymbol{\ell}}_{\mathbf{m}}\,.$$

Using that $\mathbf{m}_i\mathbf{n}_{i,k} = -\mathbf{n}_i\mathbf{m}_{i,k}$, on account of (5.2) we also have

$$A^m_n = -\mathbf{m}_l\mathbf{m}_k\mathbf{n}_i\mathbf{n}_j\mathbf{m}_{j,l}\mathbf{m}_{i,k} = -\Lambda^{\mathbf{m}}_{\boldsymbol{\ell}}$$

and again by cyclic permutations

$$A^l_m = -\Lambda^{\boldsymbol{\ell}}_{\mathbf{n}}\,, \quad A^n_l = -\Lambda^{\mathbf{n}}_{\mathbf{m}}\,.$$

Moreover, multiplying by $\mathbf{n}_i\mathbf{n}_i = 1$ and by (4.6), we have

$$\Omega^n_m = \mathbf{m}_l\mathbf{m}_k\mathbf{n}_{j,l}\mathbf{n}_i(\mathbf{n}_i\mathbf{n}_{j,k}) = -\mathbf{m}_l\mathbf{m}_k\mathbf{m}_j\mathbf{m}_{i,k}\mathbf{n}_i\mathbf{n}_{j,l} - \mathbf{m}_l\mathbf{m}_k\mathbf{n}_i\mathbf{n}_{j,l}\boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k} = -A^m_n - B_m$$

on account of (5.9), and correspondingly

$$\Omega^m_l = -A^l_m - B_l\,, \quad \Omega^l_n = -A^n_l - B_n\,.$$

Similarly, multiplying by $\mathbf{m}_i\mathbf{m}_i = 1$ and by (4.6), we have

$$\Omega^m_n = \mathbf{n}_l\mathbf{n}_k\mathbf{m}_{j,l}\mathbf{m}_i(\mathbf{m}_i\mathbf{m}_{j,k}) = -\mathbf{n}_l\mathbf{n}_k\mathbf{n}_j\mathbf{n}_{i,k}\mathbf{m}_i\mathbf{m}_{j,l} - \mathbf{n}_l\mathbf{n}_k\mathbf{m}_i\mathbf{m}_{j,l}\boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k} = -A^n_m - B_n,$$

and hence also

$$\Omega^l_m = -A^m_l - B_m\,, \quad \Omega^n_l = -A^l_n - B_l\,.$$

The above relations readily follow. □

Next, we claim that

$$\Omega^n_m + \Omega^n_l = N - \mathbf{N}\,, \quad \Omega^m_l + \Omega^m_n = M - \mathbf{M}\,, \quad \Omega^l_n + \Omega^l_m = L - \mathbf{L}, \tag{5.11}$$

where

$$N := |\nabla\mathbf{n}|^2\,, \quad M := |\nabla\mathbf{m}|^2\,, \quad L := |\nabla\boldsymbol{\ell}|^2\,.$$

In fact, by using (4.4) and (5.10), we have, on account of (4.2),

$$\begin{array}{rcl} \Omega^n_m & = & (\delta_{lk} - \mathbf{n}_l\mathbf{n}_k - \boldsymbol{\ell}_l\boldsymbol{\ell}_k)\mathbf{n}_{j,l}\mathbf{n}_{j,k} \\ & = & \mathbf{n}_{j,k}\mathbf{n}_{j,k} - \mathbf{n}_l\mathbf{n}_k\mathbf{n}_{j,l}\mathbf{n}_{j,k} - \boldsymbol{\ell}_l\boldsymbol{\ell}_k\mathbf{n}_{j,l}\mathbf{n}_{j,k} \\ & = & N - \mathbf{N} - \Omega^n_l, \end{array}$$

where δ_{lk} denotes the Kronecker tensor. The other equations are proved similarly.

We are now able to compute the terms B_n, B_m, and B_l in (5.9).

Lemma 5.4. *We have*

$$B_n = 2^{-1}(N-M-L) + \mathbf{M} + \mathbf{L} - \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} - \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}},$$
$$B_m = 2^{-1}(M-L-N) + \mathbf{L} + \mathbf{N} - \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} - \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}},$$
$$B_l = 2^{-1}(L-N-M) + \mathbf{N} + \mathbf{M} - \Lambda^{\mathbf{n}}_{\mathbf{m}} - \Lambda^{\mathbf{m}}_{\mathbf{n}}\,.$$

Proof. By the previous lemma, we know that

$$\begin{array}{c} \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} - \Omega^m_n = B_n = \Lambda^{\mathbf{n}}_{\mathbf{m}} - \Omega^l_n \\ \Lambda^{\mathbf{m}}_{\mathbf{n}} - \Omega^l_m = B_m = \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} - \Omega^n_m \\ \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} - \Omega^n_l = B_l = \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} - \Omega^m_l\,. \end{array} \tag{5.12}$$

By summation, we thus have

$$2(B_n + B_m + B_l) = \Lambda - \Omega,$$

where we have set

$$\Lambda := \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} + \Lambda^{\mathbf{n}}_{\mathbf{m}} + \Lambda^{\mathbf{m}}_{\mathbf{n}} + \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} + \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} + \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}}$$

and

$$\Omega := \Omega^n_m + \Omega^n_l + \Omega^m_l + \Omega^m_n + \Omega^l_n + \Omega^l_m\,.$$

By (5.3), we know that

$$\Lambda = \mathbf{N} + \mathbf{M} + \mathbf{L},$$

whereas by (5.11)

$$\Omega = N + M + L - (\mathbf{N} + \mathbf{M} + \mathbf{L}),$$

which implies

$$B_n + B_m + B_l = (\mathbf{N} + \mathbf{M} + \mathbf{L}) - \frac{1}{2}\,(N + M + L)\,. \tag{5.13}$$

From (5.12), we also have

$$\begin{array}{c} B_m + B_l = \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} - \Omega^n_m + \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} - \Omega^n_l \\ B_l + B_n = \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} - \Omega^m_l + \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} - \Omega^m_n \\ B_n + B_m = \Lambda^{\mathbf{n}}_{\mathbf{m}} - \Omega^l_n + \Lambda^{\mathbf{m}}_{\mathbf{n}} - \Omega^l_m \end{array}$$

and hence, by (5.11),

$$\begin{array}{c} B_m + B_l = \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} + \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} - N + \mathbf{N} \\ B_l + B_n = \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} + \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} - M + \mathbf{M} \\ B_n + B_m = \Lambda^{\mathbf{n}}_{\mathbf{m}} + \Lambda^{\mathbf{m}}_{\mathbf{n}} - L + \mathbf{L}\,. \end{array}$$

The claimed formulas follow by subtracting each of the above lines from (5.13). □

Now, by (5.8) and (5.13), we obtain

$$a_{123} = 4(\mathbf{N} + \mathbf{M} + \mathbf{L}) - 2(N + M + L)\,. \tag{5.14}$$

Moreover, by Lemmas 5.3 and 5.4, on account of the relations (5.3) we find

$$\begin{cases} a_{12} = (N - M + L) + 2(\boldsymbol{\Lambda} - 2\mathbf{N} - \mathbf{L}) \\ a_{23} = (M - L + N) + 2(\boldsymbol{\Lambda} - 2\mathbf{M} - \mathbf{N}) \\ a_{31} = (L - N + M) + 2(\boldsymbol{\Lambda} - 2\mathbf{L} - \mathbf{M}) \\ a_{21} = (M + L - N) + 2(\mathbf{N} - \mathbf{M} - \boldsymbol{\Lambda}) \\ a_{32} = (L + N - M) + 2(\mathbf{M} - \mathbf{L} - \boldsymbol{\Lambda}) \\ a_{13} = (N + M - L) + 2(\mathbf{L} - \mathbf{N} - \boldsymbol{\Lambda}) \end{cases} \tag{5.15}$$

where, for simplicity, we have denoted

$$\mathbf{\Lambda} := \Lambda^{\mathbf{n}}_{\mathbf{m}} + \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} + \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}}\,.$$

In fact, as for the first expression, we have

$$\alpha_{12} = (N - M + L) + 2(\Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} + \Lambda^{\boldsymbol{\ell}}_{\mathbf{n}} - \Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} - \mathbf{N} - \mathbf{L})$$

and by (5.3) we replace $-\Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} = -\mathbf{N} + \Lambda^{\mathbf{n}}_{\mathbf{m}}$. As for the fourth expression, we have instead

$$\alpha_{21} = (M + L - N) + 2(\Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} + \Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} - \Lambda^{\mathbf{m}}_{\boldsymbol{\ell}} - \mathbf{M} - \mathbf{L})$$

and this time we replace $\Lambda^{\mathbf{n}}_{\boldsymbol{\ell}} = \mathbf{N} - \Lambda^{\mathbf{n}}_{\mathbf{m}}$ and $\Lambda^{\boldsymbol{\ell}}_{\mathbf{m}} = \mathbf{L} - \Lambda^{\boldsymbol{\ell}}_{n}$. The other identities in (5.15) follow by similar computations.

