A LANDAU–DE GENNES THEORY OF LIQUID CRYSTAL ELASTOMERS

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Abstract. In this article, we study minimization of the energy of a Landau-de Gennes liquid crystal elastomer. The total energy consists of the sum of the Lagrangian elastic stored energy function of the elastomer and the Eulerian Landau-de Gennes energy of the liquid crystal.

There are two related sources of anisotropy in the model, that of the rigid units represented by the traceless nematic *order tensor* Q, and the positive definite *step-length tensor* L characterizing the anisotropy of the network. This work is motivated by the study of cytoskeletal networks which can be regarded as consisting of rigid rod units crosslinked into a polymeric-type network. Due to the mixed Eulerian-Lagrangian structure of the energy, it is essential that the deformation maps $\boldsymbol{\varphi}$ be invertible. For this, we require sufficient regularity of the fields $(\boldsymbol{\varphi}, Q)$ of the problem, and that the deformation map satisfies the Ciarlet-Nečas injectivity condition. These, in turn, determine what boundary conditions are admissible, which include the case of Dirichlet conditions on both fields. Alternatively, the approach of including the Rapini-Papoular surface energy for the *pull-back* tensor $\tilde{Q}$ is also discussed. The regularity requirements also lead us to consider powers of the gradient of the order tensor Q higher than quadratic in the energy.

We assume polyconvexity of the stored energy function with respect to the effective deformation tensor and apply methods of calculus of variations from isotropic nonlinear elasticity. Recovery of minimizing sequences of deformation gradients from the corresponding sequences of effective deformation tensors requires invertibility of the anisotropic shape tensor L. We formulate a necessary and sufficient condition to guarantee this invertibility property in terms of the growth to infinity of the bulk liquid crystal energy $f(Q)$, as the minimum eigenvalue of Q approaches the singular limit of $-\frac{1}{3}$. It turns out that L becomes singular as the minimum eigenvalue of Q reaches $-\frac{1}{3}$. Lower bounds on the eigenvalues of Q are needed to ensure compatibility between the theories of Landau-de Gennes and Maier-Saupe of nematics [5].

1. **Introduction.** We investigate existence of minimizers of the energy of a liquid crystal elastomer that in the reference configuration occupies a domain $\Omega \subset \mathbf{R}^3$. We assume that the total energy consists of the Lagrangian contribution of the anisotropic elastomer and the Landau-de Gennes liquid crystal energy in the Eulerian frame. The mixed Lagrangian-Eulerian setting of the problem requires injectivity of the deformation map. For this, we require the admissible deformation maps to have sufficent regularity and to satisfy the Ciarlet-Necas condition as well. This work aims at investigation the coupling of elastic energy and nematic order, and it applies to, both, thermotropic and lyotropic systems.

Liquid crystal elastomers are anisotropic nonlinear elastic materials, with the source of anisotropy stemming from the presence of elongated rigid monomer units, that are either inserted in the back-bone as part of the polymer main-chain or are present as side groups. They are elastic solids that may also present fluid and mixed regimes [18], [20], [21], [27], [43]. In nematic fluids, molecules tend to align themselves along preferential directions but do not present ordering of centers of mass.

The nature of the connections between polymer chains and rigid monomer units plays a main role in determining the behavior of liquid crystal elastomers [43]. From a different perspective, studies of actin and cytoskeletal networks ([11], [28], [42]) show lyotropic rigid rod systems crosslinked into networks by elastomer chains or linkers that present qualitative properties of liquid crystal elastomoers. A main feature of these networks is the average number of connections between rods and the location of these connections in the rod. These motivates us to consider two limiting types of lyotropic systems, the first one corresponding to a nematic liquid with rods weakly coupled into the network. The second case is that of a solid where rod rotation occurs uniquely as a result of elastic deformation, such as an elastomer made of material fibers. Consequeantly, we postulate Eulerian and Lagrangian Landau-de Gennes liquid crystal energies, respectively, for these systems. Many physical systems are found having intermediate properties between these two limiting cases, and it, then, may be appropriate to postulate the energy as a weighted sum of the Eulerian and Lagrangian energies, scaled according to a macroscopic parameter representing the density of crosslinks. The analogous property holds for the elastic energy of the system that we discuss in this article.

The study of a lyotropic elastomer with Lagrangian liquid crystal energy was carried out in previous work where we also analyzed liquid crystal phase transitions triggered by change in rod density [11]. In this work, we assume that the anisotropic behavior of the rigid units is represented by a liquid-like, Eulerian liquid crystal energy. Sufficient regularity of the deformation map is required to guarantee its invertibility, in order to pass from the current configuration of the nematic liquid crystal to the reference configuration of the elastic solid.

There are two main quantities that describe the anisotropy associated with a liquid crystal elastomer: the traceless order tensor Q describing the nematic order of rigid rod units, and the positive definite step-length tensor L that encodes the shape of the network. L is spherical for isotropic polymers and spheroidal for uniaxial nematic elastomers, in which case, it has eigenvalues $l_\parallel$ and $l_\perp$ (double). The quantity $r := \frac{l_\parallel}{l_\perp} - 1$ measures the degree of anisotropy of the network, with positive values corresponding to prolate shape and negative ones to oblate. In the prolate geometry, the eigenvector $\boldsymbol{n}$ associated with $l_\parallel$ is the director of the theory, giving the average direction of alignment of the rods and also the direction of shape

elongation of the network. It is natural to assume that L and Q share the same eigenvectors. In this article, we set $Q = L - \frac{1}{3}(\mathrm{tr}L)I$ so as to obtain a traceless Q, from a given positive definite tensor L ([43], page 49). The free energy may also carry information on the anisotropy L_0 imprinted in the network at crosslinking the original polymer melt. In this work, we choose $L_0 = I$.

