On the elastic energy density of constrained Q-tensor models for biaxial nematics

Domenico Mucci and Lorenzo Nicolodi

Abstract

Within the Landau–de Gennes theory, the order parameter describing a biaxial nematic liquid crystal assigns a symmetric traceless 3×3 matrix $\mathbf{Q}$ with three distinct eigenvalues to every point of the region Ω occupied by the system. In the constrained case of matrices $\mathbf{Q}$ with constant eigenvalues, the order parameter space is diffeomorphic to the eightfold quotient $\mathbb{S}^3/\mathcal{H}$ of the 3-sphere $\mathbb{S}^3$, where $\mathcal{H}$ is the quaternion group, and a configuration of a biaxial nematic liquid crystal is described by a map from Ω to $\mathbb{S}^3/\mathcal{H}$. We express the (simplest form of the) Landau–de Gennes elastic free-energy density as a density defined on maps $q : \Omega \to \mathbb{S}^3$, whose functional dependence is restricted by the requirements that (1) it is well defined on the class of configuration maps from Ω to $\mathbb{S}^3/\mathcal{H}$ (residual symmetry) and (2) it is independent of arbitrary superposed rigid rotations (frame indifference). As an application of this representation, we then discuss some properties of the corresponding energy functional, including coercivity, lower semicontinuity and strong density of smooth maps. Other invariance properties are also considered. In the discussion, we take advantage of the identification of $\mathbb{S}^3$ with the Lie group of unit quaternions $Sp(1) \cong SU(2)$ and of the relations between quaternions and rotations in $\mathbb{R}^3$ and $\mathbb{R}^4$.

1 Introduction

A liquid crystal is a state of matter, called mesomorphic, intermediate between the crystal state and the liquid state, in which the molecules retain preferential orientations relative to one another over large distances [9]. There are many different types of liquid crystals, the main classes being nematics, cholesterics and smectics. In nematic liquid crystals the constituent rod-like molecules have a locally preferred direction.

According to the continuum description in the Landau–de Gennes theory [9, 24], the state of alignment of a nematic liquid crystal which occupies a region Ω is characterized, at each point x of Ω, by a symmetric traceless 3×3 matrix $\mathbf{Q}(x)$, the so-called tensor order parameter. By definition, $\mathbf{Q}$ vanishes in the isotropic phase and thus measures the extent to which the system is ordered in the region Ω. In a general nematic phase, the 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. A nematic phase is said biaxial when $\mathbf{Q}$ has three distinct eigenvalues, uniaxial when $\mathbf{Q}$ has two non-zero equal eigenvalues. While the existence of uniaxial nematics has been known for more than a century, the experimental evidence of biaxial nematic liquid crystals is only recent [20]. A general tensor order parameter $\mathbf{Q}$ can be written as

$$\mathbf{Q} = S_1\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big) + S_2\Big(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3}\mathbf{I}\Big), \quad S_1, S_2 \in \mathbb{R},\ \mathbf{n}, \mathbf{m} \in \mathbb{S}^2, \tag{1.1}$$

where $\mathbf{n}$, $\mathbf{m}$ are orthonormal eigenvectors of $\mathbf{Q}$ and S_1, S_2 are scalar order parameters given by $S_1 = \lambda_1 - \lambda_3 = 2\lambda_1 + \lambda_2$, $S_2 = \lambda_2 - \lambda_3 = \lambda_1 + 2\lambda_2$ in terms of the eigenvalues $\lambda_1, \lambda_2, \lambda_3$ of $\mathbf{Q}$. (Observe that a different numbering of the eigenvalues would lead to different S_1 and S_2.) In the uniaxial case, $\mathbf{Q}$ takes the form

$$\mathbf{Q} = s\Big(\mathbf{r} \otimes \mathbf{r} - \frac{1}{3}\mathbf{I}\Big), \quad s \in \mathbb{R},\ \mathbf{r} \in \mathbb{S}^2, \tag{1.2}$$

where s is the only scalar order parameter. A tensor order parameter $\mathbf{Q}$ can be visualized by a rectangular box which is built from the eigensystem of the tensor. The eigenvalues, suitably augmented by $\sqrt{(2/3)\,\mathrm{tr}(\mathbf{Q}^2)}$ to ensure positivity, can be used as the edge lengths of the box. For a uniaxial $\mathbf{Q}$ two edges have the same length, while for a biaxial $\mathbf{Q}$ all three edges are of different lengths. The Landau–de Gennes free-energy functional is a nonlinear integral functional of $\mathbf{Q}$ and its spatial derivatives. In general, it is required that any energy density $\Psi = \Psi(\mathbf{Q}, \nabla\mathbf{Q})$ satisfy the condition of *frame indifference* which amounts to

$$\Psi(\mathbf{Q}, \nabla\mathbf{Q}) = \Psi(M\mathbf{Q}M^T, \mathbf{D}^*) \qquad \forall M = (M^i_j) \in SO(3)\,, \tag{1.3}$$

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 $\mathbf{Q}_{ij,k} = \frac{\partial}{\partial x_k}\mathbf{Q}_{ij}$ denote the first order partial derivatives of $\mathbf{Q}$, compare e.g. [1].

A commonly used expression for the free energy of a biaxial nematic liquid crystal is [9, 24, 27]

$$\mathcal{F}(\mathbf{Q},\Omega) := \int_\Omega [\psi(\mathbf{Q},\nabla\mathbf{Q}) + f_B(\mathbf{Q})]\, dx\,, \tag{1.4}$$

where $f_B(\mathbf{Q}) = f_B(\mathrm{tr}(\mathbf{Q}^2), \mathrm{tr}(\mathbf{Q}^3))$ is the bulk free-energy density (a function of the principal invariants of $\mathbf{Q}$) and

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

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

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

where summation over repeated indices is assumed. The bulk energy $f_B(\mathbf{Q})$ is invariant under the $SO(3)$-action by conjugation on the five-dimensional space of $\mathbf{Q}$-tensors, so that the critical points of the bulk energy form an orbit of solutions in the five-dimensional space of $\mathbf{Q}$-tensors. In particular, the $SO(3)$-orbit corresponding to the general case of a biaxial minimizer is a 3-manifold, while in the special case corresponding to a uniaxial minimizer the orbit reduces to a 2-manifold (see Section 2). Clearly, a tensor order parameter taking values in a group orbit has constant scalar order parameters. Actually, in many applications, it suffices to work within the so-called *constrained Landau–de Gennes theory* in which the tensor order parameter $\mathbf{Q}$ is assumed to have constant scalar order parameters S_1 and S_2, and hence constant eigenvalues [3]. In the constrained theory, the bulk energy is constant and we only have to consider the elastic free energy.

In the constrained uniaxial case, when the order parameter is constant, the more common and popular *director* approach to continuum modeling can be used only on simply-connected domains (see [3] for the non simply-connected case). In this theory, often referred to as the Oseen–Frank theory [26, 13], a configuration of a uniaxial liquid crystal is described mathematically as a unitary vector field $\mathbf{r}(x)$ in Ω, referred to as the director, which represents the direction of preferred molecular alignment. In the Oseen-Frank model, the elastic energy associated to the configuration $\mathbf{r}$ is given by

$$\mathcal{E}(\mathbf{r},\Omega) := \int_\Omega w(\mathbf{r},\nabla\mathbf{r})\, dx\,. \tag{1.7}$$

The energy density $w(\mathbf{r},\nabla\mathbf{r})$ was derived by Oseen [26] on the basis of a molecular theory, and by Frank [13] as a consequence of Galilean invariance. This energy density satisfies the *invariance properties*

$$\begin{aligned} &w(\mathbf{r},\nabla\mathbf{r}) = w(-\mathbf{r},-\nabla\mathbf{r}), \\ &w(H\mathbf{r}, H\,\nabla\mathbf{r}\,H^T) = w(\mathbf{r},\nabla\mathbf{r}), \qquad \forall\, H \in O(3)\,, \end{aligned} \tag{1.8}$$

so that the functional (1.7) is well defined on vector fields in Ω, regardless of the orientation. The first equation in (1.8) accounts for the lack of polarity of nematics, while the second one expresses the frame indifference of the energy density and the condition of material symmetry corresponding to the lack of chirality of nematics. Requiring that the second line condition in (1.8) hold for the special orthogonal group only is equivalent to the frame indifference condition (1.3) for constrained uniaxial $\mathbf{Q}$-tensors (see Section 3). The director approach to continuum modeling has been further developed by Ericksen and Leslie [11, 18] in their hydrodynamic theory of nematic liquid crystals, which reduces to the Oseen–Frank theory in the static case. In the more recent *Ericksen theory* [12], also a spatially varying orientational order is taken into account, i.e., the state of the liquid crystal is described by a pair $(s,\mathbf{r}) \in \mathbb{R}\times\mathbb{S}^2$, depending on $x \in \Omega$.

However, although the director representation of uniaxial nematics is quite intuitive, it is not completely appropriate from a physical point of view as it does not respect the inversion symmetry, in which $\mathbf{r}$ and $-\mathbf{r}$ represent the same state. This means that the vector field $\mathbf{r}$ in the Oseen-Frank approach should actually take values in the projective plane $\mathbb{R}P^2$, obtained by identification of antipodal points in $\mathbb{S}^2$. This problem is overcome by the $\mathbf{Q}$-tensor approach as the representation (1.2) is invariant under the transformation $\mathbf{r} \mapsto -\mathbf{r}$.

A variational theory that takes into account the *lack of orientability* of $\mathbb{RP}^2$ is discussed by the first author in [25]. In particular, for any Sobolev map $u \in W^{1,2}(\Omega,\mathbb{RP}^2)$, where $\Omega \subset \mathbb{R}^3$ is a simply-connected domain, there exists, up to the action of an element of $\pi_1(\mathbb{R}P^2) = \mathbb{Z}_2$, a unique map $\mathbf{r} \in W^{1,2}(\Omega, \mathbb{S}^2)$ such that $u = \Pi \circ \mathbf{r}$, where $\Pi : \mathbb{S}^2 \to \mathbb{R}P^2$ is the canonical projection map. This lifting property was obtained in a more general setting and with different techniques by Bethuel and Chiron [5], who also showed that the property is no longer true for the Sobolev classes $W^{1,p}$, when $p < 2$.

The lifting problem has been studied using the $\mathbf{Q}$-tensor approach by Ball and Zarnescu in [3], where the orientability problem has been discussed also in the non simply-connected case. They also prove that the existence of a lifting of class $W^{1,2}$ implies the existence of a lifting for the *trace* on the boundary of Ω, in the corresponding fractional Sobolev space $W^{\frac{1}{2},2}$. As for non simply-connected two-dimensional domains, they specialized to the subclass of (1.2) where $\mathbf{r}$ has the third component identically zero. Such subclass of $\mathbf{Q}$-tensors is identified with the real projective line $\mathbb{R}P^1$. In this framework, they showed examples in which the minimum energy in the class of $W^{1,2}$ maps $\mathbf{Q}(\mathbf{r})$ is strictly lower than the minimum energy in the corresponding class $W^{1,2}(\Omega, \mathbb{S}^1)$.

In this paper we restrict ourselves to the constrained theory of biaxial nematic liquid crystals. Let $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ be the set of all $\mathbf{Q}$-tensors of the form (1.1) such that S_1, S_2 are constant, independent of $x \in \Omega$, ad assume that the three distinct eigenvalues $\lambda_1, \lambda_2, \lambda_3 \in (-\frac{1}{3}, \frac{2}{3})$ (see [2] for a discussion on the physical meaning of these constraints). Any element $\mathbf{Q} \in \mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ can be written in the form

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

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. We can then identify $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ with the homogeneous space $SO(3)/D_2$, where D_2 is the abelian four-element dihedral group. Using the 2:1 universal covering map $\Phi : \mathbb{S}^3 \cong Sp(1) \to SO(3)$, the order parameter space of constrained biaxial nematics is then diffeomorphic to the homogeneous manifold $\mathbb{S}^3/\mathcal{H}$, where $\mathcal{H}$ is the non-abelian eight-element quaternion group (see Section 2 for more details). In this model, a configuration of a biaxial nematic liquid crystal is described by a map from Ω to $\mathbb{S}^3/\mathcal{H}$.

In the constrained theory of uniaxial nematics, it is known that the Landau–de Gennes elastic free-energy density $\psi(\mathbf{Q}, \nabla\mathbf{Q})$ as given in (1.5) reduces to the Oseen–Frank energy density $w(\mathbf{r}, \nabla\mathbf{r})$, i.e., it is possible to choose the material constants L_i in order that $\psi(\mathbf{Q}, \nabla\mathbf{Q}) = w(\mathbf{r}, \nabla\mathbf{r})$ (see [3, 24] and also Section 4). In analogy to the uniaxial case, one purpose of this article is to express the Landau–de Gennes elastic free-energy density of biaxial nematics as a density on maps $q : \Omega \to \mathbb{S}^3$, whose functional dependence is restricted by requiring that it is well defined on the class of configuration maps into $\mathbb{S}^3/\mathcal{H}$ and is independent of arbitrary superposed rigid rotations. In our discussion, we will take advantage of the identification of $\mathbb{S}^3$ with the Lie group of unit quaternions $Sp(1) \cong SU(2)$ and of the relations between quaternions and rotations in $\mathbb{R}^3$ and $\mathbb{R}^4$.

In Section 3, for a generic energy density depending on a map $(u, \mathbf{v}) : \Omega \to \mathbb{S}^3 \subset \mathbb{R} \times \mathbb{R}^3$ and its first order derivatives, we introduce an invariance condition and prove that it is indeed equivalent to the frame indifference condition (1.3) for $\mathbf{Q}$-tensors. We then introduce an additional symmetry condition for this density which takes into account the *residual symmetry* (characterized by the group $\mathcal{H}$) of a constrained biaxial state. In the uniaxial case, it clearly corresponds to the first equation in (1.8).

In Section 4, working in the constrained biaxial case, we consider the simplest form of the elastic free-energy density,

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

which corresponds to the Dirichlet energy density $2s^2|\nabla\mathbf{r}|^2$ in the uniaxial case (1.2). The situation considered here can be regarded as a limit case of the unconstrained $\mathbf{Q}$-tensor theory, in the spirit of the analysis in [22] (see also [3]), where the limit $L \to 0$ for the the Landau–de Gennes free-energy functional

$$\mathcal{F}(\mathbf{Q}, \Omega) := \int_\Omega \left[\frac{L}{2}\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k} - \frac{a}{2}\operatorname{tr}(\mathbf{Q}^2) - \frac{b}{3}\operatorname{tr}(\mathbf{Q}^3) + \frac{1}{4}\operatorname{tr}(\mathbf{Q}^2)^2 \right] dx \tag{1.9}$$

is considered and referred to as “the Oseen–Frank limit” (in the formula above, a, b, c are temperature and material dependent constants and $L > 0$ is the elastic constant). If instead of a bulk free-energy density with only three terms one uses a bulk free-energy density truncated at the sixth order, e.g.,

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

where A, B, C, D, E and E' are material bulk constants (see, for instance, [8, 9]), then the theory considered here can be obtained as a limit theory for $L \to 0$ (and appropriate boundary conditions) and can then be regarded as a generalization to biaxial nematics of the limit theory in the sense of [22].