By (5.6), (5.7), (5.14), and (5.15), the elastic functional I_4 on $\mathbf{Q}$ takes the form

$$\begin{aligned} I_4 \;&= \lambda_1^3\, 2\mathbf{N} + \lambda_2^3\, 2\mathbf{M} + \lambda_3^3\, 2\mathbf{L} \\ &+\lambda_1\lambda_2\lambda_3\,[4(\mathbf{N}+\mathbf{M}+\mathbf{L}) - 2(N+M+L)] \\ &+\lambda_1^2\lambda_2\,[(N-M+L) + 2(\mathbf{\Lambda} - 2\mathbf{N} - \mathbf{L})] \\ &+\lambda_2^2\lambda_3\,[(M-L+N) + 2(\mathbf{\Lambda} - 2\mathbf{M} - \mathbf{N})] \\ &+\lambda_3^2\lambda_1\,[(L-N+M) + 2(\mathbf{\Lambda} - 2\mathbf{L} - \mathbf{M})] \\ &+\lambda_2^2\lambda_1\,[(M+L-N) + 2(\mathbf{N} - \mathbf{M} - \mathbf{\Lambda})] \\ &+\lambda_3^2\lambda_2\,[(L+N-M) + 2(\mathbf{M} - \mathbf{L} - \mathbf{\Lambda})] \\ &+\lambda_1^2\lambda_3\,[(N+M-L) + 2(\mathbf{L} - \mathbf{N} - \mathbf{\Lambda})]\,. \end{aligned}$$

Writing the above formula as

$$I_4 = c_{\mathbf{N}}\,\mathbf{N} + c_{\mathbf{M}}\,\mathbf{M} + c_{\mathbf{L}}\,\mathbf{L} + c_N\,N + c_M\,M + c_L\,L + c_{\mathbf{\Lambda}}\,\mathbf{\Lambda},$$

we now compute the coefficients of the terms $\mathbf{\Lambda}, \mathbf{N}, \mathbf{M}, \mathbf{L}, N, M, L$. We have

$$c_{\mathbf{\Lambda}} = 2(\lambda_1 - \lambda_2)(2\lambda_1^2 + 2\lambda_2^2 + 5\lambda_1\lambda_2)$$

which, by the relations (1.2), and using that $\lambda_1 + \lambda_2 + \lambda_3 = 0$, can be expressed in terms of S_1, S_2 as

$$c_{\mathbf{\Lambda}} = 2S_1S_2(S_1 - S_2)\,.$$

Moreover, we similarly have

$$\begin{aligned} c_{\mathbf{N}} &= 2\,(2\lambda_1^3 + \lambda_2^3 - 3\lambda_1^2\lambda_2) = 2S_1(S_2 - S_1)^2 \\ c_{\mathbf{M}} &= 2\,(2\lambda_2^3 + \lambda_3^3 - 3\lambda_2^2\lambda_3) = 2S_2^2(S_2 - S_1) \\ c_{\mathbf{L}} &= 2\,(2\lambda_3^3 + \lambda_1^3 - 3\lambda_3^2\lambda_1) = -2S_1^2S_2\,. \end{aligned}$$

Finally, we get:

$$\begin{aligned} c_N &= \lambda_1(-2\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2) = 3^{-1}\,S_1(2S_1 - S_2)(S_2 - S_1) \\ c_M &= \lambda_2(-2\lambda_2^2 + \lambda_3^2 + \lambda_2\lambda_3) = 3^{-1}\,S_2(2S_2 - S_1)(S_1 - S_2) \\ c_L &= \lambda_3(-2\lambda_3^2 + \lambda_1^2 + \lambda_3\lambda_1) = 3^{-1}\,(S_1 + S_2)S_1S_2, \end{aligned}$$

which completes the proof of Theorem 5.1. □

6. Coercivity conditions. Let $\psi_E(\mathbf{Q},\nabla\mathbf{Q}) = L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4$ be the elastic free-energy density of a biaxial nematic liquid crystal considered in (1.6), where the L_i are material constants and the I_i are the elastic invariants (1.7).

Davis and Gartland [8] proved that, if $L_4 = 0$ and

$$L_3 > 0\,, \quad -L_3 < L_2 < 2L_3\,, \quad L_1 > -\frac{3}{5}L_3 - \frac{1}{10}L_2\,, \tag{6.1}$$

compare [21], the energy functional $\mathcal{F}_E[\mathbf{Q}] := \int_\Omega \psi_E(\mathbf{Q},\nabla\mathbf{Q})\,dx$, defined on general $\mathbf{Q}$-tensors, is sequentially weakly lower semicontinuous in $W^{1,2}$, provided that the domain Ω has smooth boundary. In fact, if (6.1) holds, there exist two positive constants $K > \mu > 0$, such that

$$K\,|\nabla\mathbf{Q}|^2 \geq L_1 I_1 + L_2 I_2 + L_3 I_3 \geq \mu\,|\nabla\mathbf{Q}|^2\,.$$

In the constrained case, one expects that coercivity holds true for suitable ranges of the L_i, even in the case $L_4 \neq 0$. This is indeed what happens in the uniaxial case. It is well known, in fact, that the general form of the Oseen–Frank energy cannot be recovered when $L_4 = 0$. Let us first recall the computation for the coercivity property in the constrained uniaxial case [3, 11, 21, 15, 34].

6.1. The uniaxial case. According to Remarks 4.6 and 5.2, if $\lambda_1 = \lambda_2$ the density $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ reduces to the Oseen–Frank energy density $w(\mathbf{r},\nabla\mathbf{r})$ of *nematic liquid crystals*:

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

provided that one chooses

$$\begin{aligned} &K_1 := L_1 s^2 + L_2 s^2 + 2L_3 s^2 - \frac{2}{3}L_4 s^3\,, \quad K_2 := 2L_3 s^2 - \frac{2}{3}L_4 s^3\,, \\ &K_3 := L_1 s^2 + L_2 s^2 + 2L_3 s^2 + \frac{4}{3}L_4 s^3\,, \quad K_4 := L_2 s^2\,. \end{aligned}$$

We now recall that necessary and sufficient conditions for

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

are the Ericksen inequalities

$$2K_1 > K_2 + K_4\,, \quad K_3 > 0\,, \quad K_2 > |K_4|\,. \tag{6.2}$$

To prove this, using the frame invariance (3.4) and arguing as in Lemma 3.6, it suffices to consider the case when $\mathbf{r} = \mathbf{r}_0 := (0,0,1)^T$. Since $(\nabla\mathbf{r})^T\mathbf{r} = 0$, it follows that the gradient matrix $\nabla\mathbf{r}$ has the third row equal to zero, and hence we can write

$$w(\mathbf{r}_0,\nabla\mathbf{r}) = f(\mathbf{r}_0,\nabla\mathbf{r}),$$

where, for every $G = (G^i_j) \in \mathbb{M}_{3\times 3}$ such that $G^T\mathbf{r}_0 = 0$, we have set

$$\begin{aligned} f(\mathbf{r}_0, G) \;&:= K_1\left(G^1_1 + G^2_2\right)^2 + K_2\left(G^1_2 - G^2_1\right)^2 + K_3\left[(G^1_3)^2 + (G^2_3)^2\right] \\ &\quad + 2(K_2+K_4)\left[G^1_2 G^2_1 - G^1_1 G^2_2\right]\,. \end{aligned}$$