The standard Landau-de Gennes free energy density consists of the sum of scalar quadratic terms of ∇Q and the bulk scalar function $f(Q)$, usually a polynomial of the trace of powers of Q, describing the phase transition between the isotropic and the nematic phases of the liquid crystal [29], [38]. In this work, we take a departure from these forms but still keeping consistentcy with the original Landau-de Gennes theory. We first observe that the polynomial growth is not physically realistic, since it is expected that the energy should grow unboundedly near limiting alignment configurations. In the uniaxial case, these correspond to perfect alignment, characterized by scalar order parameter $s = 1$, and configurations where the rods are confined to the plane perpendicular to the director $\boldsymbol{n}$ [12], [23]. In terms of the order tensor, the limiting configuration is represented by the minimum eigenvalue taking the value $-\frac{1}{3}$. Bounds on eigenvalues of Q are not part of the original theory, but are needed for it to be compatible with the Maier-Saupe theory from statistical physics [5]. This turns out to be as well an essential element of our analysis. Also, we take the gradient of Q with respect to space variables in the deformed configuration, in which case the coupling with the deformation gradient F emerges naturally. It turns out that powers of gradient of Q, higher than quadratic, in the energy, are required for compactness.

The elastic energy density proposed by Blandon, Terentjev and Warner is given by the trace form [43]:

$$\mathcal{W}_{\mathrm{BTW}} = \mu \mathrm{tr}(L_0 F^T L^{-1} F - \frac{1}{3}I). \qquad (1.1)$$

This is the analog of the Neo-Hookean energy of isotropic elasticity and is also derived from Gaussian statistical mechanics. Let us call $G = L^{-\frac{1}{2}} F L_0^{\frac{1}{2}}$ the effective deformation tensor of the network; of course, in general, G is not itself a gradient. Then $\mathcal{W}_{\mathrm{BTW}} = \mu(|G|^2 - 1)$. Motivated by the theory of existence of minimizers of isotropic nonlinear elasticity ([3]), in his PhD, thesis [32], Luo generalizes $\mathcal{W}_{\mathrm{BTW}}$ to polyconvex stored energy density functions $\hat{w}(G(\boldsymbol{x}))$; that is, $\hat{w}(G) = \Psi(G, \mathrm{adj}\, G, \det G)$ is a convex function of $(G, \mathrm{adj}\, G, \det G)$. This approach was used later in [11]) to model phase transitions in rod networks. In order to recover the limiting deformation gradient F^* from the minimizing sequences $\{G_k\}_{k \geq 1}$, it is necessary that the minimizing sequences $\{L_k\}$ yield a nonsingular limit. This is achieved by requiring the blowup of $f(Q)$ as the minimum eigenvalue of Q tends to $-\frac{1}{3}$, that is, $f(Q) \to \infty$ as $\det(Q + \frac{1}{3}I) = \det L \to 0$. We point out that this lends another significance to the minimum eigenvalue limit.

In a related work [14], Calderer and Luo carried out a mixed finite element analysis of the elastomer trace energy coupled with that of the Ericksen model of uniaxial nematic liquid crystals. This was later used in numerical simulations of domain formation in two-dimensional extensional deformations. From a different persepective, a study of uniaxial elastomers with variable length director was carried out in [13], for a restricted set of deformation maps.

Let us now comment on the deeper mechanical significance of G (also denoted F_{eff}) in connection with the special class of spontaneous deformation as brought up

by Agostiniani, DeSimone and Teresi [1], [22]. Spontaneous deformations are those that do not cost any elastic energy. In uniaxial nematics, they correspond to volume preserving uniaxial extensions along the eigenvector $\boldsymbol{n}$, the latter being defined in the current configuration of the elastomer. (In the context of biaxial nematics, volume preserving biaxial extensions are also spontaneous deformations represented by $F_s = \sqrt{L_s}$, where, in its (unit) eigenvector representation, $L_s := a\boldsymbol{m} \otimes \boldsymbol{m} + \mathbf{r} \otimes \mathbf{r}) + c\boldsymbol{n} \otimes \boldsymbol{n}, \ a, b, c > 0, \ abc = 1$). Spontaneous strains have crystallographic significance in that they represent variants in domain patterns present in low energy microstructure. The chevron domains observed by Sanchez and Finkelman in liquid crystal elastomers realize the microstructure in these materials. [31], [40] and [44].

We note that F_{eff} does not represent the deformation of the elastomer with respect to the identity but with respect to spontaneous deformations $\sqrt{L_s}$. Consequently, the Trieste group also pointed out that F_{eff} is the only deformation tensor that contributes to the elastic energy of the elastomer, this energy being isotropic, since it has the same form regardless the current value of $\boldsymbol{n}$. These authors proposed to include as well an anisotropic component in the energy depending on $F^T F$ (2.8). We observe the regularizing role of the latter part of the energy. Without loss of generality, in this work, we neglect the latter term and address the more challenging problem of the energy depending only on G (F_{eff}).

In addition to the trace models of liquid crystal elastomer energy studied by Terentjev and Warner ([43] and references therein), generalizations of these earlier forms have been proposed and studied by several authors ([2] and [26]; [1], [15], [16] and [22]). In these references, the authors propose energies based on powers of the earlier trace form, including Ogden type energies, and study their extensions to account for semisoft elasticity. Also, the analysis of equilibrium states presented in [1] applies to elastomer energy density functions that are not quasiconvex, these being appropriate to model crystal-like phase transitions.

The types of boundary conditions that we consider include prescribing the deformation map on the boundary or part of it. In such cases, we also prescribe components of the order tensor Q there. In an alternate approach, instead of prescribing boundary conditions on Q, we include a surface free energy of the Rapini-Papoular type. The latter also extends to those parts of the boundary with no prescribed Dirichlet conditions on the deformation map. In such a case, the energy integral is formulated in terms of the *pull-back* order tensor $\tilde{Q}(\boldsymbol{x})$, $\boldsymbol{x} \in \Omega$.

This article is organized as follows. Section 2 is devoted to modeling, with special emphasis on analyzing the type of coupling between the Landau-de Gennes model of nematic liquid crystal and the nonlinear elasticity of the anisotropic network. In Section 3, we study the admissible set of fields corresponding to finite energy, focusing on classes of deformation maps and boundary conditions for which the invertibility property of the maps holds. Section 4 addresses minimization of the energy. The conclusions are described in Section 5.