We express I_3 in terms of maps $(u, \mathbf{v}) : \Omega \to \mathbb{S}^3$, namely, we explicitly compute $f_3 : \mathbb{S}^3 \times \mathbb{M}_{4\times 3} \to [0, +\infty]$ so that

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

provided that $\mathbf{Q}$ corresponds to $(u, \mathbf{v})$, that is, $\mathbf{Q} = \mathbf{G}\mathbf{A}\mathbf{G}^T$ with $\mathbf{G} = \Phi((u, \mathbf{v}))$. (In principle, similar calculations can be performed also for the elastic invariants I_1, I_2 and I_4. In the final section, according to [28], we write these invariants in terms of the varying orthonormal frame $(\mathbf{n}, \mathbf{m}, \boldsymbol{\ell})$.)

In Section 5, we prove that the energy density model $f_3((u, \mathbf{v}), \nabla(u, \mathbf{v}))$ actually satisfies a general invariance property, that corresponds to the symmetry of the Dirichlet energy density $2s^2|\nabla\mathbf{r}|^2$ in the uniaxial case. Such an invariance property implies the above mentioned frame indifference and residual symmetry conditions. Therefore, f_3 may be interpreted as the elastic energy density model for the configuration maps $(u, \mathbf{v}) : \Omega \to \mathbb{S}^3/\mathcal{H}$ of a constrained biaxial nematic liquid crystal.

The corresponding elastic energy functional

$$
\mathcal{F}_3((u, \mathbf{v}), \Omega) := \int_\Omega f_3((u, \mathbf{v})(x), \nabla(u, \mathbf{v})(x))\, dx
$$

is well defined, e.g., on Sobolev maps $(u, \mathbf{v}) : \Omega \to \mathbb{S}^3/\mathcal{H}$, where Ω is a bounded domain of $\mathbb{R}^3$, i.e., a bounded connected open subset. Now, by ordering the eigenvalues as $\lambda_1 < \lambda_2 < \lambda_3$, with the notation from (1.1) we clearly have $S_1 < S_2 < 0$. Moreover, following [22] (see also Remark 2.6), we deduce that either

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

Using this and the invariance property, we are then able to prove that the energy density f_3 satisfies the following *coercivity* property:

$$
f_3((u, \mathbf{v}), \nabla(u, \mathbf{v})) \ge 8S^2|\nabla(u, \mathbf{v})|^2\,, \qquad \text{where} \quad S \ne 0\,.
$$

As a consequence, it is readily seen that *the class of measurable and a.e. weakly differentiable functions from Ω to $\mathbb{S}^3/\mathcal{H}$ with finite $\mathcal{F}_3$-energy agrees with the Sobolev class $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$.*

Now, since the second homotopy group $\pi_2(\mathbb{S}^3/\mathcal{H}) = 0$, as a consequence of the strong density result of Bethuel [4], it turns out that if the domain $\Omega \subset \mathbb{R}^3$ is bounded and simply connected, then *for each Sobolev map $w \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$ there exists a sequence of smooth maps $\{w_k\} \subset C^\infty(\Omega, \mathbb{S}^3/\mathcal{H})$ such that $w_k \to w$ strongly in $W^{1,2}$ and $\mathcal{F}_3(w_k) \to \mathcal{F}_3(w)$.* Moreover, we have that *the functional $\mathcal{F}_3$ is sequentially lower semicontinuous with respect to the weak $W^{1,2}$-topology in the class $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$.* This yields that no gap phenomenon occurs in the relaxation process, see Section 5. The proof uses the lifting result of Bethuel–Chiron [5, Theorem 1] asserting that if the domain Ω is bounded and simply connected, then for any exponent $p \ge 2$ and every Sobolev map $w \in W^{1,p}(\Omega, \mathbb{S}^3/\mathcal{H})$, there exists a Sobolev map $\widetilde{w} \in W^{1,p}(\Omega, \mathbb{S}^3)$ such that $\Pi \circ \widetilde{w} = w$, unique up to the action of an element of $\pi_1(\mathbb{S}^3/\mathcal{H}) = \mathcal{H}$, where $\Pi : \mathbb{S}^3 \to \mathbb{S}^3/\mathcal{H}$ is the canonical projection. Note that $\mathbb{S}^3/\mathcal{H}$ can be endowed with a unique Riemannian structure so that Π is a Riemannian covering map and that $\pi_1(\mathbb{S}^3/\mathcal{H}) = \mathcal{H}$ naturally acts by isometries on $\mathbb{S}^3$.

We conclude with some comments on the question of defects in our framework. It is well-known that in the Oseen-Frank theory, based on the classical Sobolev approach, when minimizing the energy among maps satisfying a zero degree boundary condition, only point defects with total degree equal to zero can be explained. Using the more geometric approach based on Cartesian currents [14, 15], see also [25], point defects connected by lines of concentration can be described. Within the Ginzburg–Landau theory, Chiron [7] was able to describe line defects (disclinations) in the uniaxial case. See also [16, 17, 19] for discussions on the configuration of liquid crystals and on the static and dynamic theories of defects. In the constrained biaxial case, our coercivity property and the triviality of the second homotopy group of $\mathbb{S}^3/\mathcal{H}$ suggest that the line singularities of biaxial nematics [23] cannot be described by means of Cartesian currents.

Acknowledgements. The authors wish to thank the referee for the many useful remarks and comments.

2 Preliminaries and notation: Q-tensors and order parameter spaces

To fix notation, we start by recalling some known facts about quaternions which will be used in our discussion, see [10]. Let $\mathbb{H}$ be the real non-commutative algebra of quaternions, with the standard basis $\{1, \mathsf{i}, \mathsf{j}, \mathsf{k}\}$. Multiplication is determined by the rules

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

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

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

The real part of q is q_0 and the pure quaternion part is $q_1\mathsf{i} + q_2\mathsf{j} + q_3\mathsf{k}$. The conjugate of q is given by $\bar{q} = q_0 - q_1\mathsf{i} - q_2\mathsf{j} - q_3\mathsf{k}$ 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 non-zero quaternion is $q^{-1} = \bar{q}/|q|^2$. As a vector space, $\mathbb{H}$ is identified with $\mathbb{R}^4$ via the usual isomorphism,

$$q = q_0 + q_1\mathsf{i} + q_2\mathsf{j} + q_3\mathsf{k} \longleftrightarrow (q_0, q_1, q_2, q_3)^T$$

which in turn induces an isomorphism between the subspace of pure quaternions and $\mathbb{R}^3$. In view of this isomorphism, when convenient, the elements $1, \mathsf{i}, \mathsf{j}, \mathsf{k}$ of $\mathbb{H}$ will be identified with the elements of the canonical basis $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ of $\mathbb{R}^4$, respectively. We will also make use of the decomposition $\mathbb{H} = \mathbb{R} \oplus \mathbb{R}^3 = \operatorname{span}\{1\} \oplus \operatorname{span}\{\mathsf{i}, \mathsf{j}, \mathsf{k}\}$ into the real and imaginary parts, and write $q = (q_0, \mathbf{q})$, where $\mathbf{q} := (q_1, q_2, q_3)$.

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

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

Let q be a unit quaternion and consider the $\mathbb{R}$-linear transformation $C_q : \mathbb{H} \to \mathbb{H}$, defined by $C_q(w) = qw\bar{q}$, for all $w \in \mathbb{H}$. The map C_q is an isometry, that is, $|C_q(w)| = |w|$, and preserves the decomposition $\mathbb{H} = \mathbb{R} \oplus \mathbb{R}^3$ of w into its 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, i.e., $M(q) \in O(4)$. The continuity of the determinant and the connectedness of $\mathbb{S}^3$ imply that the determinant of $M(q)$ is positive, so that $M(q) \in SO(4)$. The first column of $M(q)$ is the vector representing the quaternion $q1\bar{q} = q\bar{q} = 1$, that is, e_0. The fact that $M(q)$ belongs to $SO(4)$ now forces $M(q)$ to be of the form

$$M(q) = \begin{pmatrix} 1 & 0 \\ 0 & \Phi(q) \end{pmatrix}, \tag{2.1}$$

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

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

is a homomorphism of groups which is surjective and has kernel $\{\pm 1\}$ (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

$$\Phi(q) = \mathbf{G}(q_0, \mathbf{q}) := \begin{pmatrix} q_0^2 + q_1^2 - (q_2^2 + q_3^2) & 2(q_1q_2 - q_0q_3) & 2(q_1q_3 + q_0q_2) \\ 2(q_1q_2 + q_0q_3) & q_0^2 + q_2^2 - (q_1^2 + q_3^2) & 2(q_2q_3 - q_0q_1) \\ 2(q_1q_3 - q_0q_2) & 2(q_2q_3 + q_0q_1) & q_0^2 + q_3^2 - (q_1^2 + q_2^2) \end{pmatrix}. \tag{2.2}$$

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

$$\Phi(q) = \begin{pmatrix} u_1^2(1-\cos\theta)+\cos\theta & u_1u_2(1-\cos\theta)-u_3\sin\theta & u_1u_3(1-\cos\theta)+u_2\sin\theta \\ u_1u_2(1-\cos\theta)+u_3\sin\theta & u_2^2(1-\cos\theta)+\cos\theta & u_2u_3(1-\cos\theta)-u_1\sin\theta \\ u_1u_3(1-\cos\theta)-u_2\sin\theta & u_2u_3(1-\cos\theta)+u_1\sin\theta & u_3^2(1-\cos\theta)+\cos\theta \end{pmatrix}.$$

For future reference, we write the orthogonality conditions of $\mathbf{G} = \mathbf{G}(q_0, \mathbf{q})$,

$$\mathbf{G}^T\mathbf{G} = \mathbf{I}, \qquad \mathbf{G}\mathbf{G}^T = \mathbf{I}, \tag{2.3}$$

expressing, respectively, the orthonormality and the completeness of the column vectors of $\mathbf{G}$. We also record that

$$\Phi(\pm 1) = \mathbf{I}, \quad \Phi(\pm\mathsf{i}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \Phi(\pm\mathsf{j}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \Phi(\pm\mathsf{k}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2.4}$$

Remark 2.1 For any quaternion $q = q_0 + \mathsf{i}q_1 + \mathsf{j}q_2 + \mathsf{k}q_3$, let $L(q)$ and $R(q)$ denote the matrix representations of the real linear maps on $\mathbb{H}$ defined by $w \mapsto q\,w$ and $w \mapsto w\,\overline{q}$, relative to the standard basis $\{1, \mathsf{i}, \mathsf{j}, \mathsf{k}\}$. It follows that

$$L(q) = \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix}, \qquad R(q) = \begin{pmatrix} q_0 & q_1 & q_2 & q_3 \\ -q_1 & q_0 & -q_3 & q_2 \\ -q_2 & q_3 & q_0 & -q_1 \\ -q_3 & -q_2 & q_1 & q_0 \end{pmatrix}. \tag{2.5}$$

¿From the definition, one sees that $L(pq) = L(p)L(q)$, $R(pq) = R(p)R(q)$ and that the matrices $L(p)$ and $R(q)$ commute. It also follows that $L(\overline{q}) = L(q)^T$ and $R(\overline{q}) = R(q)^T$. So, if $|q| = 1$, $L(q)$ and $R(q)$ must be orthogonal matrices. One can verify by direct computation that these matrices have determinant one, i.e., belong to $SO(4)$. Moreover, in this case we have that $L(q)R(q) = M(q)$, where

$$M(q) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & q_0^2 + q_1^2 - (q_2^2 + q_3^2) & 2(q_1q_2 - q_0q_3) & 2(q_1q_3 + q_0q_2) \\ 0 & 2(q_1q_2 + q_0q_3) & q_0^2 + q_2^2 - (q_1^2 + q_3^2) & 2(q_2q_3 - q_0q_1) \\ 0 & 2(q_1q_3 - q_0q_2) & 2(q_2q_3 + q_0q_1) & q_0^2 + q_3^2 - (q_1^2 + q_2^2) \end{pmatrix}.$$

This means that for every $(q_0, \mathbf{q}) \in \mathbb{S}^3$, the matrix in (2.2) can be written in the form

$$G(q_0, \mathbf{q})^i_j = \sum_{\alpha=1}^{4} L((q_0, \mathbf{q}))^{i+1}_{\alpha} R((q_0, \mathbf{q}))^{\alpha}_{j+1} \qquad \forall\, i, j = 1, 2, 3.$$

In general, the 2:1 group homomorphism $\Phi : Sp(1) \to SO(3)$ is given, for every $q \in Sp(1)$, by

$$\Phi(q)^i_j = \sum_{\alpha=1}^{4} L(q)^{i+1}_{\alpha} R(q)^{\alpha}_{j+1} \qquad \forall\, i, j = 1, 2, 3. \tag{2.6}$$

Constrained theory of nematic liquid crystals. In the sequel, we shall think of vectors in $\mathbb{R}^3$ 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 $(\mathbf{n} \otimes \mathbf{m})^i_j = \mathbf{n}_i \mathbf{m}_j$, if $\mathbf{n} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)^T$, $\mathbf{m} = (\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)^T$. We shall also denote by $\mathbf{n} \cdot \mathbf{m}$ and $\mathbf{n} \times \mathbf{m}$ the scalar and vector products, respectively.