Writing

$$
\begin{aligned}
f(\mathbf{r}_0, G) \quad &= K_1\left[(G_1^1)^2+(G_2^2)^2\right]+2(K_1-K_2-K_4)G_1^1G_2^2 \\
&+K_2\left[(G_2^1)^2+(G_1^2)^2\right]+2K_4G_2^1G_1^2+K_3\left[(G_3^1)^2+(G_3^2)^2\right],
\end{aligned}
$$

it follows that the quadratic form $f(\mathbf{r}_0, G)$ is positive definite if and only if

$$
K_1>0\,,\quad |K_1-K_2-K_4|<K_1\,,\quad K_2>0\,,\quad |K_4|<K_2\,,\quad K_3>0\,.
$$

The above system is equivalent to the Ericksen conditions (6.2), which can be rewritten in terms of the coefficients L_i as

$$
2L_1+L_2+2L_3>\frac{2}{3}L_4s\,,\quad L_1+L_2+2L_3+\frac{4}{3}L_4s>0\,,\quad 2L_3-\frac{2}{3}L_4s>|L_2|\,. \tag{6.3}
$$

Now, assume that in addition a Dirichlet type condition similar to the one described in the introduction holds. By (4.1) and (4.3), for any $\nu>0$, we can write

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

where the last term is a null Lagrangian. This yields the coercivity property

$$
\int_\Omega w(\mathbf{r},\nabla\mathbf{r})\,dx \ge \nu\int_\Omega|\nabla\mathbf{r}|^2\,dx+c, \qquad \text{for some } \nu>0 \text{ and } c\in\mathbb{R},
$$

provided that $K_1>0$, $K_2>0$, and $K_3>0$, which in terms of the coefficients L_i takes the form

$$
L_1+L_2+2L_3>\frac{2}{3}L_4s\,,\quad L_1+L_2+2L_3+\frac{4}{3}L_4s>0\,,\quad 2L_3-\frac{2}{3}L_4s>0\,. \tag{6.4}
$$

Notice that the coercivity conditions $K_1,\,K_2,\,K_3>0$ are weaker than the Ericksen conditions (6.2), whence the system (6.4) is weaker than the system (6.3). Depending on the sign of L_4s, the above formulas may be further simplified.

6.2. Coercivity of I_3. We now briefly recall how in [29] we proved coercivity for the integral

$$
\mathcal{I}_3(\mathbf{Q}) := \int_\Omega I_3(\mathbf{Q},\nabla\mathbf{Q})\,dx\,.
$$

First, recall that, according to the model for constrained biaxial nematic systems discussed in Section 3, to any unit quaternion $(u,\mathbf{v})=(u,v_1,v_2,v_3)^T\in\mathbb{S}^3$ there corresponds a tensor order parameter

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

such that

$$
\mathbf{Q}(u,\mathbf{v})=\mathbf{G}(u,\mathbf{v})\mathbf{A}\mathbf{G}(u,\mathbf{v})^T,\quad \mathbf{G}(u,\mathbf{v})\in SO(3),\quad \mathbf{A}=\operatorname{diag}(\lambda_1,\lambda_2,\lambda_3),
$$

where $\mathbf{n}(u,\mathbf{v})$, $\mathbf{m}(u,\mathbf{v})$, and $\boldsymbol{\ell}(u,\mathbf{v})$ agree with the columns $G_1(u,\mathbf{v})$, $G_2(u,\mathbf{v})$, and $G_3(u,\mathbf{v})$ of

$$
\mathbf{G}(u,\mathbf{v})=\begin{pmatrix} u^2+v_1^2-(v_2^2+v_3^2) & 2(v_1v_2-uv_3) & 2(v_1v_3+uv_2) \\ 2(v_1v_2+uv_3) & u^2+v_2^2-(v_1^2+v_3^2) & 2(v_2v_3-uv_1) \\ 2(v_1v_3-uv_2) & 2(v_2v_3+uv_1) & u^2+v_3^2-(v_1^2+v_2^2) \end{pmatrix}. \tag{6.5}
$$

In [29], we showed that

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

where, according to the alternative in (3.2), by assuming $S_1 < S_2 < 0$, we have set

$$S := \begin{cases} S_2 & \text{if} \quad \dfrac{S_1}{2} \leq S_2 < 0 \\ S_1 & \text{if} \quad S_2 \leq \dfrac{S_1}{2} < 0 \end{cases} \qquad S \neq 0\,. \tag{6.6}$$

To prove the claim, we assumed that $(u,\mathbf{v}) = p_0 := (1,0,0,0)^T$, so that $\mathbf{n} = (1,0,0)^T$, $\mathbf{m} = (0,1,0)^T$, $\boldsymbol{\ell} = (0,0,1)^T$. Since $|(u,\mathbf{v})| \equiv 1$, the 4×3 gradient matrix $\nabla(u,\mathbf{v})$ satisfies $(\nabla(u,\mathbf{v}))^T(u,\mathbf{v}) = 0$, which implies that the first row of $\nabla(u,\mathbf{v})$ is zero, that is $\partial_i u = 0$ at p_0, for $i=1,2,3$. At p_0, we thus have

$$\partial_i\mathbf{n} = 2\begin{pmatrix} 0 \\ \partial_i v_3 \\ -\partial_i v_2 \end{pmatrix}, \quad \partial_i\mathbf{m} = 2\begin{pmatrix} -\partial_i v_3 \\ 0 \\ \partial_i v_1 \end{pmatrix}, \quad \partial_i\boldsymbol{\ell} = 2\begin{pmatrix} \partial_i v_2 \\ -\partial_i v_1 \\ 0 \end{pmatrix}, \tag{6.7}$$

which yields

$$|\nabla\mathbf{n}|^2 = 4(|\nabla v_2|^2 + |\nabla v_3|^2)\,,\ |\nabla\mathbf{m}|^2 = 4(|\nabla v_1|^2 + |\nabla v_3|^2)\,,\ |\nabla\boldsymbol{\ell}|^2 = 4(|\nabla v_1|^2 + |\nabla v_2|^2)\,.$$

As a consequence, by Proposition 4.2, for $\mathbf{Q} = \mathbf{Q}_0 := \mathbf{Q}(p_0)$, we obtain

$$\frac{1}{8}\,I_3(\mathbf{Q}_0,\nabla\mathbf{Q}) = (\Lambda_2+\Lambda_3)|\nabla v_1|^2 + (\Lambda_3+\Lambda_1)|\nabla v_2|^2 + (\Lambda_1+\Lambda_2)|\nabla v_3|^2, \tag{6.8}$$

where, according to (4.14),

$$(\Lambda_2+\Lambda_3) = S_2^2\,, \quad (\Lambda_3+\Lambda_1) = S_1^2\,, \quad (\Lambda_1+\Lambda_2) = (S_1-S_2)^2\,. \tag{6.9}$$

It then follows that

$$I_3(\mathbf{Q}_0,\nabla\mathbf{Q}) = f_3(p_0,\nabla(u,\mathbf{v})),$$

where, for every 4×3 matrix $H = (H^i_j)$, $i=0,1,2,3$, $j=1,2,3$, such that $H^T p_0 = 0$, i.e. $H^0_j = 0$ for all j, we have set

$$f_3(p_0,H) := 8\left[S_2^2\sum_{j=1}^3 (H^1_j)^2 + S_1^2\sum_{j=1}^3 (H^2_j)^2 + (S_1-S_2)^2\sum_{j=1}^3 (H^3_j)^2\right]. \tag{6.10}$$

By frame indifference, on account of Lemma 3.6, we are thus reduced to prove that, for every $H\in\mathbb{M}_{4\times 3}$ such that $H^T p_0 = 0$,

$$f_3(p_0,H) \geq 8\,S^2\,|H|^2. \tag{6.11}$$

Now, if the first alternative in (6.6) holds, we have

$$(\Lambda_2+\Lambda_3) = S_2^2\,, \quad (\Lambda_3+\Lambda_1) \geq 4S_2^2\,, \quad (\Lambda_1+\Lambda_2) \geq S_2^2,$$

whereas, if the second alternative holds,

$$(\Lambda_3+\Lambda_1) = S_1^2\,, \quad (\Lambda_2+\Lambda_3) \geq 4S_1^2\,, \quad (\Lambda_1+\Lambda_2) \geq S_1^2,$$

which yield the coercivity condition (6.11).