2. **The Landau-de Gennes liquid crystal elastomer.** Equilibrium configurations of nematic liquid crystal elastomers are characterized by the deformation gradient F together with the symmetric tensors L and Q, describing the shape of the material and the nematic order, respectively. Within the point of view of the mean-field theory, the state of alignment of a nematic liquid crystal is given by a probability distribution function ρ in the unit sphere. The order tensor is defined as the second order moment of ρ:

FIGURE 1. Representation of the step-lenght tensor L: isotropic polymer (left) and nematic polymer (right).

$$Q = \int_{\mathbb{S}^2} (\boldsymbol{m} \otimes \boldsymbol{m} - \frac{1}{3}I)\rho(\boldsymbol{m}) \, d\boldsymbol{m}. \tag{2.1}$$

From this definition, it follows that Q is a symmetric, traceless, 3×3 matrix with bounded eigenvalues ([25] and [5])

$$-\frac{1}{3} \leq \lambda_i(Q) \leq \frac{2}{3}, \quad i = 1, 2, 3, \quad \sum_{i=1}^{3} \lambda_i(Q) = 0. \tag{2.2}$$

For biaxial nematic, Q admits the representation

$$Q = r(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1 - \frac{1}{3}I) + s(\boldsymbol{e}_2 \otimes \boldsymbol{e}_2 - \frac{1}{3}I), \tag{2.3}$$

where r and s correspond to the biaxial order parameters

$$s = \lambda_1 - \lambda_3 = 2\lambda_1 + \lambda_2, \quad r = \lambda_2 - \lambda_3 = \lambda_1 + 2\lambda_2,$$

and $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are unit eigenvectors. If $r = 0$, then (2.3) yields the uniaxial order tensor $Q = s(\boldsymbol{e}_2 \otimes \boldsymbol{e}_2 - \frac{1}{3}I)$, where $s \in (-\frac{1}{2}, 1)$ corresponds to the uniaxial nematic order parameter and $\boldsymbol{n} = \mathbf{e}_2$ is the unit director field of the theory.

In a rigorous study of the Landau-De Gennes model [34], Majumdar observes that the definition of Q given by (2.1) is that of the Maier-Saupe mean-field theory [33]. In the original theory by Landau and de Gennes [19], [29], Q has a phenomenological role as a dielectric or magnetic susceptibility tensor, and its eigenvalues do not satisfy any inequality constraints. It is the latter that bring compatibility to these theories.

Following the property of freely joined rods, we assume that L and Q have common eigenvectors and propose the constitutive relation

$$L = a_0(Q + \frac{1}{3}I), \tag{2.4}$$

where $a_0 = \text{tr}L > 0$ is constant. The linear constitutive equation (2.4) is analogous to those proposed by Terentjev and Warner [43] and Fried and Sellers [26] stating that, given a symmetric and traceless tensor Q and a constant $\beta > 0$, there is a one α-parameter family of step-length tensors L with $\text{tr}L = \beta$, and such that $L = \beta(\alpha Q + \frac{1}{3}I)$. The form (2.4) corresponds to taking $\alpha = 1$ and $\beta = a_0$.

Letting l_1, l_2, l_3 denote the eigenvalues of L, it reduces to the uniaxial nematic with director $\boldsymbol{n}$ and order parameter a multiple of s in the case that

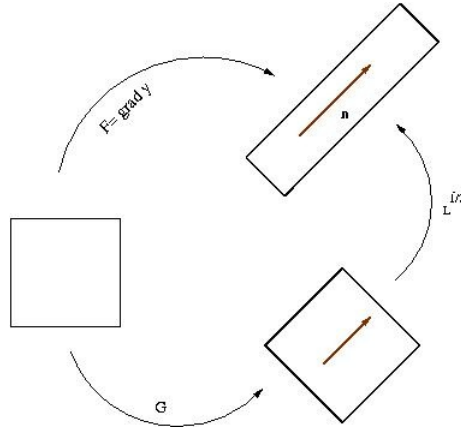$$l_2 = l_1 := l_\perp, \ l_3 := l_\parallel.$$

FIGURE 2. Relation between the deformation gradient F and the effective deformation tensor F_{eff}.

The mechanical response of the elastomer along $\boldsymbol{n}$ is distinguished from that along any of the transverse directions.

From the constitutive assumption (2.4) it follows that

$$\det L = 0 \iff \det(Q + \frac{1}{3}I) = 0 \iff \lambda_{\min}(Q) = -\frac{1}{3}, \qquad (2.5)$$

where $\lambda_{\min}(Q)$ stands for the minimal eigenvalue of a symmetric tensor Q. This shows another consequence of requiring $\lambda_{\min}(Q) > -\frac{1}{3}$: to gurantee the invertibility of L, and so, to be able to recover the gradient of deformation from the effective deformation tensor G.

We assume that, in the reference configuration, a liquid crystal elastomer occupies a bounded domain $\Omega \subset \mathbf{R}^3$ with smooth boundary $\partial\Omega$. We denote the deformation map of the elastomer and its gradient as

$$\boldsymbol{\varphi} : \Omega \to \boldsymbol{\varphi}(\Omega), \quad \boldsymbol{y} = \boldsymbol{\varphi}(\boldsymbol{x}), \qquad (2.6)$$

$$F(\boldsymbol{x}) = \nabla\boldsymbol{\varphi}(\boldsymbol{x}), \quad \det F(\boldsymbol{x}) \geq \delta_0, \qquad (2.7)$$

where $\delta_0 > 0$ is a given constant. This last constraint on the determinant expresses the maximum degree of compressibility allowed to the material.

The trace-form free energy density $\mathcal{W}_{\text{BTW}} = \mu\text{tr}(L_0 F^T L^{-1} F - \frac{1}{3}I)$ expresses the coupling between the step length tensor L and the deformation gradient F and also encodes the anisotropy L_0 of the reference configuration. Usually, L_0 is a constant positive definite symmetric tensor and, by rescaling, in what follows, we assume $L_0 = I$. Define $G = F_{\text{eff}} = L^{-\frac{1}{2}}F$.

In general, scalar functions of the invariants of the tensors FF^T and $F_{\text{eff}}^T F_{\text{eff}}$ are admissible. Let us examine how vectors transform in each of these cases as illustrated in figure (2).