In the Landau–de Gennes approach to nematic liquid crystals [9, 24], the order parameter describing the orientational properties of molecules is a function that assigns to every point of the region $\Omega \subset \mathbb{R}^3$ occupied by the liquid crystal a traceless real symmetric 3×3-matrix $\mathbf{Q}$, the so-called $\mathbf{Q}$-*tensor order parameter*. A nematic liquid crystal is said to be in the (1) *isotropic* phase if $\mathbf{Q}$ has three equal eigenvalues, i.e. $\mathbf{Q} = 0$, (2) *uniaxial* phase if $\mathbf{Q}$ has two equal non-zero eigenvalues, (3) *biaxial* phase if $\mathbf{Q}$ has three distinct eigenvalues. By the spectral theorem, a generic biaxial $\mathbf{Q}$ can be written in the form [22, 24]

$$\mathbf{Q} = S_1\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big) + S_2\Big(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3}\mathbf{I}\Big), \tag{2.7}$$

where S_1, S_2 are scalar order parameters and $\mathbf{n}$, $\mathbf{m}$, and $\mathbf{n}\times\mathbf{m}$ are orthonormal eigenvectors of $\mathbf{Q}$ corresponding to the eigenvalues

$$\lambda_1 = \frac{2S_1 - S_2}{3}, \quad \lambda_2 = \frac{2S_2 - S_1}{3}, \quad \lambda_3 = -\frac{S_1 + S_2}{3}\,. \tag{2.8}$$

(We henceforth assume the ordering $\lambda_1 \le \lambda_2 \le \lambda_3$.) Equivalently, if $\mathbf{A} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ denotes the traceless diagonal matrix of the eigenvalues, the representation (2.7) of the symmetric matrix $\mathbf{Q}$ amounts to

$$\mathbf{Q} = \mathbf{G}\mathbf{A}\mathbf{G}^T\,, \tag{2.9}$$

for some rotation matrix $\mathbf{G} \in SO(3)$. 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

$$\mathbf{Q} = s\Big(\mathbf{r}\otimes\mathbf{r} - \frac{1}{3}\mathbf{I}\Big)\,, \tag{2.10}$$

where s is a scalar order parameter and $\mathbf{r} \in \mathbb{S}^2$. When $S_1 = S_2$, the uniaxial representation for $\mathbf{Q}$ is readily obtained from the completeness property of the eigenvectors, i.e.

$$\mathbf{n}\otimes\mathbf{n} + \mathbf{m}\otimes\mathbf{m} + \boldsymbol{\ell}\otimes\boldsymbol{\ell} = \mathbf{I}\,, \qquad \boldsymbol{\ell} := \mathbf{n}\times\mathbf{m} \in \mathbb{S}^2\,. \tag{2.11}$$

Remark 2.2 The eigenvalues of physical $\mathbf{Q}$-tensors are bounded by the inequalities $-\frac{1}{3} < \lambda_i < \frac{2}{3}$, $i = 1, 2, 3$ (see e.g. [2] for a thorough discussion on the physical constraints of the eigenvalues).

In the *constrained Landau–de Gennes theory* [3, 22, 23], 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 (2.8) are constant. In the constrained uniaxial case, according to (2.10), 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 (2.10), $\mathbf{Q}$ 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 $\mathbb{R}P^2$ (see Remark 2.5 below). In the constrained biaxial case, $\mathbf{Q}$ has instead three degrees of freedom, given, e.g., by the three Euler angles corresponding to the orthonormal frame $\mathbf{n}, \mathbf{m}, \boldsymbol{\ell}$. In the following, we discuss the constrained biaxial case in more detail.

Definition 2.3 *Let $\mathcal{S}_0$ denote the vector space of traceless symmetric 3×3 matrices over $\mathbb{R}$. For fixed distinct constants $\lambda_1, \lambda_2, \lambda_3 \in (-\frac{1}{3}, \frac{2}{3})$, ordered by $\lambda_1 < \lambda_2 < \lambda_3$, let $\mathbf{A} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$. The space $\mathcal{Q}(\lambda_1, \lambda_2, \lambda_3)$ of all elements of $\mathcal{S}_0$ of the form (2.7) so that (2.8) holds is known as the order parameter space of the system.*

By (2.9), we have

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

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

$$\mathbf{G}\star\mathbf{Q} := \mathbf{G}\mathbf{Q}\mathbf{G}^T, \quad \mathbf{G} \in SO(3),\ \mathbf{Q} \in \mathcal{S}_0, \tag{2.12}$$

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

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

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

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

(This is the dihedral group D_2 which consists of the identity and 180°-rotations about three mutually perpendicular axes.) Now, from the theory of homogeneous spaces [6, 29], we know that the coset space $SO(3)/SO(3)_{\mathbf{A}} = SO(3)/D_2$ can be given a structure of differentiable manifold, so that the bijective map

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

provides $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ with a differentiable structure with this map becoming a diffeomorphism. The coset space $SO(3)/D_2$ is an eightfold quotient of the 3-sphere. In fact, according to (2.4), the preimage of D_2 in $\mathbb{S}^3$ under the 2:1 group homomorphism $\Phi : \mathbb{S}^3 \cong Sp(1) \to SO(3)$ coincides with the non-abelian eight-element quaternion group $\mathcal{H} := \{\pm 1,\ \pm\mathsf{i},\ \pm\mathsf{j},\ \pm\mathsf{k}\}$. The parameter space $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ is thus diffeomorphic to the coset space $\mathbb{S}^3/\mathcal{H}$,

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

Remark 2.4 Note that $\mathbb{S}^3/\mathcal{H}$ can be endowed with a unique Riemannian structure so that the canonical projection $\Pi : \mathbb{S}^3 \to \mathbb{S}^3/\mathcal{H}$ is a Riemannian covering map. Moreover, since $\mathbb{S}^3$ is simply connected, Π is the universal covering map and $\pi_1(\mathbb{S}^3/\mathcal{H}) = \mathcal{H}$ acts isometrically on $\mathbb{S}^3$ (see for instance [30]).

According to formula (2.9), to any unit quaternion $(u,\mathbf{v}) \in \mathbb{S}^3$ there corresponds a tensor order parameter $\mathbf{Q}(u,\mathbf{v})$,

$$\mathbf{Q}(u,\mathbf{v}) = \mathbf{G}(u,\mathbf{v})\mathbf{A}\mathbf{G}(u,\mathbf{v})^T, \tag{2.13}$$

where $\mathbf{G} = \mathbf{G}(u,\mathbf{v})$ is given by (2.2). Using (2.3) and (2.8), we can write $\mathbf{Q}(u,\mathbf{v})$ as in (2.7), where

$$\mathbf{n}(u,\mathbf{v}) = G_1(u,\mathbf{v}) := \begin{pmatrix} u^2+v_1^2-(v_2^2+v_3^2) \\ 2(v_1v_2+uv_3) \\ 2(v_1v_3-uv_2) \end{pmatrix}, \quad \mathbf{m}(u,\mathbf{v}) = G_2(u,\mathbf{v}) := \begin{pmatrix} 2(v_1v_2-uv_3) \\ u^2+v_2^2-(v_1^2+v_3^2) \\ 2(v_2v_3+uv_1) \end{pmatrix} \tag{2.14}$$

and $\boldsymbol{\ell} = \mathbf{n}\times\mathbf{m}$ agrees with the third column $G_3(u,\mathbf{v})$ of the matrix in (2.2). Notice that if $\widetilde{\mathbf{G}} = \mathbf{G}\mathbf{B}$, where $\mathbf{B} = \Phi(q)$ for some $q \in \mathcal{H} = \{\pm 1,\ \pm\mathsf{i},\ \pm\mathsf{j},\ \pm\mathsf{k}\}$, then

$$\widetilde{\mathbf{G}}\mathbf{A}\widetilde{\mathbf{G}}^T = \mathbf{G}\mathbf{A}\mathbf{G}^T\,.$$

In fact, since $\mathbf{B} = \Phi(q) \in SO(3)_{\mathbf{A}}$, we have $\mathbf{B}\mathbf{A}\mathbf{B}^T = \mathbf{A}$, and hence $\widetilde{\mathbf{G}}\mathbf{A}\widetilde{\mathbf{G}}^T = \mathbf{G}\mathbf{B}\mathbf{A}\mathbf{B}^T\mathbf{G}^T = \mathbf{G}\mathbf{A}\mathbf{G}^T$. This implies that if $p = (u,\mathbf{v}) \in \mathbb{S}^3$, using quaternion product, one has

$$\mathbf{Q}(p) = \mathbf{Q}(p\,q) \quad \forall\, q \in \mathcal{H}\,.$$

Moreover, if $(\mathbf{n},\mathbf{m},\boldsymbol{\ell})$, where $\boldsymbol{\ell} = \mathbf{n}\times\mathbf{m}$, is the oriented frame corresponding to $\pm p$ as in (2.14), the oriented frames corresponding to $p\cdot q$ are $(\mathbf{n},-\mathbf{m},-\boldsymbol{\ell})$, $(-\mathbf{n},\mathbf{m},-\boldsymbol{\ell})$, and $(-\mathbf{n},-\mathbf{m},\boldsymbol{\ell})$, if $q = \mathsf{i},\mathsf{j}$, and k, respectively.

In conclusion, to each $\mathbf{Q} \in \mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ there corresponds a set of eight elements $(u,\mathbf{v}) \in \mathbb{S}^3$, a right coset of $\mathcal{H}$ in $\mathbb{S}^3 \cong Sp(1)$.

Remark 2.5 With reference to the left action of $SO(3)$ on $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ given by (2.12), if two of the eigenvalues $\lambda_1,\lambda_2,\lambda_3$ are equal, it easily seen that the isotropy subgroup of $\mathbf{A}$, $SO(3)_{\mathbf{A}}$, is isomorphic to the orthogonal group $O(2)$. (More precisely, $SO(3)_{\mathbf{A}}$ is the group D_∞ of rotations about the molecular axis and 180°-rotations about axes perpendicular to the molecular axis.) Thus $\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ is diffeomorphic to the coset space $SO(3)/O(2)$, which is just a coset space description of real projective plane $\mathbb{R}P^2$, the order parameter space in the constrained uniaxial case.

Remark 2.6 From (2.8) and the specific ordering $\lambda_1 < \lambda_2 < \lambda_3$ of the eigenvalues, in the representation (2.7), it follows that $S_1 < S_2 < 0$. Moreover, according to the analysis in the proof of Proposition 1 in [22], one can conclude indeed that either

$$\frac{S_1}{2} \le S_2 < 0 \quad \text{or} \quad S_2 \le \frac{S_1}{2} < 0\,. \tag{2.15}$$

In fact, using the notation from [22], condition $\lambda_1 < \lambda_2 < \lambda_3$ yields that R_2^- and R_3^+ are the only admissible regions. This will be used in the proof of Proposition 5.3 below.

3 Frame-indifference

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

$$\psi(\mathbf{Q},\nabla\mathbf{Q}) = \psi(M\mathbf{Q}M^T,\mathbf{D}^*) \qquad \forall M \in SO(3)\,, \tag{3.1}$$

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

$$\mathbf{Q}_{ij,k} = \frac{\partial}{\partial x_k} \mathbf{Q}_{ij} \,.$$

Remark 3.1 Note that the elastic free-energy densities I_1, I_2, I_3, I_4 as given in (1.6) satisfy the condition (3.1) for the full orthogonal group $O(3)$. This is a material symmetry reflecting the lack of chirality of the molecules constituting nematic liquid crystals (see [1]).

THE UNIAXIAL CASE. The above condition is equivalent to the well-known frame invariance

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

that is satisfied by an energy density in the framework of Oseen-Frank theory of uniaxial liquid crystals. In fact, in the (constrained) uniaxial case we have $\mathbf{Q} = s\Big(\mathbf{r} \otimes \mathbf{r} - \dfrac{1}{3}\mathbf{I}\Big)$, with s a non-zero constant and $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_2)^T \in \mathbb{S}^2$ varying with the position $x \in \Omega$, whence

$$\mathbf{Q}_{ij} = s\Big(\mathbf{r}_i \mathbf{r}_j - \frac{1}{3}\,\delta_{ij}\Big) \,, \qquad \mathbf{Q}_{ij,k} = s(\mathbf{r}_i \mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j) \,. \tag{3.2}$$

We first observe that $\mathbf{Q}(M\mathbf{r}) = M\mathbf{Q}(\mathbf{r})M^T$. Setting

$$\mathbf{D}_{ijk}(\mathbf{r}, H) := s(H^i_k \mathbf{r}_j + \mathbf{r}_i H^j_k) \,, \qquad \mathbf{r} \in \mathbb{S}^2, \quad H = (H^i_j) \in \mathbb{M}_{3\times 3} \,,$$

it suffices to check that

$$\mathbf{D}_{ijk}(M\mathbf{r}, MHM^T) = M^i_l M^j_m M^k_p \, \mathbf{D}_{lmp}(\mathbf{r}, H) \,,$$

or, equivalently, if $\mathbf{D}_k$ is the 3×3 matrix with coefficients $(\mathbf{D}_k)^i_j = \mathbf{D}_{ijk}$, that

$$\mathbf{D}_k(M\mathbf{r}, MHM^T) = MM^k_p \mathbf{D}_p(\mathbf{r}, H) M^T.$$

Let H_j denote the jth column of H. By a direct computation,

$$\begin{aligned}
\mathbf{D}_k(M\mathbf{r}, MHM^T) &= s\left[(MHM^T)_k (M\mathbf{r})^T + M\mathbf{r}((MHM^T)_k)^T\right] \\
&= s\left[MM^k_p H_p \mathbf{r}^T M^T + M\mathbf{r}(H_p)^T M^k_p M^T\right] \\
&= s\left[MM^k_p H_p \mathbf{r}^T M^T + MM^k_p \mathbf{r}(H_p)^T M^T\right] \\
&= s\, MM^k_p \left[H_p \mathbf{r}^T + \mathbf{r}(H_p)^T\right] M^T = MM^k_p \mathbf{D}_p M^T,
\end{aligned}$$

as required.

THE BIAXIAL CASE. We now show that an equivalent property holds true for an energy density f in the framework of constrained biaxial liquid crystals. Let $\Phi : \mathbb{S}^3 \to SO(3)$ denote the 2:1 group homomorphism introduced in Section 2.

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

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

where $L(q)$ *is as in Remark 2.1 and* $\Phi(q)$ *is as in* (2.2).

Theorem 3.3 *For constrained biaxial nematics, the frame invariance condition of Definition* 3.2 *is equivalent to the frame invariance* (3.1) *in the sense of* $\mathbf{Q}$*-tensors.*

To prove Theorem 3.3, for each function $w(x) : \Omega \to \mathbb{S}^3$ we set

$$\widetilde{\mathbf{Q}}_{ij}(w) := (L(w)R(w)\widetilde{\mathbf{A}}R(w)^T L(w)^T)^i_j \,, \qquad i, j = 0, 1, 2, 3 \,,$$

where we have denoted $\widetilde{\mathbf{A}} := \mathrm{diag}(\widetilde{\lambda}_0, \widetilde{\lambda}_1, \widetilde{\lambda}_2, \widetilde{\lambda}_3) \in \mathbb{M}_{4\times 4}$, with $\widetilde{\lambda}_0 := 0$ and $\widetilde{\lambda}_i := \lambda_i$ for $i = 1, 2, 3$. Notice that $\widetilde{\mathbf{Q}}_{ij}(w) = 0$ if $i = 0$ or $j = 0$, and $\widetilde{\mathbf{Q}}_{ij}(w) = \mathbf{Q}_{ij}(w)$ otherwise, where $\mathbf{Q}(w)$ is defined as in (2.13). By linearity, we thus compute

$$\begin{aligned} \frac{\partial}{\partial x_k}\widetilde{\mathbf{Q}}_{ij}(w) &= (L(\nabla_k w)R(w)\widetilde{\mathbf{A}}R(w)^T L(w)^T)^i_j + (L(w)R(\nabla_k w)\widetilde{\mathbf{A}}R(w)^T L(w)^T)^i_j \\ &\quad + (L(w)R(w)\widetilde{\mathbf{A}}R(\nabla w_k)^T L(w)^T)^i_j + (L(w)R(w)\widetilde{\mathbf{A}}R(w)^T L(\nabla_k w)^T)^i_j\,. \end{aligned} \tag{3.3}$$

Identifying the gradient ∇w with a 4×4-matrix $\widetilde{H} = (H_0, H_1, H_2, H_3)$, where $H_0 \equiv 0$ and $H_k = \nabla_k w$ for $k = 1, 2, 3$, for each $(w, \widetilde{H}) \in \mathbb{S}^3 \times \mathbb{M}_{4\times 4}$, we are led to define

$$\begin{aligned} \widetilde{\mathbf{D}}_{ijk}(w, \widetilde{H}) &:= \big(L(H_k)R(w)\widetilde{\mathbf{A}}R(w)^T L(w)^T + L(w)R(H_k)\widetilde{\mathbf{A}}R(w)^T L(w)^T \\ &\quad + L(w)R(w)\widetilde{\mathbf{A}}R(H_k)^T L(w)^T + L(w)R(w)\widetilde{\mathbf{A}}R(w)^T L(H_k)^T\big)^i_j\,, \end{aligned} \tag{3.4}$$

where $i, j, k = 0, 1, 2, 3$. To our purposes, it then suffices to prove the following.