6.3. A first general case. Let the functional $\mathcal{F}[\mathbf{Q}]$ be as in (1.5), where the elastic energy density is of the form (1.6), for some constants $L_i \in \mathbb{R}$.

In the constrained biaxial case, according to Remark 3.2, we may assume that $S_1 < S_2 < 0$. In addition, the alternatives (3.2) hold. Let us denote

$$\sigma := S_1/S_2 = \frac{\lambda_1 - \lambda_3}{\lambda_2 - \lambda_3} = \frac{2\lambda_1 + \lambda_2}{\lambda_1 + 2\lambda_2} > 1.$$

With this notation, for the two related cases in (6.6), we have

$$\frac{S_1}{2} \le S_2 < 0 \Longleftrightarrow \sigma \ge 2\,, \quad S_2 \le \frac{S_1}{2} < 0 \Longleftrightarrow 1 < \sigma \le 2\,.$$

Remark 6.1. In the following proofs, we shall use the fact that a quadratic function of the form $Q_1(x,y) = ax^2 + by^2 - 2txy$ is positive definite if and only if $a > 0$, $b > 0$ and $t^2 < ab$. Furthermore, assuming $a \le b \le c$, a quadratic form $Q_2(x,y,z) = ax^2 + by^2 + cz^2 - 2t(xy - xz + yz)$ is positive definite if and only if $a > 0$, $t^2 < ab$, and $abc + 2t^3 - (a+b+c)t^2 > 0$. Notice that if $a = b = c$, the last inequality reads as $(a-t)^2(2t+a) > 0$, whence the quadratic form $Q_2(x,y,z) = a(x^2+y^2+z^2) - 2t(xy - xz + yz)$ is positive definite if and only if $a > |t|$ and $a + 2t > 0$.

We first deal with the simpler case when $L_4 = 0$, and prove the following.

Theorem 6.2. *In the constrained biaxial case, the quadratic form* $L_1I_1 + L_2I_2 + L_3I_3$ *is positive definite if and only if we have:*

$$L_2 + L_3 > 0\,, \quad 2L_3 - L_2 > 0 \quad \textit{and} \quad 2L_1 + L_2 + 2L_3 > 0\,. \tag{6.12}$$

Proof. Assume as above that $(u, \mathbf{v}) = p_0$, so that $\mathbf{n} = (1,0,0)^T$, $\mathbf{m} = (0,1,0)^T$, $\boldsymbol{\ell} = (0,0,1)^T$ and (6.7) holds true. At p_0, we then compute

$$\begin{aligned}
\operatorname{curl}\mathbf{n} &= 2(-\partial_2 v_2 - \partial_3 v_3, \partial_1 v_2, \partial_1 v_3),\\
\operatorname{curl}\mathbf{m} &= 2(\partial_2 v_1, -\partial_3 v_3 - \partial_1 v_1, \partial_2 v_3),\\
\operatorname{curl}\boldsymbol{\ell} &= 2(\partial_3 v_1, \partial_3 v_2, -\partial_1 v_1 - \partial_2 v_2),
\end{aligned}$$

and

$$\begin{aligned}
(\operatorname{div}\mathbf{n})^2 &= 4[(\partial_2 v_3)^2 + (\partial_3 v_2)^2 - 2\partial_2 v_3 \partial_3 v_2],\\
\operatorname{tr}[(\nabla\mathbf{n})^2] &= 4[(\partial_2 v_3)^2 + (\partial_3 v_2)^2 - 2\partial_2 v_2 \partial_3 v_3],\\
(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 &= 4[(\partial_2 v_2)^2 + (\partial_3 v_3)^2 + 2\partial_2 v_2 \partial_3 v_3],\\
|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 &= 4[(\partial_1 v_2)^2 + (\partial_1 v_3)^2],\\
(\operatorname{div}\mathbf{m})^2 &= 4[(\partial_1 v_3)^2 + (\partial_3 v_1)^2 - 2\partial_1 v_3 \partial_3 v_1],\\
\operatorname{tr}[(\nabla\mathbf{m})^2] &= 4[(\partial_1 v_3)^2 + (\partial_3 v_1)^2 - 2\partial_3 v_3 \partial_1 v_1],\\
(\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2 &= 4[(\partial_3 v_3)^2 + (\partial_1 v_1)^2 + 2\partial_3 v_3 \partial_1 v_1],\\
|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2 &= 4[(\partial_2 v_3)^2 + (\partial_2 v_1)^2],\\
(\operatorname{div}\boldsymbol{\ell})^2 &= 4[(\partial_1 v_2)^2 + (\partial_2 v_1)^2 - 2\partial_1 v_2 \partial_2 v_1],\\
\operatorname{tr}[(\nabla\boldsymbol{\ell})^2] &= 4[(\partial_1 v_2)^2 + (\partial_2 v_1)^2 - 2\partial_1 v_1 \partial_2 v_2],\\
(\boldsymbol{\ell}\cdot\operatorname{curl}\boldsymbol{\ell})^2 &= 4[(\partial_1 v_1)^2 + (\partial_2 v_2)^2 + 2\partial_1 v_1 \partial_2 v_2],\\
|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2 &= 4[(\partial_3 v_1)^2 + (\partial_3 v_2)^2].
\end{aligned}$$

By Propositions 4.3, 4.5, and 4.2, and formulas (4.14) and (6.9), if $(u, \mathbf{v}) = p_0$, we thus have

$$\begin{aligned}
I_1(\mathbf{Q}_0, \nabla\mathbf{Q}) &= 4\,S_2^2\,[(\partial_2 v_1)^2 + (\partial_3 v_1)^2] + 4\,S_1^2\,[(\partial_3 v_2)^2 + (\partial_1 v_2)^2]\\
&\quad +4\,(S_1 - S_2)^2\,[(\partial_1 v_3)^2 + (\partial_2 v_3)^2]\\
&\quad -8\,[S_1(S_1 - S_2)\,\partial_2 v_3 \partial_3 v_2 + S_2(S_2 - S_1)\,\partial_3 v_1 \partial_1 v_3 + S_1 S_2\,\partial_1 v_2 \partial_2 v_1],
\end{aligned} \tag{6.13}$$

$$
\begin{aligned}
I_2(\mathbf{Q}_0,\nabla\mathbf{Q}) = {} & 4\,S_2^2\,[(\partial_2 v_1)^2+(\partial_3 v_1)^2]+4\,S_1^2\,[(\partial_3 v_2)^2+(\partial_1 v_2)^2] \\
& +4\,(S_1-S_2)^2\,[(\partial_1 v_3)^2+(\partial_2 v_3)^2] \\
& -8\,[S_1(S_1-S_2)\,\partial_2 v_2\partial_3 v_3+S_2(S_2-S_1)\,\partial_3 v_3\partial_1 v_1+S_1S_2\,\partial_1 v_1\partial_2 v_2],
\end{aligned}
\tag{6.14}
$$

and, according to (6.8),

$$
\begin{aligned}
I_3(\mathbf{Q}_0,\nabla\mathbf{Q}) = {} & 8\,S_2^2\,[(\partial_1 v_1)^2+(\partial_2 v_1)^2+(\partial_3 v_1)^2] \\
& +8\,S_1^2\,[(\partial_1 v_2)^2+(\partial_2 v_2)^2+(\partial_3 v_2)^2] \\
& +8\,(S_1-S_2)^2\,[(\partial_1 v_3)^2+(\partial_2 v_3)^2+(\partial_3 v_3)^2]\,.
\end{aligned}
\tag{6.15}
$$