In [22], the authors propose an elastomer energy of the form

$$W(F, L, L_0) = \alpha W_\alpha(F_{\text{eff}} F_{\text{eff}}^T) + \beta W_\beta(F^T F), \qquad (2.8)$$

with F_{eff} representing the deformation tensor with respect to spontaneous deformations. The α-component of this energy was also analyzed in previous work [11], [32], and in [13] and [14] for the Neo-Hookean trace form of the energy. As indicated in

the introduction, these terms correspond to two limiting liquid crystal elastomer behaviors, perhaps ideal, the first corresponding to the case that the material is made of pure fibers and the second to a standard liquid crystal elastomer but showing interaction between alignment and deformation.

We focus on the cases of nontrivial coupling between Q and F and propose a Landau-de Gennes elastomer energy of the following form:

$$\mathcal{E}(\boldsymbol{\varphi}, Q) = \int_\Omega \hat{W}(G)\, d\boldsymbol{x} + \int_{\boldsymbol{\varphi}(\Omega)} \big(\mathcal{L}(\nabla_{\boldsymbol{y}} Q, Q) + f(Q) \big)\, d\boldsymbol{y}, \tag{2.9}$$

where, for certain given $\boldsymbol{\varphi}$ and Q,

$$L(\boldsymbol{y}) = a_0(Q(\boldsymbol{y}) + \tfrac{1}{3}I), \text{ where } a_0 > 0 \text{ is a constant,} \tag{2.10}$$

$$G = G(\boldsymbol{x}) := \tilde{L}(\boldsymbol{x})^{-\frac{1}{2}} F, \ F = \nabla \boldsymbol{\varphi}(\boldsymbol{x}), \ \tilde{L}(\boldsymbol{x}) = L(\boldsymbol{\varphi}(\boldsymbol{x})), \tag{2.11}$$

$$(\nabla_{\boldsymbol{y}} Q)_{ijk} = \tfrac{\partial Q_{ij}}{\partial y_k}, \ 1 \le i, j, k \le 3. \tag{2.12}$$

In what follows, we denote $\mathbb{M}^3$ the space of three-dimensional tensors and $\mathbb{M}^3_+ = \{M \in \mathbb{M}^3 : \det M > 0\}$. According to (2.2), we define

$$\mathcal{Q} = \{Q \in \mathbb{M}^3 : Q = Q^T, \ \mathrm{tr} Q = 0, \ -\frac{1}{3} < \lambda_{\min}(Q) \le \lambda_{\max}(Q) \le \frac{2}{3}\}. \tag{2.13}$$

Then, for $Q \in \mathcal{Q}$, it follows that $|Q| \le \frac{2}{\sqrt{3}}$ and the tensor L defined by (2.4) is invertible.

As for the density functions $\hat{W}$, $\mathcal{L}$ and f in (2.9), we make the following assumptions motivated by the analogous ones in isotropic nonlinear elasticity [3].

Polyconvexity and coerciveness of $\hat{W}$: There exists a convex function $\Psi : \mathbb{M}^3_+ \times \mathbb{M}^3 \times \mathbb{R}^+ \to \mathbb{R}$ such that $\hat{W}$ in (2.9) satisfies

$$\hat{W}(G) = \Psi(G, \mathrm{adj}\, G, \det G). \tag{2.14}$$

Also, there exist constants $\alpha > 0$, $p > 3$ such that

$$\hat{W}(G) \ge \alpha |G|^p, \quad \forall G \in \mathbb{M}^3_+. \tag{2.15}$$

Convexity and growth of $\mathcal{L}$: The Landau-de Gennes energy function $\mathcal{L}(\nabla_{\boldsymbol{y}} Q, Q)$ is convex in $\nabla_{\boldsymbol{y}} Q$. Moreover, there exists a constant $\kappa > 0$ such that

$$\mathcal{L}(\nabla_{\boldsymbol{y}} Q, Q) \ge \kappa |\nabla_{\boldsymbol{y}} Q|^r, \tag{2.16}$$

where r is a constant satisfying

$$r > \max\{3, \frac{p}{p-3}\}. \tag{2.17}$$

Blow-up of f: The bulk free energy density $f : \mathcal{Q} \to \mathbb{R}^+$ is continuous and satisfies

$$\lim_{\lambda_{\min}(Q) \to -\frac{1}{3}} f(Q) = +\infty. \tag{2.18}$$

Notation. For r as in (2.17), we define

$$q = \frac{pr}{p+r}. \tag{2.19}$$

We point out that $q > \max\{\frac{p}{p-2}, \frac{3p}{p+3}\} > 1$.

Remarks.

1. If L is given by (2.4), then $0 < \det L \le (a_0)^3$ when $Q \in \mathcal{Q}$. So, in the case that $\det F \ge \delta_0$, we have that $\det G \ge \delta_0(a_0)^{-\frac{3}{2}}$. Therefore, no condition on the growth near zero-determinant has to be imposed on $\hat{W}(G)$.

2. We observe that $\det L$ can become arbitrarily small. This corresponds to the polymer adopting a needle or plate shape.

3. The growth condition (2.18) has been applied in [5] in the context of studying of minimization of the Landau-de Gennes energy. Its restriction to the uniaxial case was first proposed by Ericksen [23] and used in analysis of defects in liquid crystal flow [7, 8, 9, 12].

In order to achieve a better understanding of the gradient part of the of the Landau-de Gennes energy (2.16), let us give a brief review of the standard liquid crystal theory [38]. The total energy is of the form

$$\mathcal{E}_{\mathrm{LdeG}} = \int_\Omega (\Psi(\nabla Q, Q) + f_{\mathrm{B}}(Q; T))\, d\boldsymbol{x},$$

$$\Psi(\nabla Q, Q) = \sum_{i=1}^4 L_i I_i,$$

$$f_{\mathrm{B}}(Q; T) = \frac{a(T)}{2} \mathrm{tr} Q^2 - \frac{b}{3} \mathrm{tr} Q^3 + \frac{c}{4} \mathrm{tr} Q^4,$$

where $a(T) = \alpha(T - T^*)$, $T > 0$ denotes the absolute temperature, $\alpha, T^*, b, c, L_i = L_i(T)$ are constants, and

$$I_1 = Q_{ij,j} Q_{ik,k},\ I_2 = Q_{ik,j} Q_{ij.k},$$
$$I_3 = Q_{ij,k} Q_{ij,k},\ I_4 = Q_{lk} Q_{ij.l} Q_{ij.k}.$$

In the special case of a single constant, the energy (2.20) reduces to $L|\nabla Q|^2$. For this energy, existence of global minimizer was discussed in [36], with further studies of regularity, characterization of uniaxial and biaxial states, and structure of defect sets presented in [35].