Proposition 3.4 *With the previous notation, for every $q \in \mathbb{S}^3$ we have*

$$\widetilde{\mathbf{D}}_{ijk}(qw, L(q)\widetilde{H}M(q)^T) = M^i_l(q)M^j_m(q)M^k_p(q)\,\widetilde{\mathbf{D}}_{lmp}(w, \widetilde{H})\,,$$

where $M(q) = L(q)R(q)$.

In fact, $\widetilde{\mathbf{D}}_{ijk}(w, \widetilde{H}) \equiv 0$ if $i = 0$ or $j = 0$ or $k = 0$. Since property (2.6) yields $M(q) = \begin{pmatrix} 1 & 0 \\ 0 & \Phi(q) \end{pmatrix}$,

$$\mathbf{Q}(qw) = \Phi(q)\mathbf{Q}(w)\Phi(q)^T \iff \widetilde{\mathbf{Q}}(qw) = M(q)\widetilde{\mathbf{Q}}(w)M(q)^T.$$

This combined with Proposition 3.4 implies Theorem 3.3.

Proof of Proposition 3.4: We divide the proof into two steps.

Step 1: We first collect some useful formulas.

Lemma 3.5 *For every $q, w \in \mathbb{R}^4$, we have:*

$$L(L(q)w) = L(q)L(w)\,, \quad R(L(q)w) = R(q)R(w)\,, \quad L(q)R(w) = R(w)L(q)\,.$$

Moreover, for matrices $H, M \in \mathbb{M}_{4\times 4}$, let $(HM)_k$ denote the kth column vector of the matrix HM. Then,

$$L((HM)_k) = L(HM_k) = M^h_k L(H_h)\,, \quad R((HM)_k) = R(HM_k) = M^h_k R(H_h)\,.$$

As a consequence, we have:

$$L(L(q)H(M(q)^T)_k) = M(q)^k_h L(q)L(H_h)\,, \quad R(L(q)H(M(q)^T)_k) = M(q)^k_h R(q)R(H_h)\,.$$

Proof: The equations in the first centered line follow from the definition of the matrices $L(q)$ and $R(q)$. Moreover, denoting by $(\mathbf{e}_0, \ldots, \mathbf{e}_3)$ the column vectors of the canonical basis in $\mathbb{R}^4$, we have

$$(HM)_k = HM_k = H^i_h M^h_k \mathbf{e}_i = M^h_k H^i_h \mathbf{e}_i = M^h_k H_h$$

and hence, by linearity, we deduce the formulas in the second line. The last two formulas are obtained by using the equations in the first and then in the second line. □

Step 2: Denote by $\widetilde{\mathbf{D}}_k \in \mathbb{M}_{4\times 4}$ the symmetric matrix with coefficients $(\widetilde{\mathbf{D}}_k)^i_j := \widetilde{\mathbf{D}}_{ijk}$. Then the claim is equivalent to the formula

$$\widetilde{\mathbf{D}}_k(qw, L(q)\widetilde{H}M(q)^T) = M(q)^k_h M(q)\widetilde{\mathbf{D}}_h(w, \widetilde{H})M(q)^T\,, \tag{3.5}$$

by replacing h with p. By (3.4), we have

$$\begin{aligned}\widetilde{\mathbf{D}}_k(qw, L(q)\widetilde{H}M(q)^T) &= L(L(q)\widetilde{H}(M(q)^T)_k)R(qw)\widetilde{\mathbf{A}}R(qw)^T L(qw)^T \\ &\quad + L(qw)R(L(q)\widetilde{H}(M(q)^T)_k)\widetilde{\mathbf{A}}R(qw)^T L(qw)^T \\ &\quad + L(qw)R(qw)\widetilde{\mathbf{A}}R(L(q)\widetilde{H}(M(q)^T)_k)^T L(qw)^T \\ &\quad + L(qw)R(qw)\widetilde{\mathbf{A}}R(qw)^T L(L(q)\widetilde{H}(M(q)^T)_k)^T .\end{aligned}$$

According to Lemma 3.5 and by the linearity of $p \mapsto L(p)$ and $p \mapsto R(p)$, we get

$$\begin{aligned}\widetilde{\mathbf{D}}_k(qw, L(q)\widetilde{H}M(q)^T) &= M(q)^k_h L(q)L(H_h)R(q)R(w)\widetilde{\mathbf{A}}M(w)^T M(q)^T \\ &\quad + L(q)L(w)M(q)^k_h R(q)R(H_h)\widetilde{\mathbf{A}}M(w)^T M(q)^T \\ &\quad + M(q)M(w)\widetilde{\mathbf{A}}[M(q)^k_h R(q)R(H_h)]^T L(w)^T L(q)^T \\ &\quad + M(q)M(w)\widetilde{\mathbf{A}}R(w)^T R(q)^T [M(q)^k_h L(q)L(H_h)]^T \\ &= M(q)^k_h M(q)L(H_h)R(w)\widetilde{\mathbf{A}}M(w)^T M(q)^T \\ &\quad + M(q)^k_h M(q)L(w)R(H_h)\widetilde{\mathbf{A}}M(w)^T M(q)^T \\ &\quad + M(q)^k_h M(q)M(w)\widetilde{\mathbf{A}}[M(q)L(w)R(H_h)]^T \\ &\quad + M(q)^k_h M(q)M(w)\widetilde{\mathbf{A}}[M(q)L(H_h)R(w)]^T ,\end{aligned}$$

from which follows

$$\begin{aligned}\widetilde{\mathbf{D}}_k(qw, L(q)\widetilde{H}M(q)^T) = M(q)^k_h M(q)\big\{&L(H_h)R(w)\widetilde{\mathbf{A}}M(w)^T + L(w)R(H_h)\widetilde{\mathbf{A}}M(w)^T \\ &+ M(w)\widetilde{\mathbf{A}}R(H_h)^T L(w)^T + M(w)\widetilde{\mathbf{A}}R(w)^T L(H_h)^T\big\}M(q)^T,\end{aligned}$$

that is (3.5), as claimed. □

Residual symmetry. In order to deal with a functional defined on maps taking values in the coset space $\mathbb{S}^3/\mathcal{H}$, where $\mathcal{H} = \{\pm 1, \pm \mathsf{i}, \pm \mathsf{j}, \pm \mathsf{k}\}$, we also introduce the following symmetry condition.

Definition 3.6 *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*

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

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.

Remark 3.7 Note that the two conditions in Definition 3.2 and 3.6 are necessary conditions 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. In Section 5, we will introduce an energy density, f_3, which satisfies both the invariance and the symmetry properties in the sense of Definitions 3.2 and 3.6 (see Proposition 5.1).

4 The elastic energy density

In a special case of the Landau–de Gennes theory, compare e.g. [3, 24], the elastic energy density is defined by

$$\psi(\mathbf{Q}, \nabla\mathbf{Q}) = L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4 \tag{4.1}$$

where the L_i are constant and the four elastic invariants I_i are

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

The uniaxial case. In the (constrained) uniaxial case we have (3.2). For the sake of completeness, we now recover the well-known related formulas.

Proposition 4.1 *In the constrained uniaxial case* (3.2)*, we have*

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

PROOF: We first recall that $\mathbf{r}_i\mathbf{r}_i = 1$, so that $\mathbf{r}_i\mathbf{r}_{i,\alpha} = 0$ for each i,α. Moreover,

$$\begin{array}{rcl} |\operatorname{curl}\mathbf{r}|^2 &=& (\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 + |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2\,,\\ |\nabla\mathbf{r}|^2 &=& \operatorname{tr}[(\nabla\mathbf{r})^2] + |\operatorname{curl}\mathbf{r}|^2\,,\\ |\nabla\mathbf{r}|^2 &=& \operatorname{tr}[(\nabla\mathbf{r})^2] + (\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 + |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2\,. \end{array} \tag{4.2}$$

In fact, one has

$$\begin{array}{rcl} \operatorname{curl}\mathbf{r} &=& (a_{32}, a_{13}, a_{21})\,, \qquad a_{ij} := (\mathbf{r}_{i,j} - \mathbf{r}_{j,i})\,,\\ |\operatorname{curl}\mathbf{r}|^2 &=& a_{32}^2 + a_{13}^2 + a_{21}^2\,,\\ (\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 &=& (\mathbf{r}_1 a_{32} + \mathbf{r}_2 a_{13} + \mathbf{r}_3 a_{21})^2\,,\\ \mathbf{r}\times\operatorname{curl}\mathbf{r} &=& (\mathbf{r}_2 a_{21} - \mathbf{r}_3 a_{13}, \mathbf{r}_3 a_{32} - \mathbf{r}_1 a_{21}, \mathbf{r}_1 a_{13} - \mathbf{r}_2 a_{32})\\ |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2 &=& (\mathbf{r}_1 a_{13} - \mathbf{r}_2 a_{32})^2 + (\mathbf{r}_1 a_{21} - \mathbf{r}_3 a_{32})^2 + (\mathbf{r}_2 a_{21} - \mathbf{r}_3 a_{13})^2\,. \end{array}$$

On the other hand,

$$\begin{array}{rcl} |\operatorname{curl}\mathbf{r}|^2 - (\mathbf{r}\cdot\operatorname{curl}\mathbf{r})^2 &=& (1-\mathbf{r}_1^2)a_{32}^2 + (1-\mathbf{r}_2^2)a_{13}^2 + (1-\mathbf{r}_3^2)a_{21}^2\\ && -2(\mathbf{r}_1\mathbf{r}_2 a_{32}a_{13} + \mathbf{r}_1\mathbf{r}_3 a_{32}a_{21} + \mathbf{r}_2\mathbf{r}_3 a_{13}a_{21})\\ &=& (\mathbf{r}_2^2+\mathbf{r}_3^2)a_{32}^2 + (\mathbf{r}_1^2+\mathbf{r}_3^2)a_{13}^2 + (\mathbf{r}_1^2+\mathbf{r}_2^2)a_{21}^2\\ && -2(\mathbf{r}_1\mathbf{r}_2 a_{32}a_{13} + \mathbf{r}_1\mathbf{r}_3 a_{32}a_{21} + \mathbf{r}_2\mathbf{r}_3 a_{13}a_{21})\\ &=& (\mathbf{r}_1 a_{13} - \mathbf{r}_2 a_{32})^2 + (\mathbf{r}_1 a_{21} - \mathbf{r}_3 a_{32})^2 + (\mathbf{r}_2 a_{21} - \mathbf{r}_3 a_{13})^2\,, \end{array}$$

that gives the first equality in (4.2). Also,

$$\begin{array}{rcl} \operatorname{tr}[(\nabla\mathbf{r})^2] &=& \mathbf{r}_{k,j}\mathbf{r}_{j,k} = \mathbf{r}_{1,1}^2 + \mathbf{r}_{2,2}^2 + \mathbf{r}_{3,3}^2 + 2(\mathbf{r}_{1,2}\mathbf{r}_{2,1} + \mathbf{r}_{1,3}\mathbf{r}_{3,1} + \mathbf{r}_{2,3}\mathbf{r}_{3,2})\\ |\operatorname{curl}\mathbf{r}|^2 &=& \mathbf{r}_{1,2}^2 + \mathbf{r}_{2,1}^2 + \mathbf{r}_{1,3}^2 + \mathbf{r}_{3,1}^2 + \mathbf{r}_{2,3}^2 + \mathbf{r}_{3,2}^2 - 2(\mathbf{r}_{1,2}\mathbf{r}_{2,1} + \mathbf{r}_{1,3}\mathbf{r}_{3,1} + \mathbf{r}_{2,3}\mathbf{r}_{3,2}) \end{array} \tag{4.3}$$

hence the second equality in (4.2) holds by summation, whereas the third one is a direct consequence.

Remark 4.2 Using that $\mathbf{r}_i\mathbf{r}_{i,\alpha} = 0$, one also obtains

$$\mathbf{r}_1 a_{13} - \mathbf{r}_2 a_{32} = -(\nabla\mathbf{r})^3\mathbf{r}\,, \quad \mathbf{r}_3 a_{32} - \mathbf{r}_1 a_{21} = -(\nabla\mathbf{r})^2\mathbf{r}\,, \quad \mathbf{r}_2 a_{21} - \mathbf{r}_3 a_{13} = -(\nabla\mathbf{r})^1\mathbf{r}\,,$$

where we have denoted $(\nabla\mathbf{r})^i\mathbf{r} := \mathbf{r}_k\mathbf{r}_{i,k}$, so that

$$\mathbf{r}_l\mathbf{r}_k\mathbf{r}_{i,l}\mathbf{r}_{i,k} = \sum_{i=1}^{3}\big((\nabla\mathbf{r})^i\mathbf{r}\big)^2 = |\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2\,. \tag{4.4}$$

As for the first energy term, using that $\mathbf{r}_i\mathbf{r}_i = 1$ and $\mathbf{r}_i\mathbf{r}_{i,\alpha} = 0$, we have

$$\begin{array}{rcl} I_1 &=& s^2(\mathbf{r}_i\mathbf{r}_{j,j} + \mathbf{r}_{i,j}\mathbf{r}_j)(\mathbf{r}_i\mathbf{r}_{k,k} + \mathbf{r}_{i,k}\mathbf{r}_k)\\ &=& s^2(\mathbf{r}_i\mathbf{r}_i\mathbf{r}_{j,j}\mathbf{r}_{k,k} + \mathbf{r}_j\mathbf{r}_k\mathbf{r}_{i,j}\mathbf{r}_{i,k} + (\mathbf{r}_i\mathbf{r}_{i,k})\mathbf{r}_k\mathbf{r}_{j,j} + (\mathbf{r}_i\mathbf{r}_{i,j})\mathbf{r}_j\mathbf{r}_{k,k})\\ &=& s^2(\mathbf{r}_{j,j}\mathbf{r}_{k,k} + \mathbf{r}_j\mathbf{r}_k\mathbf{r}_{i,j}\mathbf{r}_{i,k})\,, \end{array}$$

so that the above formula follows from (4.4) and from the equality $\mathbf{r}_{j,j}\mathbf{r}_{k,k} = (\operatorname{div}\mathbf{r})^2$.