We can thus write

$$
I_i(\mathbf{Q}_0,\nabla\mathbf{Q}) = f_i(p_0,\nabla(u,\mathbf{v})),\qquad i=1,2,3
$$

where, for every matrix $H=(H^i_j)\in\mathbb{M}_{4\times 3}$, such that $H^Tp_0=0$, we have set

$$
\begin{aligned}
f_1 = f_1(p_0,H) := {} & 4\,S_2^2\,\big[(H^1_2)^2+(H^1_3)^2\big]+4\,S_1^2\,\big[(H^2_3)^2+(H^2_1)^2\big] \\
& +4\,(S_1-S_2)^2\,\big[(H^3_1)^2+(H^3_2)^2\big] \\
& -8\,\big[S_1(S_1-S_2)\,H^3_2H^2_3+S_2(S_2-S_1)\,H^1_3H^3_1+S_1S_2\,H^2_1H^1_2\big]\,,
\end{aligned}
\tag{6.16}
$$

$$
\begin{aligned}
f_2 = f_2(p_0,H) := {} & 4\,S_2^2\,\big[(H^1_2)^2+(H^1_3)^2\big]+4\,S_1^2\,\big[(H^2_3)^2+(H^2_1)^2\big] \\
& +4\,(S_1-S_2)^2\,\big[(H^3_1)^2+(H^3_2)^2\big] \\
& -8\,\big[S_1(S_1-S_2)\,H^2_2H^3_3+S_2(S_2-S_1)\,H^3_3H^1_1+S_1S_2\,H^1_1H^2_2\big]\,,
\end{aligned}
\tag{6.17}
$$

and $f_3=f_3(p_0,H)$ is given by (6.10). Dividing by $4S_2^2$ and using $\sigma=S_1/S_2$, we then compute:

$$
\begin{aligned}
\frac{1}{4\,S_2^2}\,(L_1f_1+L_2f_2+L_3f_3) = {} & 2L_3\,\big[(H^1_1)^2+(\sigma H^2_2)^2+((\sigma-1)H^3_3)^2\big] \\
& -2L_2\,\big[H^1_1\,\sigma H^2_2-H^1_1\,(\sigma-1)H^3_3+\sigma H^2_2\,(\sigma-1)H^3_3\big] \\
& +(L_1+L_2+2L_3)\,\big[(H^1_3)^2+((\sigma-1)H^3_1)^2\big]+2L_1\,H^1_3\,(\sigma-1)H^3_1 \\
& +(L_1+L_2+2L_3)\,\big[(H^1_2)^2+(\sigma H^2_1)^2\big]-2L_1\,H^1_2\,\sigma H^2_1 \\
& +(L_1+L_2+2L_3)\,\big[(\sigma H^2_3)^2+((\sigma-1)H^3_2)^2\big]-2L_1\,\sigma H^2_3\,(\sigma-1)H^3_2\,.
\end{aligned}
$$

Therefore, see Remark 6.1, the quadratic form $L_1f_1+L_2f_2+L_3f_3$ is positive definite if and only if the following inequalities are satisfied:

$$
2L_3>0\,,\quad |L_2|<2|L_3|\,,\quad 8L_3^3+2L_2^3-6L_2^2L_3>0
$$

and

$$
L_1+L_2+2L_3>0\,,\quad |L_1|<|L_1+L_2+2L_3|\,.
$$

Since $8L_3^3+2L_2^3-6L_2^2L_3=2(2L_3-L_2)^2(L_2+L_3)$, these conditions are clearly equivalent to (6.12). The claim follows by frame indifference through Lemma 3.6. □

We now consider Dirichlet boundary conditions, specified by the admissible set of tensor $W^{1,2}_\varphi$ defined in the introduction.

THEOREM 6.3. *For a constrained biaxial nematic system, let $\mathcal{F}[\mathbf{Q}]$ be of the form (1.5), and let $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ be of the form (1.6), for some constants $L_1,L_2,L_3\in\mathbb{R}$, and $L_4=0$. Then, the functional $\mathcal{F}[\mathbf{Q}]$ is coercive on the admissible set $W^{1,2}_\varphi$ provided that*

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

REMARK 6.4. If $L_1 \neq 0$, then the sufficient conditions in Theorem 6.3 are *strictly weaker* than the positivity conditions from Theorem 6.2 for several choices of L_1 and L_2, that depend on the sign of the sum $L_1 + L_2$:

1. $L_1 + L_2 = 0$;
2. $L_1 + L_2 > 0$ and one of the following additional inequalities holds:

$$\frac{L_1 + L_2}{2} < -L_2\,, \quad \frac{L_1 + L_2}{2} < \frac{L_2}{2}\,, \quad \frac{L_1 + L_2}{2} < -L_1 - \frac{L_2}{2}\,;$$

3. $L_1 + L_2 < 0$ and one of the following additional inequalities holds:

$$-(L_1 + L_2) < -L_2\,, \quad -(L_1 + L_2) < \frac{L_2}{2}\,, \quad -(L_1 + L_2) < -L_1 - \frac{L_2}{2}\,.$$

The above choices are equivalent to the following complete list:

- $L_1 + L_2 = 0$;
- $L_1 + L_2 > 0$, $L_1 > 0$, $L_2 < 0$, and $L_1 + 3L_2 < 0$;
- $L_1 + L_2 > 0$, $L_1 < 0$, and $L_2 > 0$;
- $L_1 + L_2 < 0$, $L_1 > 0$, and $L_2 < 0$;
- $L_1 + L_2 < 0$, $L_1 < 0$, and $L_2 > 0$.

Proof of Theorem 6.3. Assuming as above that $(u, \mathbf{v}) = p_0$, by (4.3), the surface terms read as

$$\begin{aligned}
&(\operatorname{div}\mathbf{n})^2 - \operatorname{tr}[(\nabla\mathbf{n})^2] = \operatorname{div}\Phi_1\,, && \Phi_1 := 4(0, v_2\partial_3 v_3 - v_3\partial_3 v_2, v_3\partial_2 v_2 - v_2\partial_2 v_3),\\
&(\operatorname{div}\mathbf{m})^2 - \operatorname{tr}[(\nabla\mathbf{m})^2] = \operatorname{div}\Phi_2\,, && \Phi_2 := 4(v_1\partial_3 v_3 - v_3\partial_3 v_1, 0, v_3\partial_1 v_1 - v_1\partial_1 v_3),\\
&(\operatorname{div}\boldsymbol{\ell})^2 - \operatorname{tr}[(\nabla\boldsymbol{\ell})^2] = \operatorname{div}\Phi_3\,, && \Phi_3 := 4(v_1\partial_2 v_2 - v_2\partial_2 v_1, v_2\partial_1 v_1 - v_1\partial_1 v_2, 0)\,.
\end{aligned}$$

We thus have:

$$I_1(\mathbf{Q}, \nabla\mathbf{Q}) = I_2(\mathbf{Q}, \nabla\mathbf{Q}) + \operatorname{div}(\Lambda_1\Phi_1 + \Lambda_2\Phi_2 + \Lambda_3\Phi_3)\,. \tag{6.18}$$