3. **Admissible classes of fields.** In what follows, we let $p > 3$ and $r > \max\{3, \frac{p}{p-3}\}$ be as in (2.17). We consider the admissible classes of $(\boldsymbol{\varphi}, Q)$ for the energy $\mathcal{E}(\boldsymbol{\varphi}, Q)$, from subclasses of functions $\boldsymbol{\varphi} \in W^{1,p}(\Omega, \mathbb{R}^3)$ and $Q \in W^{1,r}(\boldsymbol{\varphi}(\Omega), \mathbb{M}^3)$. Throughout the paper, given a measurable set $B \subset \mathbb{R}^3$ and a measurable function ω on B, we define $\omega \in W^{1,s}(B)$, provided there exist an open set O containing B and a function $\tilde{\omega} \in W^{1,s}(O)$ such that $\tilde{\omega} = \omega$ on B.

We assume $\boldsymbol{\varphi} \in W^{1,p}(\Omega, \mathbb{R}^3)$ and that the condition (2.7) above is satisfied. To avoid material inter-penetration, we also require that $\boldsymbol{\varphi}$ be injective. The latter issue is addressed in forthcoming lemmas.

Since $p > 3$, by Sobolev embedding, every map $\boldsymbol{\varphi} \in W^{1,p}(\Omega, \mathbb{R}^3)$ is Hölder continuous on $\bar{\Omega}$. Moreover, in [37] Marcus and Mizel proved that, for every measurable set $A \subseteq \Omega$, the set $\boldsymbol{\varphi}(A)$ is also measurable and

$$|\boldsymbol{\varphi}(A)| \le C\, |A|^{1 - \frac{3}{p}} \|\nabla \boldsymbol{\varphi}\|_{L^p(A)}^3. \tag{3.1}$$

In particular, $|\boldsymbol{\varphi}(A)| = 0$ for all $A \subset \bar{\Omega}$ with $|A| = 0$ (that is, $\boldsymbol{\varphi}$ satisfies the so-called **Lusin (N) property**). Furthermore, the following change of variable formula (or area formula) holds (see also [30]): if $g \ge 0$ is measurable, then

$$\int_{\boldsymbol{\varphi}(\Omega)} N(\boldsymbol{\varphi}, \boldsymbol{y}) g(\boldsymbol{y})\, d\boldsymbol{y} = \int_\Omega g(\boldsymbol{\varphi}(\boldsymbol{x})) \det \nabla \boldsymbol{\varphi}(\boldsymbol{x})\, d\boldsymbol{x}, \tag{3.2}$$

where

$$N(\boldsymbol{\varphi}, \boldsymbol{y}) = \mathcal{H}^0(\boldsymbol{\varphi}^{-1}(\boldsymbol{y})) = \#\{\boldsymbol{x} \in \Omega \colon \boldsymbol{\varphi}(\boldsymbol{x}) = \boldsymbol{y}\}. \tag{3.3}$$

Consequently, the injectivity of φ corresponds to the condition $N(\varphi, y) = 1$, for all $y \in \varphi(\Omega)$. In the context of nonlinear elasticity, this condition has been addressed by Ball [4], for pure displacement one-to-one boundary conditions, and also by Ciarlet and Nečǎs [17], in terms of the inequality:

$$\int_\Omega \det \nabla \varphi(x) \, dx \leq |\varphi(\Omega)|. \tag{3.4}$$

The following result is useful for our purpose.

Lemma 3.1. *Let* $\varphi \in W^{1,p}(\Omega, \mathbb{R}^3)$ *satisfy conditions* (2.7) *and* (3.4). *Then,* $N(\varphi, y) = 1$ *for a.e.* $y \in \varphi(\Omega)$*; hence, for all measurable* $g \geq 0$*, it follows that*

$$\int_{\varphi(\Omega)} g(y) \, dy = \int_\Omega g(\varphi(x)) \det \nabla \varphi(x) \, dx. \tag{3.5}$$

Moreover, $|\varphi^{-1}(B)| \leq |B|/\delta_0$ *for all measurable sets* $B \subseteq \varphi(\Omega)$*. In particular,* $|\varphi^{-1}(B)| = 0$ *for all* $B \subset \varphi(\Omega)$ *with* $|B| = 0$.

Proof. With $g(y) \equiv 1$ in (3.2), by (3.4), we obtain that

$$|\varphi(\Omega)| \leq \int_{\varphi(\Omega)} N(\varphi, y) \, dy = \int_\Omega \det \nabla \varphi(x) \, dx \leq |\varphi(\Omega)|.$$

Therefore, $N(\varphi, y) = 1$ for a.e. $y \in \varphi(\Omega)$. Hence (3.5) follows from (3.2). In (3.5), let $g(y) = \chi_B(y)$, where $B \subseteq \varphi(\Omega)$ is any measurable set, and χ_B denotes the characteristic function. So, we have

$$|B| = \int_B dy = \int_\Omega \chi_B(\varphi(x)) \det \nabla \varphi \, dx = \int_{\varphi^{-1}(B)} \det \nabla \varphi \, dx \geq \delta_0 |\varphi^{-1}(B)|,$$

which completes the proof. $\qquad \square$

Remark 1. From the arguments of the proof, we see that for maps $\varphi \in W^{1,p}(\Omega, \mathbb{R}^3)$ with $\det \nabla \varphi(x) > 0$ a.e. Ω, if inequality (3.4) holds then it must be an equality.

We also need the following result on invertibility of the deformation map. For related results under weaker regularity conditions, we refer the reader to [24].