For the second energy term, we similarly compute

$$\begin{array}{rcl} I_2 &=& s^2(\mathbf{r}_i\mathbf{r}_{k,j} + \mathbf{r}_{i,j}\mathbf{r}_k)(\mathbf{r}_i\mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j)\\ &=& s^2(\mathbf{r}_i\mathbf{r}_i\mathbf{r}_{k,j}\mathbf{r}_{j,k} + \mathbf{r}_j\mathbf{r}_k\mathbf{r}_{i,j}\mathbf{r}_{i,k} + (\mathbf{r}_i\mathbf{r}_{i,k})\mathbf{r}_j\mathbf{r}_{k,j} + (\mathbf{r}_i\mathbf{r}_{i,j})\mathbf{r}_k\mathbf{r}_{j,k})\\ &=& s^2(\mathbf{r}_{k,j}\mathbf{r}_{j,k} + \mathbf{r}_j\mathbf{r}_k\mathbf{r}_{i,j}\mathbf{r}_{i,k})\,, \end{array}$$

and then use the first equality in (4.3) and again (4.4).

The third energy term similarly reads as

$$\begin{aligned} I_3 &= s^2(\mathbf{r}_i\mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j)(\mathbf{r}_i\mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j) \\ &= s^2(\mathbf{r}_i\mathbf{r}_i\mathbf{r}_{j,k}\mathbf{r}_{j,k} + \mathbf{r}_j\mathbf{r}_j\mathbf{r}_{i,k}\mathbf{r}_{i,k} + 2(\mathbf{r}_i\mathbf{r}_{i,k})\mathbf{r}_j\mathbf{r}_{j,k}) \\ &= 2s^2\mathbf{r}_{j,k}\mathbf{r}_{j,k}\,, \end{aligned}$$

so that this time we use that $\mathbf{r}_{j,k}\mathbf{r}_{j,k} = |\nabla\mathbf{r}|^2$ and the third equality in (4.2).

Finally, we decompose the fourth term as $I_4 = I_4^1 + I_4^2$, where

$$\begin{aligned} I_4^1 &:= s^3\mathbf{r}_l\mathbf{r}_k(\mathbf{r}_i\mathbf{r}_{j,l} + \mathbf{r}_{i,l}\mathbf{r}_j)(\mathbf{r}_i\mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j)\,, \\ I_4^2 &:= -\frac{1}{3}s^3\delta_{lk}(\mathbf{r}_i\mathbf{r}_{j,l} + \mathbf{r}_{i,l}\mathbf{r}_j)(\mathbf{r}_i\mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j) = -\frac{1}{3}s^3(\mathbf{r}_i\mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j)(\mathbf{r}_i\mathbf{r}_{j,k} + \mathbf{r}_{i,k}\mathbf{r}_j)\,. \end{aligned}$$

Similarly to as for I_3, we get $I_4^2 = -\dfrac{2}{3}s^3\,|\nabla\mathbf{r}|^2$, whereas

$$\begin{aligned} I_4^1 &= s^3\mathbf{r}_l\mathbf{r}_k(\mathbf{r}_i\mathbf{r}_i\mathbf{r}_{j,l}\mathbf{r}_{j,k} + \mathbf{r}_j\mathbf{r}_j\mathbf{r}_{i,l}\mathbf{r}_{i,k} + (\mathbf{r}_i\mathbf{r}_{i,k})\mathbf{r}_j\mathbf{r}_{j,l} + (\mathbf{r}_i\mathbf{r}_{i,l})\mathbf{r}_j\mathbf{r}_{j,k}) \\ &= 2s^3\mathbf{r}_l\mathbf{r}_k\mathbf{r}_{\alpha,l}\mathbf{r}_{\alpha,k}\,, \end{aligned}$$

so that (4.4) gives $I_4^1 = 2s^3|\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2$. Adding the two terms, we obtain

$$I_4 = 2s^3\big(|\mathbf{r}\times\operatorname{curl}\mathbf{r}|^2 - \frac{1}{3}|\nabla\mathbf{r}|^2\big)\,,$$

and hence the formula for I_4 follows from the third equality in (4.2). □

As a consequence, compare [3], choosing

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

by Proposition 4.1 we deduce that the energy density $\psi(\mathbf{Q},\nabla\mathbf{Q})$ in (4.1) agrees with the Oseen-Frank energy density $w(\mathbf{r},\nabla\mathbf{r})$ of *nematic liquid crystals*:

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

We finally recall that the last energy term of $w(\mathbf{r},\nabla\mathbf{r})$ is a null-Lagrangian, as

$$\big[\operatorname{tr}[(\nabla\mathbf{r})^2] - (\operatorname{div}\mathbf{r})^2\big] = \operatorname{div}[(\nabla\mathbf{r})\mathbf{r} - (\operatorname{div}\mathbf{r})\mathbf{r})]\,.$$

THE BIAXIAL CASE. In the (constrained) biaxial case, we have (2.7), where $S_1 \neq S_2$ are non-zero constants and $\mathbf{n}$, $\mathbf{m}\in\mathbb{S}^2$ satisfy $\mathbf{n}\cdot\mathbf{m} = 0$ and depend on the position $x\in\Omega$, see Definition 2.3.

We shall focus on the third elastic invariant

$$I_3(\mathbf{Q},\nabla\mathbf{Q}) := \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}\,. \tag{4.5}$$

Using (2.11), we have that

$$\mathbf{Q} = \lambda_1\mathbf{n}\otimes\mathbf{n} + \lambda_2\mathbf{m}\otimes\mathbf{m} + \lambda_3\boldsymbol{\ell}\otimes\boldsymbol{\ell}\,, \tag{4.6}$$

with $\lambda_1,\lambda_2,\lambda_3$ as in (2.8), hence

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

Proposition 4.3 *Under the previous hypotheses, we have*

$$I_3(\mathbf{Q},\nabla\mathbf{Q}) = 2(2\lambda_1^2 + \lambda_2\lambda_3)|\nabla\mathbf{n}|^2 + 2(2\lambda_2^2 + \lambda_3\lambda_1)|\nabla\mathbf{m}|^2 + 2(2\lambda_3^2 + \lambda_1\lambda_2)|\nabla\boldsymbol{\ell}|^2\,.$$

PROOF: We first decompose $I_3 = I_3^1 + I_3^2 + I_3^3 + I_3^4 + I_3^5 + I_3^6$, where

$$\begin{array}{rcl} I_3^1 &=& \lambda_1^2(\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_{i,k}\mathbf{n}_j)(\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_{i,k}\mathbf{n}_j)\,, \\ I_3^2 &=& \lambda_2^2(\mathbf{m}_i\mathbf{m}_{j,k} + \mathbf{m}_{i,k}\mathbf{m}_j)(\mathbf{m}_i\mathbf{m}_{j,k} + \mathbf{m}_{i,k}\mathbf{m}_j)\,, \\ I_3^3 &=& \lambda_3^2(\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_j)(\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_j)\,, \\ I_3^4 &=& 2\lambda_1\lambda_2(\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_{i,k}\mathbf{n}_j)(\mathbf{m}_i\mathbf{m}_{j,k} + \mathbf{m}_{i,k}\mathbf{m}_j)\,, \\ I_3^5 &=& 2\lambda_2\lambda_3(\mathbf{m}_i\mathbf{m}_{j,k} + \mathbf{m}_{i,k}\mathbf{m}_j)(\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_j)\,, \\ I_3^6 &=& 2\lambda_3\lambda_1(\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_j)(\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_{i,k}\mathbf{n}_j)\,. \end{array}$$

Arguing exactly as in Proposition 4.1, we get

$$I_3^1 = 2\lambda_1^2|\nabla\mathbf{n}|^2\,, \qquad I_3^2 = 2\lambda_2^2|\nabla\mathbf{m}|^2\,, \qquad I_3^3 = 2\lambda_3^2|\nabla\boldsymbol{\ell}|^2\,,$$

compare the third equality in (4.2). As for the fourth term, using that $\mathbf{n}_i\mathbf{m}_i = 0$, we get

$$\begin{array}{rcl} I_3^4 &=& 2\lambda_1\lambda_2(\mathbf{n}_i\mathbf{m}_i\mathbf{n}_{j,k}\mathbf{m}_{j,k} + \mathbf{n}_j\mathbf{m}_j\mathbf{n}_{i,k}\mathbf{m}_{i,k} + \mathbf{n}_i\mathbf{m}_j\mathbf{n}_{j,k}\mathbf{m}_{i,k} + \mathbf{n}_j\mathbf{m}_i\mathbf{n}_{i,k}\mathbf{m}_{j,k}) \\ &=& 4\lambda_1\lambda_2\mathbf{n}_i\mathbf{m}_j\mathbf{n}_{j,k}\mathbf{m}_{i,k}\,. \end{array}$$

In a similar way, we have:

$$I_3^5 = 4\lambda_2\lambda_3\mathbf{m}_i\boldsymbol{\ell}_j\mathbf{m}_{j,k}\boldsymbol{\ell}_{i,k}\,, \qquad I_3^6 = 4\lambda_3\lambda_1\boldsymbol{\ell}_i\mathbf{n}_j\boldsymbol{\ell}_{j,k}\mathbf{n}_{i,k}\,.$$

Denoting for simplicity

$$\begin{array}{c} X := (\mathbf{n}_i\mathbf{n}_{j,k})\mathbf{m}_j\mathbf{m}_{i,k}\,, \quad Y := (\mathbf{m}_i\mathbf{m}_{j,k})\boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k}\,, \quad Z := (\boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k})\mathbf{n}_j\mathbf{n}_{i,k}\,, \\ N := \mathbf{n}_{i,k}\mathbf{n}_{i,k}\,, \quad M := \mathbf{m}_{i,k}\mathbf{m}_{i,k}\,, \quad L := \boldsymbol{\ell}_{i,k}\boldsymbol{\ell}_{i,k}\,, \end{array}$$

we deduce the formulas:

$$X = \frac{1}{2}(L - M - N)\,, \quad Y = \frac{1}{2}(N - L - M)\,, \quad Z = \frac{1}{2}(M - N - L)\,. \tag{4.7}$$

In fact, the property (2.11) yields that for each i, j, k

$$\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_j\mathbf{n}_{i,k} + \mathbf{m}_i\mathbf{m}_{j,k} + \mathbf{m}_j\mathbf{m}_{i,k} + \boldsymbol{\ell}_i\boldsymbol{\ell}_{j,k} + \boldsymbol{\ell}_j\boldsymbol{\ell}_{i,k} = 0\,. \tag{4.8}$$

Replacing the parenthesis in X, Y, and Z with the corresponding sum of five terms coming from equation (4.8), and using that $(\mathbf{n}, \mathbf{m}, \boldsymbol{\ell})$ is an orthonormal frame, we readily obtain the system

$$\left\{ \begin{array}{l} X = -M - Y \\ Y = -L - Z \\ Z = -N - X \end{array} \right.$$

the solution of which gives (4.7). Using that

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

we thus obtain

$$\begin{array}{l} I_3^4 = 2\lambda_1\lambda_2(|\nabla\boldsymbol{\ell}|^2 - |\nabla\mathbf{m}|^2 - |\nabla\mathbf{n}|^2)\,, \\ I_3^5 = 2\lambda_2\lambda_3(|\nabla\mathbf{n}|^2 - |\nabla\boldsymbol{\ell}|^2 - |\nabla\mathbf{m}|^2)\,, \\ I_3^6 = 2\lambda_3\lambda_1(|\nabla\mathbf{m}|^2 - |\nabla\mathbf{n}|^2 - |\nabla\boldsymbol{\ell}|^2)\,. \end{array}$$

Adding the six terms I_3^h, and using that $\lambda_1 + \lambda_2 + \lambda_3 = 0$, the formula for I_3 is readily proved. □

We recall that in the previous sections we have associated to each unit vector $(u, \mathbf{v}) \in \mathbb{S}^3$ a tensor order parameter $\mathbf{Q}(u, \mathbf{v})$ that satisfies (4.6), where $\mathbf{n}(u, \mathbf{v})$, $\mathbf{m}(u, \mathbf{v})$, and $\boldsymbol{\ell}(u, \mathbf{v})$ agree with the three columns $G_1(u, \mathbf{v})$, $G_2(u, \mathbf{v})$, and $G_3(u, \mathbf{v})$ of the matrix in (2.2), respectively, compare (2.14). Using this correspondence, we now compute $|\nabla\mathbf{n}|^2$, $|\nabla\mathbf{m}|^2$, and $|\nabla\boldsymbol{\ell}|^2$ in terms of the derivatives of the vector map $(u, \mathbf{v}) : \Omega \to \mathbb{S}^3$, where $\mathbf{v} = (v_1, v_2, v_3)$. Denoting by D_i the ith partial derivative with respect to $x \in \Omega$, we now prove the following.

Proposition 4.4 *For each* $i=1,2,3$ *we have:*

$$\begin{aligned}
|D_i\mathbf{n}|^2 &= 4\Big(|D_i(u,\mathbf{v})|^2-\big(-v_1D_iu+uD_iv_1+v_3D_iv_2-v_2D_iv_3\big)^2\Big)\\
|D_i\mathbf{m}|^2 &= 4\Big(|D_i(u,\mathbf{v})|^2-\big(-v_2D_iu-v_3D_iv_1+uD_iv_2+v_1D_iv_3\big)^2\Big)\\
|D_i\boldsymbol{\ell}|^2 &= 4\Big(|D_i(u,\mathbf{v})|^2-\big(-v_3D_iu+v_2Dv_1-v_1Dv_2+uD_iv_3\big)^2\Big)
\end{aligned}$$

where $|D_i(u,\mathbf{v})|^2:=(D_iu)^2+(D_iv_1)^2+(D_iv_2)^2+(D_iv_3)^2$.