Denote for simplicity $2L := L_1 + L_2$. Putting in evidence the positive factor $8\,S_2^2$ and replacing $\sigma = S_1/S_2$, by (6.18), (6.14), and (6.15), we thus obtain

$$\begin{aligned}
\frac{1}{8\,S_2^2}\,(L_1 I_1 + L_2 I_2 + L_3 I_3) = {}& \frac{L_1}{8}\operatorname{div}(\Lambda_1\Phi_1 + \Lambda_2\Phi_2 + \Lambda_3\Phi_3)\,S_2^{-2}\\
&+L_3\left[(\partial_1 v_1)^2 + (\sigma\partial_2 v_2)^2 + ((\sigma-1)\partial_3 v_3)^2\right]\\
&-2L\left[\partial_1 v_1\,\sigma\partial_2 v_2 - \partial_1 v_1\,(\sigma-1)\,\partial_3 v_3 + \sigma\partial_2 v_2\,(\sigma-1)\partial_3 v_3\right]\\
&+(L+L_3)\left[(\partial_2 v_1)^2 + (\partial_3 v_1)^2\right]\\
&+(L+L_3)\,\sigma^2\left[(\partial_1 v_2)^2 + (\partial_3 v_2)^2\right]\\
&+(L+L_3)\,(\sigma-1)^2\left[(\partial_1 v_3)^2 + (\partial_2 v_3)^2\right].
\end{aligned} \tag{6.19}$$

Therefore, coercivity for the functional $\mathcal{F}[\mathbf{Q}]$ holds provided that the following strict inequalities hold:

$$L_3 > 0\,, \quad |L| < L_3\,, \quad 2L + L_3 > 0\,, \quad L + L_3 > 0\,,$$

which reduce to $2L_3 > L_1 + L_2$ and $L_1 + L_2 + L_3 > 0$. The claim now follows by frame invariance, on account of Lemma 3.6. □

6.4. The general case. We are now in a position to state and prove our main results for $L_4 \neq 0$.

Theorem 6.5. *In the constrained biaxial case, if $L_4 \neq 0$, the quadratic form $L_1I_1 + L_2I_2 + L_3I_3 + L_4I_4$ is positive definite if and only if the following system holds, according to the sign of L_4:*

i) $L_4 \geq 0$ *and*

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

ii) $L_4 \leq 0$ *and*

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

Remark 6.6. If $L_4 = 0$, the positivity conditions in i) and ii) are both equivalent to (6.12). Moreover, by (3.2), the coefficients $L_4(2S_1 - S_2)$ and $L_4(S_1 + S_2)$ are both negative when $L_4 > 0$, and both positive when $L_4 < 0$, whereas the sign of $L_4(2S_2 - S_1)$ depends on the two regimes described in (3.2), according to the sign of L_4. It also follows from the proof that, independently of the sign of L_4, the last three conditions in the above two systems i) and ii) are equivalent. This is due to the fact that the systems (6.23) and (6.24) below have the same solutions. Finally, in both cases the necessary condition $L_3 > 0$ is satisfied.

Proof of Theorem 6.5. First, we compute I_4 at p_0, as we did for I_1, I_2, I_3 in the proof of Theorem 6.2. The mixed terms (5.2) in the expression of I_4 given in Theorem 5.1 become

$$\Lambda_{\mathbf{m}}^{\mathbf{n}} = 4(\partial_1 v_2)^2\,, \quad \Lambda_{\boldsymbol{\ell}}^{\mathbf{m}} = 4(\partial_2 v_3)^2\,, \quad \Lambda_{\mathbf{n}}^{\boldsymbol{\ell}} = 4(\partial_3 v_1)^2\,.$$

Therefore, at p_0, the functional I_4 takes the form

$$
\begin{aligned}
I_4(\mathbf{Q}_0,\nabla\mathbf{Q}) &= 3^{-1}\, S_1(2S_1-S_2)(S_2-S_1)\left[4|\nabla v_2|^2+4|\nabla v_3|^2\right]\\
&\quad + 2S_1(S_2-S_1)^2\left[4(\partial_1 v_2)^2+4(\partial_1 v_3)^2\right]\\
&\quad + 3^{-1}\, S_2(2S_2-S_1)(S_1-S_2)\left[4|\nabla v_3|^2+4|\nabla v_1|^2\right]\\
&\quad + 2S_2^2(S_2-S_1)\left[4(\partial_2 v_3)^2+4(\partial_2 v_1)^2\right]\\
&\quad + 3^{-1}\, S_1S_2(S_1+S_2)\left[4|\nabla v_1|^2+4|\nabla v_2|^2\right]\\
&\quad - 2S_1^2S_2\left[4(\partial_3 v_1)^2+4(\partial_3 v_2)^2\right]\\
&\quad + 2S_1S_2(S_1-S_2)\left[4(\partial_1 v_2)^2+4(\partial_2 v_3)^2+4(\partial_3 v_1)^2\right].
\end{aligned}
\tag{6.20}
$$

As before, we can thus write $I_4(\mathbf{Q}_0,\nabla\mathbf{Q}) = f_4(p_0,\nabla(u,\mathbf{v}))$, where, for every 4×3 matrix $H=(H^i_j)$, such that $H^Tp_0=0$, we have set

$$
\begin{aligned}
f_4(p_0,H) \;:=\;& 3^{-1}\, S_1(2S_1-S_2)(S_2-S_1)\left[4\sum_{j=1}^3 (H^2_j)^2+4\sum_{j=1}^3 (H^3_j)^2\right]\\
&+2S_1(S_2-S_1)^2\left[4(H^2_1)^2+4(H^3_1)^2\right]\\
&+3^{-1}\, S_2(2S_2-S_1)(S_1-S_2)\left[4\textstyle\sum_{j=1}^3 (H^3_j)^2+4\sum_{j=1}^3 (H^1_j)^2\right]\\
&+2S_2^2(S_2-S_1)\left[4(H^3_2)^2+4(H^1_2)^2\right]\\
&+3^{-1}\, S_1S_2(S_1+S_2)\left[4\textstyle\sum_{j=1}^3 (H^1_j)^2+4\sum_{j=1}^3 (H^2_j)^2\right]\\
&-2S_1^2S_2\left[4(H^1_3)^2+4(H^2_3)^2\right]\\
&+2S_1S_2(S_1-S_2)\left[4(H^2_1)^2+4(H^3_2)^2+4(H^1_3)^2\right].
\end{aligned}
\tag{6.21}
$$

Using (6.16), (6.17), (6.10), and (6.21), we thus compute

$$
\begin{aligned}
\frac{1}{4\,S_2^2}\,(L_1f_1+L_2f_2+L_3f_3+L_4f_4) &= \left[2L_3+(2/3)\,L_4S_2(2\sigma-1)\right](H^1_1)^2\\
&+\left[2L_3+(2/3)\,L_4S_2(2-\sigma)\right](\sigma H^2_2)^2\\
&+\left[2L_3-(2/3)\,L_4S_2(\sigma+1)\right]((\sigma-1)H^3_3)^2\\
&-2L_2\left[H^1_1\,\sigma H^2_2 - H^1_1\,(\sigma-1)H^3_3+\sigma H^2_2\,(\sigma-1)H^3_3\right]\\
&+\left[L_1+L_2+2L_3-(2/3)\,L_4S_2(\sigma+1)\right](H^1_3)^2\\
&+\left[L_1+L_2+2L_3+(2/3)\,L_4S_2(2\sigma-1)\right]((\sigma-1)H^3_1)^2+2L_1\,H^1_3\,(\sigma-1)H^3_1\\
&+\left[L_1+L_2+2L_3+(2/3)\,L_4S_2(2-\sigma)\right](H^1_2)^2\\
&+\left[L_1+L_2+2L_3+(2/3)\,L_4S_2(2\sigma-1)\right](\sigma\,H^2_1)^2-2L_1\,H^1_2\,\sigma H^2_1\\
&+\left[L_1+L_2+2L_3-(2/3)\,L_4S_2(\sigma+1)\right](\sigma H^2_3)^2\\
&+\left[L_1+L_2+2L_3+(2/3)\,L_4S_2(2-\sigma)\right]((\sigma-1)H^3_2)^2-2L_1\,\sigma H^2_3\,(\sigma-1)H^3_2\,.
\end{aligned}
$$