Lemma 3.2. *Let* $\varphi \in W^{1,p}(\Omega, \mathbb{R}^3)$ *satisfy conditions* (2.7) *and* (3.4). *Then, there exist sets* $N \subset \Omega$ *and* $Z \subset \varphi(\Omega)$ *with* $|N| = |Z| = 0$ *such that* $\varphi \colon \Omega \setminus N \to \varphi(\Omega) \setminus Z$ *is bijective and the inverse map* $\varphi^{-1} = \psi$ *belongs to* $W^{1,p/2}(\varphi(\Omega) \setminus Z)$*, with*

$$\nabla_y \psi(y) = ((\nabla_x \varphi)^{-1} \circ \psi)(y) = \frac{\mathrm{adj}((\nabla \varphi) \circ \psi)(y)}{\det((\nabla \varphi) \circ \psi)(y)} \quad a.e. \ y \in \varphi(\Omega) \setminus Z. \tag{3.6}$$

Proof. Let $N(\varphi, y) = 1$ for $y \in \varphi(\Omega) \setminus Z_1$, where $|Z_1| = 0$. By [24, Theorem 3.1], there exists a set $N_1 \subset \Omega$, with $|N_1| = 0$, such that for each $x_0 \in \Omega \setminus N_1$, there is an open neighborhood $D_{x_0} \subset\subset \Omega$, for which there exist $\delta > 0$ and a function $\psi_0 \in W^{1,p/2}(B_\delta(y_0), D_{x_0})$, with $y_0 = \varphi(x_0)$, satisfying the following properties:

$$\psi_0 \circ \varphi(x) = x \ \ a.e. \ x \in D_{x_0}, \quad \varphi \circ \psi_0(y) = y \ \ a.e. \ y \in B_\delta(y_0),$$
$$\nabla_y \psi_0(y) = ((\nabla_x \varphi)^{-1} \circ \psi_0)(y) \quad a.e. \ y \in B_\delta(y_0).$$

Let $N = N_1 \cup \varphi^{-1}(Z_1) \subset \Omega$ and $Z = Z_1 \cup \varphi(N_1)$. By Lemma 3.1, $|Z| = |N| = 0$, and $\varphi \colon \Omega \setminus N \to \varphi(\Omega) \setminus Z$ is bijective. Let $\psi = \varphi^{-1} \colon \varphi(\Omega) \setminus Z \to \Omega \setminus N$ denote the inverse map. Let $y_0 \in \varphi(\Omega) \setminus Z$ and $x_0 = \psi(y_0) \in \Omega \setminus N$; so $x_0 \in \Omega \setminus N_1$ and $y_0 = \varphi(x_0)$. Let $\psi_0 \in W^{1,p/2}(B_\delta(y_0), D_{x_0})$ be the function determined above. It follows that $\psi = \psi_0$ a.e. $B_\delta(y_0)$. Hence ψ is weakly differentiable on $\varphi(\Omega) \setminus Z$ and the weak

gradient $\nabla\boldsymbol{\psi}(\boldsymbol{y})$ is given by (3.6). This also proves that $\nabla\boldsymbol{\psi} \in L^{p/2}(\boldsymbol{\varphi}(\Omega) \setminus Z)$, since $\mathrm{adj}\,\nabla\boldsymbol{\varphi}(\boldsymbol{x}) \in L^{p/2}(\Omega)$ and $\det\nabla\boldsymbol{\varphi}(\boldsymbol{x})) \geq \delta_0 > 0$. Finally, since clearly $\boldsymbol{\psi} \in L^{\infty}(\boldsymbol{\varphi}(\Omega) \setminus Z)$, it follows that $\boldsymbol{\psi} \in W^{1,p/2}(\boldsymbol{\varphi}(\Omega) \setminus Z)$. This completes the proof. $\quad\square$

In order to define the admissible set $\mathcal{A}$ of the variational problem, we first need to introduce the functional $\mathcal{S}$. In particular, it will help us identify types of boundary conditions of the displacement field that are compatible with the injectivity conditions previously discussed.

Let $S\colon W^{1,p}(\Omega,\mathbb{R}^3) \to \mathbb{R}^+$ be a given functional such that $S(t\boldsymbol{\varphi}) = |t|S(\boldsymbol{\varphi})$ for all $t \in \mathbb{R}$ and $\boldsymbol{\varphi}$. Assume that S is continuous under the weak convergence of $W^{1,p}(\Omega,\mathbb{R}^3)$, and that if $\boldsymbol{\varphi}$ is constant and $S(\boldsymbol{\varphi}) = 0$ then $\boldsymbol{\varphi} = 0$. Then, by the Sobolev-Rellich-Kondrachov compact embedding of $W^{1,p}(\Omega) \to L^p(\Omega)$, one easily has the following Poincaré-type inequality: there exists a constant C such that

$$\|\boldsymbol{\varphi}\|_{W^{1,p}(\Omega)} \leq C(S(\boldsymbol{\varphi}) + \|\nabla\boldsymbol{\varphi}\|_{L^p(\Omega)}) \quad \forall\,\boldsymbol{\varphi} \in W^{1,p}(\Omega,\mathbb{R}^3). \qquad (3.7)$$

For such a functional S and given a constant $\beta > 0$, let

$$\mathcal{D}_{S,\beta}(\Omega) = \{\boldsymbol{\varphi} \in W^{1,p}(\Omega,\mathbb{R}^3) : S(\boldsymbol{\varphi}) \leq \beta\}. \qquad (3.8)$$

In many applications, the functional S can be chosen as one of the following:

$$S_1(\boldsymbol{\varphi}) = \|\boldsymbol{\varphi}|_{\partial\Omega}\|_{L^p(\partial\Omega)}, \;\; \text{(Dirichlet boundary)}; \qquad (3.9)$$

$$S_2(\boldsymbol{\varphi}) = |\textstyle\int_D \boldsymbol{\varphi}\,d\boldsymbol{x}|, \;\; \text{where } D \subseteq \Omega \text{ with } |D| > 0, \;\; \text{(partial average)}; \quad (3.10)$$

$$S_3(\boldsymbol{\varphi}) = |\boldsymbol{\varphi}(\boldsymbol{x}_0)|, \;\; \text{where } \boldsymbol{x}_0 \in \bar{\Omega} \text{ is given}, \;\; \text{(one-point)}, \qquad (3.11)$$

the last choice following from the compact embedding $W^{1,p}(\Omega) \to C(\bar{\Omega})$ as $p > 3$.