Proof: We first prove the first formula, and we denote $D=D_i$ for simplicity. Since $\mathbf{n}=G_1(u,\mathbf{v})$, compare (2.14), we get

$$D\mathbf{n}=DG_1(u,\mathbf{v})=2\begin{pmatrix}uDu+v_1Dv_1-v_2Dv_2-v_3Dv_3\\ v_1Dv_2+v_2Dv_1+uDv_3+v_3Du\\ v_1Dv_3+v_3Dv_1-uDv_2-v_2Du\end{pmatrix}.$$

Using that $|(u,\mathbf{v})|=1$, we compute

$$\begin{aligned}
\frac{1}{4}|D\mathbf{n}|^2 &= (Du)^2(u^2+v_3^2+v_2^2)+(Dv_1)^2(v_1^2+v_2^2+v_3^2)\\
&\quad+(Dv_2)^2(v_2^2+v_1^2+u^2)+(Dv_3)^2(v_3^2+u^2+v_1^2)\\
&\quad+2\big[DuDv_1(uv_1+v_2v_3-v_2v_3)+DuDv_2(-uv_2+v_1v_3+uv_2)\\
&\qquad+DuDv_3(-uv_3+uv_3-v_1v_2)+Dv_1Dv_2(-v_1v_2+v_1v_2-uv_3)\\
&\qquad+Dv_1Dv_3(-v_1v_3+uv_2+v_1v_3)+Dv_2Dv_3(v_2v_3+uv_1-uv_1)\big]\\
&= (Du)^2(1-v_1^2)+(Dv_1)^2(1-u^2)+(Dv_2)^2(1-v_3^2)+(Dv_3)^2(1-v_2^2)\\
&\quad+2\big[uv_1DuDv_1+v_1v_3DuDv_2-v_1v_2DuDv_3\\
&\qquad-uv_3Dv_1Dv_2+uv_2Dv_1Dv_3+v_2v_3Dv_2Dv_3\big]
\end{aligned}$$

and hence

$$\begin{aligned}
\frac{1}{4}|D\mathbf{n}|^2 &= |D(u,\mathbf{v})|^2-(v_1Du-uDv_1)^2-(v_3Dv_2-v_2Dv_3)^2\\
&\quad+2\big[v_1v_3DuDv_2-v_1v_2DuDv_3-uv_3Dv_1Dv_2+uv_2Dv_1Dv_3\big]\\
&= |D(u,\mathbf{v})|^2-(v_1Du-uDv_1)^2-(v_3Dv_2-v_2Dv_3)^2\\
&\quad+2(v_1Du-uDv_1)(v_3Dv_2-v_2Dv_3)\\
&= |D(u,\mathbf{v})|^2-\big(v_1Du-uDv_1+v_2Dv_3-v_3Dv_2\big)^2,
\end{aligned}$$

that gives the first formula. The second and third formulas are obtained by replacing (u,v_1,v_2,v_3) with $(u,-v_2,-v_1,-v_3)$ and $(u,-v_3,-v_2,-v_1)$, respectively. □

For the sake of brevity, denote now:

$$\begin{aligned}
A^2 &:= \sum_{i=1}^{3}\big(-v_1D_iu+uD_iv_1+v_3D_iv_2-v_2D_iv_3\big)^2,\\
B^2 &:= \sum_{i=1}^{3}\big(-v_2D_iu-v_3D_iv_1+uD_iv_2+v_1D_iv_3\big)^2,\\
C^2 &:= \sum_{i=1}^{3}\big(-v_3D_iu+v_2Dv_1-v_1Dv_2+uD_iv_3\big)^2,
\end{aligned}\tag{4.9}$$

so that by Proposition 4.4 and the fact that $\lambda_1+\lambda_2+\lambda_3=0$,

$$4\big(|\nabla(u,\mathbf{v})|^2-A^2\big)=|\nabla\mathbf{n}|^2,\quad 4\big(|\nabla(u,\mathbf{v})|^2-B^2\big)=|\nabla\mathbf{m}|^2,\quad 4\big(|\nabla(u,\mathbf{v})|^2-C^2\big)=|\nabla\boldsymbol{\ell}|^2.$$

Using Proposition 4.3, we get

$$\begin{aligned}
I_3 &= 12(\lambda_1^2+\lambda_2^2+\lambda_3^2)|\nabla(u,\mathbf{v})|^2-8(2\lambda_1^2+\lambda_2\lambda_3)\,A^2\\
&\quad-8(2\lambda_2^2+\lambda_3\lambda_1)\,B^2-8(2\lambda_3^2+\lambda_1\lambda_2)\,C^2.
\end{aligned}$$

By (2.8), we compute

$$\begin{gathered}
\lambda_1^2+\lambda_2^2+\lambda_3^2=\frac{2}{3}(S_1^2+S_2^2-S_1S_2),\quad 2\lambda_3^2+\lambda_1\lambda_2=S_1S_2,\\
2\lambda_1^2+\lambda_2\lambda_3=S_1^2-S_1S_2,\quad 2\lambda_2^2+\lambda_3\lambda_1=S_2^2-S_1S_2,
\end{gathered}$$

so that we obtain:

$$\begin{aligned}\frac{1}{8}I_3 &= (S_1^2+S_2^2-S_1S_2)|\nabla(u,\mathbf{v})|^2-(S_1^2-S_1S_2)\,A^2\\ &\quad -(S_2^2-S_1S_2)\,B^2-S_1S_2\,C^2\,.\end{aligned} \tag{4.10}$$

Equivalently, by Proposition 4.3 we deduce that

$$I_3 = 2\big\{S_1(S_1-S_2)|\nabla\mathbf{n}|^2+S_2(S_2-S_1)|\nabla\mathbf{m}|^2+S_1S_2|\nabla\boldsymbol{\ell}|^2\big\}\,,$$

where we have identified $\mathbf{n},\mathbf{m},\mathbf{n}$ with the first, second, and third column of the matrix-valued map $x\mapsto\mathbf{G}(u,\mathbf{v})$.

Remark 4.5 In the uniaxial case, we have seen that

$$\lambda_2=\lambda_3\Longrightarrow S_2=0\,,\quad \lambda_1=\lambda_3\Longrightarrow S_1=0\,,\quad \lambda_2=\lambda_3\Longrightarrow S_1=S_2=-S\,.$$

We thus recover the expression of I_3 from Proposition 4.1 where, we recall, in the above three cases one has $s=S_1,S_2,S$ and $\mathbf{r}=\mathbf{n},\mathbf{m},\boldsymbol{\ell}$, respectively.

5 The elastic energy of biaxial nematic liquid crystals

In this section we discuss the functional corresponding to the energy density given by the elastic invariant (4.5), which has been considered in the previous section in the framework of constrained biaxial nematic liquid crystals.

FUNCTION SPACES. Let $\Omega\subset\mathbb{R}^3$ denote a bounded domain. Following [3], and according to Definition 2.3, for $1\le p<\infty$ we shall denote by $W^{1,p}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$ the class of measurable maps $\mathbf{Q}:\Omega\to\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3)$ such that $\mathbf{Q}(x)$ has weak derivative $\nabla\mathbf{Q}(x)$ a.e. in Ω satisfying

$$\int_\Omega|\nabla\mathbf{Q}(x)|^p\,dx<\infty\,.$$

Since

$$I_3(\mathbf{Q},\nabla\mathbf{Q}):=\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}=|\nabla\mathbf{Q}|^2\,,$$

we deduce that the energy functional

$$\mathbf{Q}\mapsto\mathcal{I}_3(\mathbf{Q}):=\int_\Omega I_3(\mathbf{Q},\nabla\mathbf{Q})\,dx \tag{5.1}$$

is well defined and finite on the Sobolev class $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$.

The above facts lead us to consider also the Sobolev classes

$$W^{1,p}(\Omega,\mathbb{S}^3):=\{(u,\mathbf{v})\in W^{1,p}(\Omega,\mathbb{R}^4)\,:\,|(u,\mathbf{v})(x)|=1\quad\text{for a.e. }x\in\Omega\}\,.$$

We also introduce the elastic energy functional

$$\widetilde{\mathcal{F}}_3(u,\mathbf{v}):=\int_\Omega f_3((u,\mathbf{v})(x),\nabla(u,\mathbf{v})(x))\,dx\,, \tag{5.2}$$

where the energy density $f_3:\mathbb{S}^3\times\mathbb{M}_{4\times3}\to[0,+\infty)$ is defined for $(u,\mathbf{v})\in\mathbb{S}^3$ and $H\in\mathbb{M}_{4\times3}$ by

$$f_3((u,\mathbf{v}),H):=(k_1-k_2+k_3)|H|^2-k_1\,A((u,\mathbf{v}),H)^2+k_2B((u,\mathbf{v}),H)^2-k_3C((u,\mathbf{v}),H)^2\,. \tag{5.3}$$

In the above formula, $H=(H_i^j)$, $j=0,1,2,3\,;\ i=1,2,3$, $|H|^2:=\sum_{i=1}^3\sum_{j=0}^3(H_i^j)^2$, and

$$k_1:=8S_1(S_1-S_2)\,,\quad k_2:=8S_2(S_1-S_2)\,,\quad k_3:=8S_1S_2.$$

From Remark 2.6, it follows that $k_1, k_2, k_3 > 0$ and $(k_1 - k_2 + k_3) = 8(S_1^2 + S_2^2 - S_1 S_2) > 0$. Moreover, by (4.9),

$$\begin{aligned} A((u,\mathbf{v}),H)^2 &:= \sum_{i=1}^{3}\big(-v_1H_i^0 + uH_i^1 + v_3H_i^2 - v_2H_i^3\big)^2\,, \\ B((u,\mathbf{v}),H)^2 &:= \sum_{i=1}^{3}\big(-v_2H_i^0 - v_3H_i^1 + uH_i^2 + v_1H_i^3\big)^2\,, \\ C((u,\mathbf{v}),H)^2 &:= \sum_{i=1}^{3}\big(-v_3H_i^0 + v_2H_1^1 - v_1H_i^2 + uH_i^3\big)^2\,. \end{aligned} \tag{5.4}$$

Therefore, by (4.10), *the energy density* f_3 *corresponds to the third elastic invariant* I_3 *in* (4.5)*, in the constrained biaxial case.*

INVARIANCE PROPERTIES. Using the above notation and Remark 2.1, we can prove the following.

Proposition 5.1 *For every* $(u,\mathbf{v}) \in \mathbb{S}^3$ *and* $H \in \mathbb{M}_{4\times 3}$*, let* f_3 *be as in* (5.3)*. Then*

$$f_3(q\cdot(u,\mathbf{v}), L(q)H) = f_3((u,\mathbf{v}),H) = f_3\big((u,\mathbf{v}), HM^T\big)$$

for any $q \in \mathbb{S}^3$ *and* $M \in SO(3)$*.*

PROOF: We first observe that by orthogonality $|H| = |L(q)H|$. Since $L(q\cdot(u,\mathbf{v}))^T = (L(q)L((u,\mathbf{v})))^T = L((u,\mathbf{v}))^T L(q)^T$, we have

$$L(q\cdot(u,\mathbf{v}))^T\,L(q)H_i = L((u,\mathbf{v}))^T L(q)^T L(q)H_i = L((u,\mathbf{v}))^T H_i\,. \tag{5.5}$$

Using that $L((u,-\mathbf{v})) = L((u,\mathbf{v}))^T$, we observe that the terms in (5.4) are actually expressed in terms of the products $L((u,\mathbf{v}))^T\,H_i$. This gives the first equality, on account of (5.5). As for the second equality, we again have $|H| = |HM^T|$. Moreover, we compute

$$(HM^T)_i^j = H_\alpha^j (M^T)_i^\alpha = H_\alpha^j M_\alpha^i\,.$$

By substituting in the first equation of (5.4), and using the orthogonality of M, we get

$$\begin{aligned} A((u,\mathbf{v}),HM^T)^2 &= \sum_{i=1}^{3}\big(-v_1(HM^T)_i^0 + u(HM^T)_i^1 + v_3(HM^T)_i^2 - v_2(HM^T)_i^3\big)^2 \\ &= \sum_{i=1}^{3}\big(-v_1H_\alpha^0M_\alpha^i + uH_\alpha^1M_\alpha^i + v_3H_\alpha^2M_\alpha^i - v_2H_\alpha^2M_\alpha^i\big)^2 \\ &= \big(-v_1H_\alpha^0M_\alpha^i + uH_\alpha^1M_\alpha^i + v_3H_\alpha^2M_\alpha^i - v_2H_\alpha^2M_\alpha^i\big) \\ &\quad\times\big(-v_1H_\beta^0M_\beta^i + uH_\beta^1M_\beta^i + v_3H_\beta^2M_\beta^i - v_2H_\beta^2M_\beta^i\big) \\ &= \big(-v_1H_\alpha^0 + uH_\alpha^1 + v_3H_\alpha^2 - v_2H_\alpha^2\big)\big(-v_1H_\beta^0 + uH_\beta^1 + v_3H_\beta^2 - v_2H_\beta^2\big)M_\alpha^iM_\beta^i \\ &= \sum_{\alpha=1}^{3}\big(-v_1H_\alpha^0 + uH_\alpha^1 + v_3H_\alpha^2 - v_2H_\alpha^2\big)^2 = A((u,\mathbf{v}),H)^2\,. \end{aligned}$$

In a similar way, it can be checked that

$$B((u,\mathbf{v}),HM^T)^2 = B((u,\mathbf{v}),H)^2\,, \qquad C((u,\mathbf{v}),HM^T)^2 = C((u,\mathbf{v}),H)^2\,.$$

The claim follows from (5.3). □

Remark 5.2 According to Theorem 3.3, by Proposition 5.1 we directly obtain that the energy density f_3 satisfies both the frame invariance and the residual symmetry properties introduced in Definitions 3.2 and 3.6. This fact will be used in our Definition 5.5 below.