We now set

$$
\begin{aligned}
a &:= 2L_3+\tfrac{2}{3}\,L_4S_2(2\sigma-1)\,,\\
b &:= 2L_3+\tfrac{2}{3}\,L_4S_2(2-\sigma)\,,\\
c &:= 2L_3-\tfrac{2}{3}\,L_4S_2(\sigma+1),
\end{aligned}
\tag{6.22}
$$

so that

$$
\begin{aligned}
\frac{1}{4\,S_2^2}\,(L_1f_1+L_2f_2+L_3f_3+L_4f_4) &= a(H^1_1)^2+b(\sigma H^2_2)^2+c((\sigma-1)H^3_3)^2\\
&-2L_2\left[H^1_1\,\sigma H^2_2-H^1_1\,(\sigma-1)H^3_3+\sigma H^2_2\,(\sigma-1)H^3_3\right]\\
&+(L_1+L_2+c)(H^1_3)^2+(L_1+L_2+a)((\sigma-1)H^3_1)^2+2L_1\,H^1_3\,(\sigma-1)H^3_1\\
&+(L_1+L_2+b)(H^1_2)^2+(L_1+L_2+a)(\sigma\,H^2_1)^2-2L_1\,H^1_2\,\sigma H^2_1\\
&+(L_1+L_2+c)(\sigma H^2_3)^2+(L_1+L_2+b)((\sigma-1)H^3_2)^2-2L_1\,\sigma H^2_3\,(\sigma-1)H^3_2.
\end{aligned}
$$

We distinguish two cases according to the sign of the coefficient L_4, recalling that $\sigma > 1$.

In the case $L_4 > 0$, we have $L_4 S_2 < 0$, and hence $a < b < c$. By Remark 6.1, the quadratic form $(L_1 f_1 + L_2 f_2 + L_3 f_3 + L_4 f_4)$ is positive definite if and only if the following inequalities hold:

$$a > 0\,, \quad L_2^2 < ab\,, \quad abc + 2L_2^3 - (a+b+c)L_2^2 > 0 \tag{6.23}$$

and also

$$L_1 + L_2 + a > 0\,, \quad L_1^2 < (L_1 + L_2 + a)(L_1 + L_2 + b),$$

where the last inequality becomes

$$L_2^2 + 2L_1 L_2 + (L_1 + L_2)(a+b) + ab > 0\,.$$

We now observe that $a + b + c = 6L_3$, whereas

$$ab = 4L_3^2 + \frac{4}{9} L_4^2 S_2^2 (2\sigma - 1)(2 - \sigma) + \frac{4}{3} L_3 L_4 S_2 (\sigma + 1)$$

and

$$abc = 8L_3^3 - \frac{8}{27} L_4^3 S_2^3 (2\sigma - 1)(2-\sigma)(\sigma+1) + \frac{8}{9} L_3 L_4^2 S_2^2 \big[(2\sigma-1)(2-\sigma) - (\sigma+1)^2\big]\,.$$

Since $(2\sigma - 1)(2 - \sigma) - (\sigma + 1)^2 = -3(\sigma^2 - \sigma + 1)$, recalling that $\sigma = S_1/S_2$ we can rewrite

$$ab = 4L_3^2 + \frac{4}{9} L_4^2 (2S_1 - S_2)(2S_2 - S_1) + \frac{4}{3} L_3 L_4 (S_1 + S_2)$$

and

$$abc = 8L_3^3 - \frac{8}{27} L_4^3 (2S_1 - S_2)(2S_2 - S_1)(S_1 + S_2) - \frac{8}{3} L_3 L_4^2 \big[S_1^2 - S_1 S_2 + S_2^2\big]\,.$$

Using that $a + b = 6L_3 - c$, we obtain the system in i).

In the case $L_4 < 0$, we have $L_4 S_2 > 0$ and hence $c < b < a$. Again by Remark 6.1, this time we deduce that the quadratic form $(L_1 f_1 + L_2 f_2 + L_3 f_3 + L_4 f_4)$ is positive definite if and only if the inequalities

$$c > 0\,, \quad L_2^2 < cb\,, \quad abc + 2L_2^3 - (a+b+c)L_2^2 > 0\,, \tag{6.24}$$

which are equivalent to the ones in (6.23), hold true, and also

$$L_1 + L_2 + c > 0\,, \quad L_1^2 < (L_1 + L_2 + c)(L_1 + L_2 + b)\,.$$

The last inequality is the same as

$$L_2^2 + 2L_1 L_2 + (L_1 + L_2)(c + b) + cb > 0\,,$$

where

$$\begin{aligned} cb &= 4L_3^2 + \tfrac{4}{9} L_4^2 S_2^2 (\sigma - 2)(\sigma + 1) - \tfrac{4}{3} L_3 L_4 S_2 (2\sigma - 1) \\ &= 4L_3^2 - \tfrac{4}{9} L_4^2 (2S_2 - S_1)(S_1 + S_2) - \tfrac{4}{3} L_3 L_4 (2S_1 - S_2)\,. \end{aligned}$$

Using that $c + b = 6L_3 - a$, this time we obtain the system in ii). The claim follows from Lemma 3.6. □

We finally consider again Dirichlet boundary conditions, specified by the admissible set of tensor $W^{1,2}_\varphi$ defined in the introduction.

THEOREM 6.7. *For a constrained biaxial nematic system, let $\mathcal{F}[\mathbf{Q}]$ be of the form* (1.5)*, and let $\psi_E(\mathbf{Q},\nabla\mathbf{Q})$ be of the form* (1.6)*, for some constants $L_1, L_2, L_3 \in \mathbb{R}$, and $L_4 \neq 0$. Then, the functional $\mathcal{F}[\mathbf{Q}]$ is coercive on the admissible set $W^{1,2}_{\varphi}$ provided that the following alternative inequalities are satisfied.*

a) $L_4 \geq 0$ *and*

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

b) $L_4 \leq 0$ *and*

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

REMARK 6.8. If $L_4 = 0$, we recover the statement of Theorem 6.3. As before, independently of the sign of L_4, the last three conditions in the above two systems a) and b) are equivalent, and in both cases the necessary condition $L_3 > 0$ is satisfied.

Moreover, if $L_1 \neq 0$, then the sufficient conditions in Theorem 6.7 are *strictly weaker* than the positivity conditions from Theorem 6.5 for several choices of the coefficients L_1 and L_2. This happens if, e.g.,

$$L_1 > 0\,, \quad L_2 < 0\,, \quad \text{and} \quad L_1 + 2L_2 \leq 0$$

independently of the sign of L_4. In fact, e.g. in the case $L_4 > 0$, comparing the systems i) and a) in Theorems 6.5 and 6.7, respectively, we observe that the fourth line in i) implies the third line in a) provided that $L_2^2 \geq (L_1 + L_2)^2$, i.e. $L_1(L_1 + 2L_2) \leq 0$. On the other hand, the last line in i) implies the last line in a) provided that

$$4L_3^3 + L_2^3 - 3L_3L_2^2 \leq 4L_3^3 + (L_1 + L_2)^3 - 3L_3(L_1 + L_2)^2\,,$$

which is equivalent to

$$3L_3\big(L_2^2 - (L_1 + L_2)^2\big) \geq -L_1(L_1^2 + 3L_1L_2 + 3L_2^2)\,.$$

Since $(L_1^2 + 3L_1L_2 + 3L_2^2) > 0$, our claim readily follows.