Assume $\mathcal{B}(\Omega)$ is any nonempty subset of $\mathcal{D}_{S,\beta}(\Omega)$ that is closed under the weak convergence of $W^{1,p}(\Omega,\mathbb{R}^3)$. We then introduce an admissible class for energy $\mathcal{E}$ by

$$\mathcal{A} = \{(\boldsymbol{\varphi},Q) : \boldsymbol{\varphi} \in \mathcal{B}(\Omega) \text{ satisfies } (2.7),\,(3.4),\; Q \in W^{1,r}(\boldsymbol{\varphi}(\Omega),\mathcal{Q})\}, \qquad (3.12)$$

where $\mathcal{Q}$ is defined by expression (2.13).

Remarks.   1. Examples of sets $\mathcal{B}(\Omega)$ include the following ones, associated with standard types of boundary conditions:

$$\mathcal{B}_1(\Omega) = \{\boldsymbol{\varphi} \in W^{1,p}(\Omega,\mathbb{R}^3) : \boldsymbol{\varphi}|_{\partial\Omega} = \boldsymbol{\varphi}_0\} \;\; (\boldsymbol{\varphi}_0 \text{ a given trace-function}),$$

$$\mathcal{B}_2(\Omega) = \{\boldsymbol{\varphi} \in W^{1,p}(\Omega,\mathbb{R}^3) : \textstyle\int_D \boldsymbol{\varphi}\,d\boldsymbol{x} = 0\} \;\; (D \subseteq \Omega \text{ with } |D| > 0),$$

$$\mathcal{B}_3(\Omega) = \{\boldsymbol{\varphi} \in W^{1,p}(\Omega,\mathbb{R}^3) : \boldsymbol{\varphi}|_A = \boldsymbol{\varphi}_0|_A\} \;\; (A \subseteq \bar{\Omega} \text{ nonempty}, \boldsymbol{\varphi}_0 \text{ bounded}).$$

2. The set $\mathcal{B}_3(\Omega)$ includes $\mathcal{B}_1(\Omega)$ and the case that partial Dirichlet boundary conditions are prescribed. $\mathcal{B}_3$ can be considered a subset of $\mathcal{D}_{S,\beta}$ with $S = S_3$ defined by (3.11). This is mainly due to the assumption $p > 3$ and the compact embedding $W^{1,p}(\Omega) \to C(\bar{\Omega})$.

3. For $\mathcal{B}_1(\Omega)$ and if $\boldsymbol{\varphi}_0|_{\partial\Omega} \in W^{1,p}(\partial\Omega)$ is injective, then $\boldsymbol{\varphi}\colon \Omega \to \boldsymbol{\varphi}_0(\Omega)$ is bijective [4]. In this case, the current domain $\boldsymbol{\varphi}(\Omega)$ is fixed. The minimization problem considered below becomes less technical, with no need of changing the Landau-de Gennes energy integral to the reference domain Ω.

4. Deformation maps corresponding to $\mathcal{B}_2$ include anti-plane shear deformation.

Note that, for all $(\boldsymbol{\varphi},Q) \in \mathcal{A}$,

$$-1/3 < \lambda_{\min}(Q(\boldsymbol{y})) \leq 2/3 \quad a.e. \; \boldsymbol{y} \in \boldsymbol{\varphi}(\Omega).$$

Hence,

$$\det(Q(\boldsymbol{y}) + \frac{1}{3}I) > 0 \ \ a.e.\, \boldsymbol{y} \in \boldsymbol{\varphi}(\Omega), \quad \|Q\|_{L^\infty(\boldsymbol{\varphi}(\Omega))} \leq \frac{2}{\sqrt{3}}. \tag{3.13}$$

We now consider the *pull-back* order, step-length and effective deformation tensors:

$$\tilde{Q}(\boldsymbol{x}) = Q(\boldsymbol{\varphi}(\boldsymbol{x})), \ \ \tilde{L}(\boldsymbol{x}) = a_0(\tilde{Q}(\boldsymbol{x}) + \frac{1}{3}I), \ \ G(\boldsymbol{x}) = \tilde{L}(\boldsymbol{x})^{-\frac{1}{2}}\nabla\boldsymbol{\varphi}(\boldsymbol{x}). \tag{3.14}$$

We first explore the relationship between $Q(\boldsymbol{y})$ and $\tilde{Q}(\boldsymbol{x})$.

Lemma 3.3. *Let $p > 3$. Suppose that r and q are given by (2.17) and in (2.19), respectively. Then, for all $(\boldsymbol{\varphi}, Q) \in \mathcal{A}$, $\tilde{Q} \in W^{1,q}(\Omega, \mathcal{Q})$. Moreover,*

$$\nabla_{\boldsymbol{x}}\tilde{Q}(\boldsymbol{x}) = \nabla_{\boldsymbol{y}}Q(\boldsymbol{\varphi}(\boldsymbol{x}))\nabla\boldsymbol{\varphi}(\boldsymbol{x}) \quad a.e.\ \boldsymbol{x} \in \Omega. \tag{3.15}$$