ENERGY BOUNDS. Clearly there exists an absolute constant $K > 0$, only depending on S_1, S_2, and hence on the fixed eigenvalues $\lambda_1, \lambda_2, \lambda_3$, such that

$$0 \le f_3(w,H) \le K\,|H|^2 \qquad \forall\,(w,H) \in \mathbb{S}^3 \times \mathbb{M}_{4\times 3}\,. \tag{5.6}$$

This yields that the energy $\widetilde{\mathcal{F}}_3$ is finite on the Sobolev class $W^{1,2}(\Omega,\mathbb{S}^3)$. Therefore, by the previous computation, we deduce that for each Sobolev map $(u,\mathbf{v})\in W^{1,2}(\Omega,\mathbb{S}^3)$ the corresponding map $x\mapsto \mathbf{Q}(x):=\mathbf{Q}((u,\mathbf{v})(x))$ belongs to the Sobolev space $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$, and for a.e. $x\in\Omega$

$$f_3((u,\mathbf{v})(x),\nabla(u,\mathbf{v})(x))=I_3(\mathbf{Q}(u,\mathbf{v}),\nabla\mathbf{Q}(u,\mathbf{v})(x))\,. \tag{5.7}$$

Using the invariance properties and (2.15) of Remark 2.6, we now prove that a coercivity property holds too. To this purpose, according to the alternative in (2.15), we set

$$S:=\begin{cases} S_2 & \text{if } \dfrac{S_1}{2}\le S_2<0 \\ S_1 & \text{if } S_2\le \dfrac{S_1}{2}<0 \end{cases} \qquad S\neq 0\,. \tag{5.8}$$

Proposition 5.3 *For every $(u,\mathbf{v})\in\mathbb{S}^3$ and $H\in\mathbb{M}_{4\times 3}$, we have*

$$f_3((u,\mathbf{v}),H)\ge 8\,S^2\,|H|^2\,.$$

PROOF: By (5.4), taking $(u,\mathbf{v})=P_N:=(1,0,0,0)$, the north pole in $\mathbb{S}^3$, for each $H\in\mathbb{M}_{4\times 3}$ we have

$$A(P_N,H)^2=\sum_{i=1}^3(H_i^1)^2\,,\quad B(P_N,H)^2=\sum_{i=1}^3(H_i^2)^2\,,\quad C(P_N,H)^2=\sum_{i=1}^3(H_i^3)^2\,.$$

Setting $|H^j|^2:=\sum_{i=1}^3(H_i^j)^2$, so that $|H|^2=\sum_{j=0}^3|H^j|^2$, by (5.3) we thus obtain

$$f_3(P_N,H)=(k_1-k_2+k_3)|H^0|^2+(k_3-k_2)|H^1|^2+(k_1+k_3)|H^2|^2+(k_1-k_2)|H^3|^2\,.$$

Assume now that the first alternative in (2.15) holds. We observe that

$$\begin{aligned}&(k_1-k_2+k_3)=8(S_1^2+S_2^2-S_1S_2)\ge 4(S_1^2+S_2^2)\ge 20S_2^2\,,\\ &(k_3-k_2)=8S_2^2\,,\quad (k_1+k_3)=8S_1^2\ge 32S_2^2\,,\quad (k_1-k_2)=8(S_1-S_2)^2\ge 8S_2^2\,.\end{aligned}$$

This yields the lower bound

$$f_3(P_N,H)\ge 8S_2^2\sum_{j=1}^4|H^j|^2=8S_2^2\,|H|^2\,. \tag{5.9}$$

We now use the invariance properties of f_3. More precisely, let $q:=(u,\mathbf{v})^{-1}=(u,-\mathbf{v})$, so that $q\cdot(u,\mathbf{v})=P_N$. Proposition 5.1 yields that

$$f_3(P_N,L(q)H)=f_3(q\cdot(u,\mathbf{v}),L(q)H)=f_3((u,\mathbf{v}),H)\,.$$

Using (5.9), this implies that

$$f_3((u,\mathbf{v}),H)\ge 8\big(S_2|L(q)H|\big)^2\,.$$

By the orthogonality of $L(q)$, we finally get $|L(q)H|=|H|$. On the other hand, if the second alternative in (2.15) holds, we similarly obtain that

$$f_3((u,\mathbf{v}),H)\ge 8\big(S_1|L(q)H|\big)^2\,,$$

which proves the claim. □

We have shown that

$$8\,S^2\int_\Omega|\nabla(u,\mathbf{v})|^2\,dx\le\widetilde{\mathcal{F}}_3(u,\mathbf{v})\le K\int_\Omega|\nabla(u,\mathbf{v})|^2\,dx\qquad\forall\,(u,\mathbf{v})\in W^{1,p}(\Omega,\mathbb{S}^3)\,, \tag{5.10}$$

with $S\neq 0$ given by (5.8). This yields that *the class of measurable and a.e. weakly differentiable functions from Ω to $\mathbb{S}^3$ with finite $\widetilde{\mathcal{F}}_3$-energy agrees with the Sobolev class $W^{1,2}(\Omega,\mathbb{S}^3)$.*

THE ENERGY OF MAPS INTO $\mathbb{S}^3/\mathcal{H}$. From now on, we let $\Omega \subset \mathbb{R}^3$ denote a bounded and simply connected domain, and $\mathcal{Y}$ a smooth, compact Riemannian manifold without boundary isometrically embedded in $\mathbb{R}^N$, equipped with the induced metric (and topology). Also, for $X = L^p$, $W^{1,p}$, C^∞, where $p \geq 1$, denote

$$\begin{aligned} X(\Omega, \mathcal{Y}) &:= \{w \in X(\Omega, \mathbb{R}^N) \mid w(x) \in \mathcal{Y} \text{ for a.e } x \in \Omega\}, \\ X(\Omega, \mathcal{Y}) \cap C^\infty &:= \{w \in X(\Omega, \mathcal{Y}) \mid w \text{ is smooth}\}. \end{aligned}$$

By the Nash–Moser isometric embedding theorem, we assume that the Riemannian homogeneous manifold $\mathbb{S}^3/\mathcal{H}$ is isometrically embedded as a submanifold $\mathcal{Y} := F(\mathbb{S}^3/\mathcal{H})$ in some Euclidean space $\mathbb{R}^N$ with induced Riemannian metric, where $F : \mathbb{S}^3/\mathcal{H} \to \mathbb{R}^N$ is an *isometric embedding.*

Remark 5.4 Observe that the diffeomorphism $\mathbb{S}^3/\mathcal{H} \cong Q(\lambda_1, \lambda_2, \lambda_3)$ yields a bijective correspondence between the Sobolev spaces $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$ and $W^{1,2}(\Omega, Q(\lambda_1, \lambda_2, \lambda_3))$.

We now make use of the lifting result of Bethuel–Chiron discussed at the end of the introduction. As in Remark 2.4, let $\Pi : \mathbb{S}^3 \to \mathbb{S}^3/\mathcal{H}$ denote the canonical projection and set $\widetilde{\Pi} := F \circ \Pi$. Then, according to [5, Theorem 1], for every $w \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$, there exists $\widetilde{w} \in W^{1,2}(\Omega, \mathbb{S}^3)$ such that $\widetilde{\Pi} \circ \widetilde{w} = w$ a.e. in Ω, that is unique up to the action of an element of $\mathcal{H} = \pi_1(\mathbb{S}^3/\mathcal{H})$. Furthermore, we have $|\nabla w| = |\nabla \widetilde{w}|$ a.e. in Ω. This suggests the following.

Definition 5.5 *The* $\mathcal{F}_3$-energy *of a Sobolev map* $w \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$ *is given by the* $\widetilde{\mathcal{F}}_3$*-energy of* any *Sobolev map* $\widetilde{w} \in W^{1,2}(\Omega, \mathbb{S}^3)$ *such that* $\widetilde{\Pi} \circ \widetilde{w} = w$*, i.e.,*

$$\mathcal{F}_3(w) := \widetilde{\mathcal{F}}_3(\widetilde{w}) \quad \textit{if} \quad \widetilde{\Pi} \circ \widetilde{w} = w \ \textit{ a.e. in } \Omega,$$

where $\widetilde{\mathcal{F}}_3(\widetilde{w})$ *is given by* (5.2)*, with* $\widetilde{w} = (u, \mathbf{v})$.

By Remark 5.2, note that *the energy functional* $\mathcal{F}_3(w)$ *is well defined on the Sobolev class* $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$. Moreover, property (5.10) and the equality $|\nabla w| = |\nabla \widetilde{w}|$ yield that

$$8\, S^2 \int_\Omega |\nabla w|^2\, dx \leq \mathcal{F}_3(w) \leq K \int_\Omega |\nabla w|^2\, dx \qquad \forall\, w \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H}), \tag{5.11}$$

with $S \neq 0$ given by (5.8), hence *the energy functional* $\mathcal{F}_3(w)$ *is finite exactly on* $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$.

DENSITY RESULTS. The following strong density result is due to Bethuel [4].

Theorem 5.6 (Bethuel) *Let* $p \geq 1$ *and* $\mathfrak{p}$ *denote the integer part of* p*. The class* $W^{1,p}(\Omega, \mathcal{Y}) \cap C^\infty$ *is strongly dense in* $W^{1,p}(\Omega, \mathcal{Y})$ *if and only if the* $\mathfrak{p}$*-th homotopy group* $\pi_{\mathfrak{p}}(\mathcal{Y}) = 0$.

Choosing $\mathcal{Y} := F(\mathbb{S}^3/\mathcal{H})$ and $p = 2$, we have $\pi_2(\mathcal{Y}) = \pi_2(\mathbb{S}^3/\mathcal{H}) = \pi_2(\mathbb{S}^3) = 0$. Therefore, *for each Sobolev map* $w \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$ *there exists a sequence of smooth maps* $\{w_k\} \subset W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H}) \cap C^\infty$ *such that* $w_k \to w$ *strongly in* $W^{1,2}$. Furthermore, we obtain:

Proposition 5.7 *For each Sobolev map* $w \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$ *there exists a sequence of smooth maps* $\{w_k\} \subset W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H}) \cap C^\infty$ *such that* $w_k \to w$ *strongly in* $W^{1,2}$ *and* $\mathcal{F}_3(w_k) \to \mathcal{F}_3(w)$.

PROOF: By uniform convexity, the strong convergence $w_k \to w$ in $W^{1,2}$ is equivalent to the a.e. convergence $w_k \to w$ joined with the energy convergence $\int_\Omega |\nabla w_k|^2\, dx \to \int_\Omega |\nabla w|^2\, dx$. Therefore, for each $w \in W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$ we find a sequence $\{w_k\} \subset W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H}) \cap C^\infty$ such that $w_k \to w$ a.e. and $\int_\Omega |\nabla w_k|^2\, dx \to \int_\Omega |\nabla w|^2\, dx$. By [5, Theorem 1], for each k we also find a (smooth) Sobolev map $\widetilde{w}_k \in W^{1,2}(\Omega, \mathbb{S}^3)$ such that $\widetilde{\Pi} \circ \widetilde{w}_k = w_k$. Using the bounds in the formula (5.10), the structure (5.3) and (5.4) of the energy density f_3, and the dominated convergence theorem, we deduce that $\widetilde{\mathcal{F}}_3(\widetilde{w}_k) \to \widetilde{\mathcal{F}}_3(\widetilde{w})$ for some Sobolev map $\widetilde{w} \in W^{1,2}(\Omega, \mathbb{S}^3)$ satisfying $\widetilde{\Pi} \circ \widetilde{w} = w$. The claim follows from Definition 5.5. □

LOWER SEMICONTINUITY. We now see that *the functional* $w \mapsto \mathcal{F}_3(w)$ *is sequentially lower semicontinuous w.r.t. the weak* $W^{1,2}$*-topology in the class* $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$.

Proposition 5.8 *Let* $\{w_k\} \subset W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$ *be a sequence such that* $\sup_k \int_\Omega |\nabla w_k|^2\,dx < \infty$ *and* $w_k \to w$ *a.e. to some* $w \in W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$. *Then*

$$\mathcal{F}_3(w) \le \liminf_{k\to\infty} \mathcal{F}_3(w_k)\,.$$

PROOF: By the preceding discussion, see Remark 5.4, to any Sobolev map $w \in W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$ there corresponds a unique $\widetilde{\mathbf{Q}}$ in $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$ given by $\widetilde{\mathbf{Q}}(x) := \mathbf{Q}(\widetilde{w}(x))$, where $\widetilde{w} \in W^{1,2}(\Omega,\mathbb{S}^3)$ is such that $\widetilde{\Pi}\circ\widetilde{w} = w$, so that by Definition 5.5, (5.7), and (5.1)

$$\mathcal{F}_3(w) = \mathcal{I}_3(\widetilde{\mathbf{Q}}) = \int_\Omega |\nabla\widetilde{\mathbf{Q}}(x)|^2\,dx\,.$$

Therefore, by (5.11), the weak $W^{1,2}$-convergence $w_k \rightharpoonup w$ implies the weak $W^{1,2}$-convergence $\widetilde{\mathbf{Q}}_k \rightharpoonup \widetilde{\mathbf{Q}}$, where $\widetilde{\mathbf{Q}}_k \in W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$ is given by $\widetilde{\mathbf{Q}}_k(x) := \mathbf{Q}(\widetilde{w}_k(x))$ for some $\widetilde{w}_k \in W^{1,2}(\Omega,\mathbb{S}^3)$ satisfying $\widetilde{\Pi}\circ\widetilde{w}_k = w_k$. Since the functional $\widetilde{\mathbf{Q}} \mapsto \mathcal{I}_3(\widetilde{\mathbf{Q}})$ is sequentially lower semicontinuous with respect to the weak topology in $W^{1,2}(\Omega,\mathcal{Q}(\lambda_1,\lambda_2,\lambda_3))$, we get

$$\mathcal{F}_3(w) = \mathcal{I}_3(\widetilde{\mathbf{Q}}) \le \liminf_{k\to\infty} \mathcal{I}_3(\widetilde{\mathbf{Q}}_k) = \liminf_{k\to\infty} \mathcal{F}_3(w_k)\,,$$

as required. □

RELAXED ENERGY. Finally, for the class of summable maps $L^1(\Omega,\mathbb{S}^3/\mathcal{H})$ we consider the *relaxed energy*

$$\overline{\mathcal{F}}_3(w) := \inf\bigl\{\liminf_{k\to\infty} \mathcal{F}_3(w_k) \mid \{w_k\} \subset C^\infty(\Omega,\mathbb{S}^3/\mathcal{H})\,,\ w_k \to w \text{ strongly in } L^1\bigr\}\,.$$

Corollary 5.9 *We have*

$$\overline{\mathcal{F}}_3(w) = \begin{cases} \mathcal{F}_3(w) & \text{if } \ w \in W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H}) \\ +\infty & \text{otherwise in } L^1(\Omega,\mathbb{S}^3/\mathcal{H})\,. \end{cases}$$

PROOF: If $\overline{\mathcal{F}}_3(w) < \infty$, from the coercivity condition (5.11) and the lower semicontinuity property established in Proposition 5.8 we infer that $w \in W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$ and that $\mathcal{F}_3(w) \le \overline{\mathcal{F}}_3(w)$. In this case, moreover, the density result from Proposition 5.7 yields the equality $\mathcal{F}_3(w) = \overline{\mathcal{F}}_3(w)$. □

6 A more general energy density

With reference to the discussion in Section 4 and according to [8], in this section we extend some of the previous results to a more general energy functional. First, following [28], we explicitly write the elastic invariants

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

in the *constrained* biaxial case. For the sake of brevity, we omit the calculations. As above, let

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

with $\lambda_1,\lambda_2,\lambda_3$ given by (2.8). Then

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

For unit vector fields $\mathbf{r},\mathbf{s},\mathbf{t}$, we adopt the following notation:

$$\begin{aligned} (\nabla\mathbf{r})\mathbf{s} &:= (\nabla\mathbf{r})^i\mathbf{s}\,\mathbf{e}_i\,, \qquad & (\nabla\mathbf{r})^i\mathbf{s} &:= \mathbf{s}_k\mathbf{r}_{i,k} \\ \mathbf{r}^T\nabla\mathbf{s} &:= (\mathbf{r}\nabla_i\mathbf{s})\,\mathbf{e}_i\,, \qquad & \mathbf{r}\nabla_i\mathbf{s} &:= \mathbf{r}_k\mathbf{s}_{k,i} \end{aligned}$$

where $(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)$ is the canonical basis in $\mathbb{R}^3$ and "$\cdot$" denotes the scalar product in $\mathbb{R}^3$, so that

$$\mathbf{r}\cdot(\nabla\mathbf{s})\mathbf{t} = \mathbf{r}_i(\mathbf{t}_k\mathbf{s}_{i,k}) = \mathbf{t}_k(\mathbf{r}_i\mathbf{s}_{i,k}) = \mathbf{t}_i(\mathbf{r}_k\mathbf{s}_{k,i}) = \mathbf{t}\cdot(\mathbf{r}^T\nabla\mathbf{s})\,.$$