Proof of Theorem 6.7. If we put in evidence the factor $(4/3)\,S_2^3$ and substitute

$\sigma := S_1/S_2$, by (6.20) we obtain

$$\begin{aligned}\frac{3}{4}\,I_4(\mathbf{Q},\nabla\mathbf{Q})\cdot {S_2}^{-3} \quad &= \sigma(2\sigma-1)(1-\sigma)\left[|\nabla v_2|^2+|\nabla v_3|^2\right]\\ &+6\sigma(\sigma-1)^2\left[(\partial_1 v_2)^2+(\partial_1 v_3)^2\right]\\ &+(2-\sigma)(\sigma-1)\left[|\nabla v_3|^2+|\nabla v_1|^2\right]\\ &+6(1-\sigma)\left[(\partial_2 v_3)^2+(\partial_2 v_1)^2\right]\\ &+\sigma(\sigma+1)\left[|\nabla v_1|^2+|\nabla v_1|^2\right]\\ &-6\sigma^2\left[(\partial_3 v_1)^2+(\partial_3 v_2)^2\right]\\ &+6\sigma(\sigma-1)\left[(\partial_1 v_2)^2+(\partial_2 v_3)^2+(\partial_3 v_1)^2\right],\end{aligned}$$

and hence, using that $|\nabla v_j|^2=(\partial_1 v_j)^2+(\partial_2 v_j)^2+(\partial_3 v_j)^2$,

$$\begin{aligned}\frac{3}{8}\,I_4(\mathbf{Q},\nabla\mathbf{Q})\,{S_2}^{-3} &= (2\sigma-1)\,(\partial_1 v_1)^2+\sigma^2(2-\sigma)\,(\partial_2 v_2)^2-(\sigma-1)^2(\sigma+1)\,(\partial_3 v_3)^2\\ &+(2-\sigma)\,(\partial_2 v_1)^2-(\sigma+1)\,(\partial_3 v_1)^2\\ &+\sigma^2(2\sigma-1)\,(\partial_1 v_2)^2-\sigma^2(\sigma+1)\,(\partial_3 v_2)^2\\ &+(\sigma-1)^2(2\sigma-1)\,(\partial_1 v_3)^2+(\sigma-1)^2(2-\sigma)\,(\partial_2 v_3)^2\,.\end{aligned}$$

On account of (6.19), and using the notation from (6.22), we then obtain the formula

$$\begin{aligned}\frac{1}{4\,S_2^2}\,\psi_E(\mathbf{Q},\nabla\mathbf{Q}) &= \frac{1}{4}\,L_1\,\operatorname{div}(\Lambda_1\Phi_1+\Lambda_2\Phi_2+\Lambda_3\Phi_3)\,S_2^{-2}\\ &+a\,(\partial_1 v_1)^2+b\,(\sigma\partial_2 v_2)^2+c\,((\sigma-1)\partial_3 v_3)^2\\ &-4L\left[-\partial_1 v_1\,(\sigma-1)\,\partial_3 v_3+\partial_1 v_1\,\sigma\partial_2 v_2+\sigma\partial_2 v_2\,(\sigma-1)\partial_3 v_3\right]\\ &+(2L+b)(\partial_2 v_1)^2+(2L+c)(\partial_3 v_1)^2+(2L+a)(\sigma\partial_1 v_2)^2\\ &+(2L+c)\,(\sigma\partial_3 v_2)^2+(2L+a)\,((\sigma-1)\partial_1 v_3)^2+(2L+b)\,((\sigma-1)\partial_2 v_3)^2.\end{aligned}$$

We again distinguish two cases according to the sign of the coefficient L_4. By the Dirichlet-type assumption, we can omit to consider the divergence term.

In the case $L_4>0$, we have $a<b<c$. By Remark 6.1, we are led to consider the following inequalities:

$$a>0\,,\quad (2L)^2<ab\,,\quad abc+2(2L)^3-(a+b+c)(2L)^2>0\,,\quad 2L+a>0\,.$$

Recalling from the proof of Theorem 6.5 the formulas for ab, abc, and $a+b+c$, and using that $2L=L_1+L_2$, we readily obtain the system a).

In the case $L_4<0$, we have $c<b<a$, and we are thus led to consider the following inequalities:

$$c>0\,,\quad (2L)^2<cb\,,\quad abc+2(2L)^3-(a+b+c)(2L)^2>0\,,\quad 2L+c>0\,.$$

Recalling the formula for bc, we obtain the system b). Therefore, our conclusions readily follow, again by frame invariance. □

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REFERENCES

[1] 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.
[2] 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.
[3] J. M. Ball and A. Zarnescu, *Orientability and energy minimization in liquid cristal models*, Arch. Ration. Mech. Anal., 202 (2011), pp. 493–535.
[4] F. Bethuel and D. Chiron, *Some questions related to the lifting problem in Sobolev spaces*, Contemp. Math., 446 (2007), pp. 125-152.
[5] D. W. Berreman and S. Meiboom, *Tensor representation of Oseen–Frank strain energy in uniaxial cholesterics*, Phys. Rev. A, 30 (1984), pp. 1955–1959.
[6] D. Chillingworth, *Perturbed hedgehogs: continuous deformation of point defects in biaxial nematic liquid crystals*, IMA J. Appl. Math., special issue in Honour of John Hogan, to appear; available online from http://eprints.soton.ac.uk/id/eprint/384172.
[7] D. Chiron, *Point topological defects in ordered media in dimension two*, preprint, Laboratoire J. A. Dieudonne, Université de Nice - Sophia Antipolis.
[8] 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.
[9] 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.
[10] H.-D. Ebbinghaus, H. Hermes, F. Hirzebruck, M. Koecher, K. Mainzer, J. Neukirch, A. Prestel, and R. Remmert, *Numbers*, Graduate Texts in Mathematics, 123, Springer, New York, 1991.
[11] J. L. Ericksen, *Inequalities in liquid crystal theory*, Phys. Fluids, 9 (1966), pp. 1205–1207.
[12] 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.
[13] F. C. Frank, *I. Liquid crystals. On the theory of liquid crystals*, Discuss. Faraday Soc., 25 (1958), pp. 19–28.
[14] M. Giaquinta, *Multiple Integrals in the Calculus of Variations and Nonlinear Elliptic Systems*, Annals of Mathematics Studies, 105, Princeton University Press, Princeton, 1983.
[15] M. Giaquinta, G. Modica, and J. Souček, *Cartesian Currents in the Calculus of Variations*, II, Ergebnisse der Mathematik und ihrer Grenzgebiete (III Ser), 38, Springer, Berlin, 1998.
[16] 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.
[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] 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.
[19] F. C. Leslie, *Some topics in equilibrium theory of liquid crystals*, 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. 211–234.
[20] F. H. Lin and C. Liu, *Static and dynamic theories of liquid crystals*, J. Partial Differential Equations, 14 (2001), pp. 289-330.
[21] 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.
[22] 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.
[23] A. Majumdar, *Equilibrium order parameters of nematic liquid crystals in the Landau–de Gennes theory*, European J. Appl. Math., 21 (2010), pp. 181-203.
[24] A. Majumdar and A. Zarnescu, *Landau–de Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond*, Arch. Ration. Mech. Anal., 196 (2010), pp. 227-280.
[25] N. D. Mermin, *The topological theory of defects in ordered media*, Rev. Modern Phys., 51 (1979), pp. 591-648.
[26] H. Mori, E. C. Gartland, Jr., J. R. Kelly, and P. J. Bos, *Multidimensional director modeling using the Q tensor representation in a liquid crystal cell and its application to the π cell with patterned electrodes*, Jap. J. App. Phys., 38 (1999), pp. 135-146.
[27] 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.
[28] D. Mucci, *Maps into projective spaces: liquid crystals and conformal energies*, Discrete Contin. Dyn. Syst. Ser. B, 17 (2012), pp. 597-635.
[29] 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.

[30] C. W. Oseen, *The theory of liquid crystals*, Trans. Faraday Soc., 29 (1933), pp. 883-899.
[31] N. Schopohl and T. J. Sluckin, *Defect core structure in nematic liquid crystals*, Phys. Rev. Lett., 59 (1987), pp. 2582–2584.
[32] S. Stallinga and G. Vertogen, *Theory of orientational elasticity*, Phys. Rev. E, 49 (1994), pp. 1483–1494.
[33] H.-R. Trebin, *Elastic energies of a directional medium*, J. Physique, 42 (1981), pp. 1573–1576.
[34] E. Virga, *Variational Theories for Liquid Crystals*, Applied Mathematics and Mathematical Computation, 8, Chapman & Hall, London, 1994.
[35] H. Zocher, *The effect of a magnetic field on the nematic state*, Trans. Faraday Soc., 29 (1933), pp. 945–957.