As for the first elastic invariant, we obtain:

$$\begin{array}{rcl}
I_1 & = & \lambda_1^2\big((\operatorname{div}\mathbf{n})^2+|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2\big)+\lambda_2^2\big((\operatorname{div}\mathbf{m})^2+|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2\big)+\lambda_3^2\big((\operatorname{div}\boldsymbol{\ell})^2+|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\big)\\
& & +2\lambda_1\lambda_2\big\{(\nabla\mathbf{n})\mathbf{n}\cdot(\nabla\mathbf{m})\mathbf{m}+(\operatorname{div}\mathbf{n})\big[\mathbf{n}\cdot(\nabla\mathbf{m})\mathbf{m}\big]+(\operatorname{div}\mathbf{m})\big[\mathbf{m}\cdot(\nabla\mathbf{n})\mathbf{n}\big]\big\}\\
& & +2\lambda_2\lambda_3\big\{(\nabla\mathbf{m})\mathbf{m}\cdot(\nabla\boldsymbol{\ell})\boldsymbol{\ell}+(\operatorname{div}\mathbf{m})\big[\mathbf{m}\cdot(\nabla\boldsymbol{\ell})\boldsymbol{\ell}\big]+(\operatorname{div}\boldsymbol{\ell})\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{m})\mathbf{m}\big]\big\}\\
& & +2\lambda_3\lambda_1\big\{(\nabla\boldsymbol{\ell})\boldsymbol{\ell}\cdot(\nabla\mathbf{n})\mathbf{n}+(\operatorname{div}\boldsymbol{\ell})\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{n})\mathbf{n}\big]+(\operatorname{div}\mathbf{n})\big[\mathbf{n}\cdot(\nabla\boldsymbol{\ell})\boldsymbol{\ell}\big]\big\}\,.
\end{array}\tag{6.1}$$

The second elastic invariant becomes:

$$\begin{array}{rcl}
I_2 & = & \lambda_1^2\big(|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2+\operatorname{tr}[(\nabla\mathbf{n})^2]\big)+\lambda_2^2\big(|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2+\operatorname{tr}[(\nabla\mathbf{m})^2]\big)+\lambda_3^2\big(|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2+\operatorname{tr}[(\nabla\boldsymbol{\ell})^2]\big)\\
& & +2\lambda_1\lambda_2\big\{(\mathbf{n}^T\nabla\mathbf{m})\cdot(\nabla\mathbf{n})\mathbf{m}+(\mathbf{m}^T\nabla\mathbf{n})\cdot(\nabla\mathbf{m})\mathbf{n}+(\nabla\mathbf{n})\mathbf{m}\cdot(\nabla\mathbf{m})\mathbf{n}\big\}\\
& & +2\lambda_2\lambda_3\big\{(\mathbf{m}^T\nabla\boldsymbol{\ell})\cdot(\nabla\mathbf{m})\boldsymbol{\ell}+(\boldsymbol{\ell}^T\nabla\mathbf{m})\cdot(\nabla\boldsymbol{\ell})\mathbf{m}+(\nabla\mathbf{m})\boldsymbol{\ell}\cdot(\nabla\boldsymbol{\ell})\mathbf{m}\big\}\\
& & +2\lambda_3\lambda_1\big\{(\boldsymbol{\ell}^T\nabla\mathbf{n})\cdot(\nabla\boldsymbol{\ell})\mathbf{n}+(\mathbf{n}^T\nabla\boldsymbol{\ell})\cdot(\nabla\mathbf{n})\boldsymbol{\ell}+(\nabla\boldsymbol{\ell})\mathbf{n}\cdot(\nabla\mathbf{n})\boldsymbol{\ell}\big\}\,.
\end{array}\tag{6.2}$$

Finally, the fourth elastic invariant takes the following form:

$$\begin{array}{rcl}
\frac{1}{2}I_4 & = & \lambda_1^3|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2+\lambda_2^3|\mathbf{m}\times\operatorname{curl}\mathbf{m}|^2+\lambda_3^3|\boldsymbol{\ell}\times\operatorname{curl}\boldsymbol{\ell}|^2\\
& & +2\lambda_1^2\lambda_2\big[\mathbf{n}\cdot(\nabla\mathbf{m})\mathbf{n}\big]\,\big[\mathbf{m}\cdot(\nabla\mathbf{n})\mathbf{n}\big]+2\lambda_2^2\lambda_1\big[\mathbf{m}\cdot(\nabla\mathbf{n})\mathbf{m}\big]\,\big[\mathbf{n}\cdot(\nabla\mathbf{m})\mathbf{m}\big]\\
& & +2\lambda_2^2\lambda_3\big[\mathbf{m}\cdot(\nabla\boldsymbol{\ell})\mathbf{m}\big]\,\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{m})\mathbf{m}\big]+2\lambda_3^2\lambda_2\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{m})\boldsymbol{\ell}\big]\,\big[\mathbf{m}\cdot(\nabla\boldsymbol{\ell})\boldsymbol{\ell}\big]\\
& & +2\lambda_3^2\lambda_1\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{n})\boldsymbol{\ell}\big]\,\big[\mathbf{n}\cdot(\nabla\boldsymbol{\ell})\boldsymbol{\ell}\big]+2\lambda_1^2\lambda_3\big[\mathbf{n}\cdot(\nabla\boldsymbol{\ell})\mathbf{n}\big]\,\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{n})\mathbf{n}\big]\\
& & +\lambda_1\lambda_2\lambda_3\big\{\big[\mathbf{m}\cdot(\nabla\boldsymbol{\ell})\mathbf{n}\big]\,\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{m})\mathbf{n}\big]+\big[\boldsymbol{\ell}\cdot(\nabla\mathbf{n})\mathbf{m}\big]\,\big[\mathbf{n}\cdot(\nabla\boldsymbol{\ell})\mathbf{m}\big]+\big[\mathbf{n}\cdot(\nabla\mathbf{m})\boldsymbol{\ell}\big]\,\big[\mathbf{m}\cdot(\nabla\mathbf{n})\boldsymbol{\ell}\big]\big\}\,.
\end{array}$$

The third elastic invariant I_3 has already been computed in Proposition 4.3 and written in terms of a map $(u,\mathbf{v})$ in Proposition 4.4. In principle, by similar computation as those in Proposition 4.4, one could express also the invariants I_1, I_2, and I_4 in terms of maps $(u,\mathbf{v}):\Omega\to\mathbb{S}^3$, hence yielding energy densities $f_i:\mathbb{S}^3\times\mathbb{M}_{4\times 3}\to[0,+\infty)$ such that

$$f_i((u,\mathbf{v})(x),\nabla(u,\mathbf{v})(x))=I_i(\mathbf{Q}(u,\mathbf{v})(x),\nabla\mathbf{Q}(u,\mathbf{v})(x)),\quad i=1,2,4,\tag{6.3}$$

see (5.3) for the case $i=3$. By Theorem 3.3, the energy densities f_i satisfy both the frame invariance and the residual symmetry properties from Definitions 3.2 and 3.6, see also Remark 3.7.

A MORE GENERAL ENERGY. Assume now that the elastic constants verify $L_4=0$ and

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

Davis and Gartland [8] proved that under these hypotheses the energy functional (defined on general $\mathbf{Q}$-tensors)

$$\mathcal{I}(\mathbf{Q}):=\int_\Omega\big(L_1I_1+L_2I_2+L_3I_3\big)\,dx$$

is sequentially weakly lower semicontinuous in $W^{1,2}$, provided that the domain Ω has smooth boundary. In fact, there exist two positive constants $K>\mu>0$ such that

$$K\,|\nabla\mathbf{Q}|^2\ge L_1I_1+L_2I_2+L_3I_3\ge\mu\,|\nabla\mathbf{Q}|^2\,.$$

With this choice of the constants L_i, since $|\nabla\mathbf{Q}|^2=I_3$, by (5.7) and Proposition 5.3 we readily obtain a similar coercivity property for the corresponding functional $\widetilde{\mathcal{F}}:=L_1\widetilde{\mathcal{F}}_1+L_2\widetilde{\mathcal{F}}_2+L_3\widetilde{\mathcal{F}}_3$ on $W^{1,2}(\Omega,\mathbb{S}^3)$, where $\widetilde{\mathcal{F}}_i$ is defined as in (5.2) with f_i as in (6.3). As a consequence, the class of measurable and a.e. weakly differentiable functions from Ω to $\mathbb{S}^3$ with finite $\widetilde{\mathcal{F}}$-energy agrees with the Sobolev class $W^{1,2}(\Omega,\mathbb{S}^3)$.

Reasoning exactly as in the second part of Section 5, with $\mathcal{F}_3$ replaced by $\mathcal{F}$, we can extend the $\mathcal{F}$-energy to the Sobolev class $W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$ as in Definition 5.5; in particular, the energy functional $\mathcal{F}(w)$ is finite exactly on $W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$.

As in Proposition 5.7, we then obtain the approximation in $\mathcal{F}$-energy with smooth maps in the class $W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$. In fact, on account e.g. of the formulas (6.1) and (6.2), recalling that $\mathbf{n}$ and $\mathbf{m}$ are given by (2.14), and that $\boldsymbol{\ell}=\mathbf{n}\times\mathbf{m}$ agrees with the third column $G_3(u,\mathbf{v})$ of the matrix in (2.2), we deduce that the dominated convergence theorem can be applied.

Moreover, arguing as in Proposition 5.8, since the functional $\widetilde{\mathbf{Q}}\mapsto\mathcal{I}(\widetilde{\mathbf{Q}})$ is sequentially lower semicontinuous with respect to the weak $W^{1,2}$-topology, we infer the weak lower semicontinuity of the functional $w\mapsto\mathcal{F}(w)$ in $W^{1,2}(\Omega,\mathbb{S}^3/\mathcal{H})$.

Finally, we deduce the representation formula of the corresponding relaxed energy as in Corollary 5.9.

References

[1] J.M. BALL, The Q-tensor theory of liquid crystals, Lecture slides, Benin Summer School, 28 June–2 July 2010.

[2] J.M. BALL, A. MAJUMDAR, Nematic liquid crystals: from Maier-Saupe to a continuum theory, *Mol. Cryst. Liq. Cryst.* **525** (2010), 1–11.

[3] J.M. BALL, A. ZARNESCU, Orientability and energy minimization in liquid cristal models, *Arch. Ration. Mech. Anal.*, **202** (2011), no. 2, 493–535.

[4] F. BETHUEL, The approximation problem for Sobolev maps between manifolds, *Acta Math.* **167** (1991), 153–206.

[5] F. BETHUEL, D. CHIRON, Some questions related to the lifting problem in Sobolev spaces, *Contemp. Math.* **446** (2007), 125-152.

[6] T. BRÖCKER, T. TOM DIECK, *Representations of compact Lie groups*, Graduate Texts in Mathematics, 98, Springer-Verlag, New York, 1985.

[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, E.C. GARTLAND, Jr., Finite element analysis of the Landau–de Gennes minimization problem for liquid crystals, *SIAM J. Numer. Anal.* **35** (1998), 336-362.

[9] P.G. DE GENNES, J. PROST, *The physics of liquid crystals*, 2nd edn. Oxford University Press, 1995.

[10] H.-D. EBBINGHAUS, H. HERMES, F. HIRZEBRUCH, M. KOECHER, K. MAINZER, J. NEUKIRCH, A. PRESTEL, R. REMMERT, *Numbers*, Graduate Texts in Mathematics, 123, Springer-Verlag, New York, 1991.

[11] J.L. ERICKSEN, Equilibrium theory of liquid crystals, In: *Advances in liquid crystals* **2**, G.H. Brown (ed.), Academic Press, New York (1976), 233–299.

[12] J.L. ERICKSEN, Liquid crystals with variable degree of orientation, *Arch. Ration. Mech. Anal.* **113** (1990), 97-120.

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

[14] M. GIAQUINTA, G. MODICA, J. SOUČEK: Liquid crystals: relaxed energies, dipoles, singular lines and singular points, *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* (4) **17** (1990), 415–437.

[15] M. GIAQUINTA, G. MODICA, J. SOUČEK: *Cartesian currents in the calculus of variations,* I, II. Ergebnisse Math. Grenzgebiete (III Ser), **37**, **38**, Springer, Berlin, 1998.

[16] R. HARDT, D. KINDERLEHRER, F. LIN, The variety of configurations of liquid crystals, in: *Variational Methods* (eds. H. Beresticky, J.M. Coron and I. Ekeland), PNDE, Birkäuser, Basel (1990), 115–131.

[17] D. KINDERLEHRER, Recent developments in liquid crystals theory, in: *Frontiers in Pure and Applied Mathemathics*, North-Holland, Amsterdam (1991), 151–178.

[18] F.C. LESLIE, Theory of flow phenomena in liquid crystals, In: *Advances in liquid crystals* **2**, G.H. Brown (ed.), Academic Press, New York (1976), 1–81.

[19] F.H. LIN, C. LIU, Static and dynamic theories of liquid crystals, *J. Partial Differential Equations* **14** (2001), no. 4, 289-330.

[20] G.R. LUCKHURST, Liquid crystals: a missing phase found at last?, *Nature* **430** (2004), 413-414.

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

[22] A. MAJUMDAR, A. ZARNESCU, Landau–de Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond, *Arch. Ration. Mech. Anal.* **196** (2010), 227-280.

[23] N.D. MERMIN, The topological theory of defects in ordered media, *Rev. Modern Phys.* **51** (1979), 591-648.

[24] N.J. MOTTRAM, C. NEWTON, Introduction to Q-tensor theory, Technical report, University of Strathclyde, Department of Mathematics (2004).

[25] D. MUCCI, Maps into projective spaces: liquid crystals and conformal energies, *Discrete Contin. Dyn. Syst. Ser. B* **17** (2012), no. 2, 597-635.

[26] C.W. OSEEN, The theory of liquid crystals, *Trans. Faraday Soc.* **29** (1933), 883-899.

[27] N. SCHOPOHL, T.J. SLUCKIN, Defect core structure in nematic liquid crystals, *Phys. Rev. Lett.* **59** (1987), 2582–2584.

[28] M. VISSENBERG, S. STALLINGA, G. VERTOGEN, Generalized Landau–de Gennes theory of uniaxial and biaxial nematic liquid crystals, *Phys. Rev. E* **55** (1997), 4367.

[29] F. WARNER, *Foundations of differentiable manifolds and Lie groups*, Graduate Texts in Mathematics, 94, Springer-Verlag, New York, 1983.

[30] J.A. WOLF, *Spaces of constant curvature*, fifth edition, Publish or Perish, Inc., Houston, TX, 1984.

Dipartimento di Matematica, Università di Parma,
Parco Area delle Scienze 53/A, I-43124 Parma, Italy
E-mail: domenico.mucci@unipr.it, lorenzo.nicolodi@unipr.it