Proof. Clearly $\tilde{Q} \in L^\infty(\Omega)$. In general, the composition $\tilde{Q} = Q \circ \boldsymbol{\varphi}$ may not be weakly differentiable. However, we show that this is the case if $(\boldsymbol{\varphi}, Q) \in \mathcal{A}$. By the approximation theorem [30, Lemma 10], there exist measurable sets $Z_j \subseteq \boldsymbol{\varphi}(\Omega)$ and Lipschitz functions Q_j in $\mathbb{R}^3$, such that $|Z_j| \to 0$ and $Q = Q_j$ in $\boldsymbol{\varphi}(\Omega) \setminus Z_j$. Let $\Omega_j = \boldsymbol{\varphi}^{-1}(\boldsymbol{\varphi}(\Omega) \setminus Z_j)$. Then $\tilde{Q}(\boldsymbol{x}) = Q_j(\boldsymbol{\varphi}(\boldsymbol{x}))$ for $\boldsymbol{x} \in \Omega_j$. Since Q_j is Lipschitz, and so $Q_j(\boldsymbol{\varphi})$ is weakly differentiable on Ω, it follows that $\tilde{Q}$ is weakly differentiable on Ω_j, with weak gradient given by

$$\nabla_{\boldsymbol{x}}\tilde{Q}(\boldsymbol{x}) = \nabla_{\boldsymbol{y}}Q_j(\boldsymbol{\varphi}(\boldsymbol{x}))\nabla\boldsymbol{\varphi}(\boldsymbol{x}) = \nabla_{\boldsymbol{y}}Q(\boldsymbol{\varphi}(\boldsymbol{x}))\nabla\boldsymbol{\varphi}(\boldsymbol{x}) \quad a.e.\ \boldsymbol{x} \in \Omega_j.$$

Note that $\Omega \setminus \Omega_j = \boldsymbol{\varphi}^{-1}(Z_j)$. Hence, $|\Omega \setminus \Omega_j| = |\boldsymbol{\varphi}^{-1}(Z_j)| \leq \frac{1}{\delta_0}|Z_j| \to 0$. This proves the weak differentiability of $\tilde{Q}$ on Ω and establishes the equation (3.15). Moreover, by relations (2.7) and (3.5),

$$\int_\Omega |\nabla_{\boldsymbol{y}}Q(\boldsymbol{\varphi}(\boldsymbol{x}))|^r d\boldsymbol{x} \leq \frac{1}{\delta_0} \int_\Omega |\nabla_{\boldsymbol{y}}Q(\boldsymbol{\varphi}(\boldsymbol{x}))|^r \det \nabla\boldsymbol{\varphi}(\boldsymbol{x})d\boldsymbol{x}$$
$$= \frac{1}{\delta_0} \int_{\boldsymbol{\varphi}(\Omega)} |\nabla_{\boldsymbol{y}}Q(\boldsymbol{y})|^r d\boldsymbol{y}. \tag{3.16}$$

So, $\nabla_{\boldsymbol{y}}Q(\boldsymbol{\varphi}(\boldsymbol{x})) \in L^r(\Omega)$. Since $\nabla\boldsymbol{\varphi} \in L^p(\Omega)$, it follows that

$$\nabla_{\boldsymbol{x}}\tilde{Q}(\boldsymbol{x}) = \nabla_{\boldsymbol{y}}Q(\boldsymbol{\varphi}(\boldsymbol{x}))\nabla\boldsymbol{\varphi}(\boldsymbol{x}) \in L^q(\Omega), \text{ where } \frac{1}{r} + \frac{1}{p} = \frac{1}{q} \text{ and } q > 1.$$

Hence $\tilde{Q} \in W^{1,q}(\Omega, \mathcal{Q})$. Furthermore, it follows that

$$\|\tilde{Q}\|_{W^{1,q}(\Omega)} \leq C(\|\nabla_{\boldsymbol{y}}Q\|_{L^r(\boldsymbol{\varphi}(\Omega))}\|\nabla\boldsymbol{\varphi}\|_{L^p(\Omega)} + 1), \tag{3.17}$$

where C is a constant independent of $(\boldsymbol{\varphi}, Q) \in \mathcal{A}$. $\qquad\square$

Let us now rewrite the total energy (2.9) for fields $(\boldsymbol{\varphi}, Q)$ in the admissible set.

It follows from (3.15) that, for $(\boldsymbol{\varphi}, Q) \in \mathcal{A}$, $\nabla_{\boldsymbol{y}}Q(\boldsymbol{\varphi}(\boldsymbol{x})) = \nabla_{\boldsymbol{x}}\tilde{Q}(\boldsymbol{x})\nabla\boldsymbol{\varphi}(\boldsymbol{x})^{-1}$. Therefore, by (3.5), we have that,

$$\mathcal{E}(\boldsymbol{\varphi}, Q) = \int_\Omega \hat{W}(G)\, d\boldsymbol{x} + \int_\Omega \left(\mathcal{L}(\nabla_{\boldsymbol{x}}\tilde{Q}\nabla\boldsymbol{\varphi}^{-1}, \tilde{Q}) + f(\tilde{Q}) \right) \det \nabla\boldsymbol{\varphi}\, d\boldsymbol{x}, \tag{3.18}$$

for all $(\boldsymbol{\varphi}, Q) \in \mathcal{A}$.

Let us now discuss appropriate boundary conditions to impose on Q, either in the form of strong anchoring (Dirichelt) or by modifying the total energy by adding a surface energy penalty of the Rapini-Papoular form [39]. For this, we first assume that $\boldsymbol{\varphi}$ satisfies Dirichlet boundary conditions on $\Gamma \subseteq \partial\Omega$ (Remarks 1 and 3, page 10), and require one of the following on Q:

1. Dirichlet boundary conditions:

$$Q(\boldsymbol{y}) = Q_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma \subseteq \partial\Omega \quad \text{with,} \tag{3.19}$$

$$\boldsymbol{y} = \boldsymbol{\varphi}_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma. \tag{3.20}$$

2. We include a surface energy contribution in the total energy. This term, of the Rapini-Papoular form is

$$\mathcal{E}_{\mathrm{S}}(\boldsymbol{\varphi}, Q) = \int_\Gamma h(\boldsymbol{x}, \tilde{Q}(\boldsymbol{x})) \, dS, \tag{3.21}$$

where $\tilde{Q}|_\Gamma$ is the L^q-trace of $\tilde{Q} \in W^{1,q}(\Omega, \mathcal{Q})$, $\alpha \geq 0$ and $h \geq 0$ denotes a continuous function satisfying

$$|h(\boldsymbol{x}, A) - h(\boldsymbol{x}, B)| \leq \alpha |A - B|^q, \tag{3.22}$$

with $A, B \in \mathbb{M}^{3\times3}$ and $\mathrm{tr}A = 0 = \mathrm{tr}B$. This energy form includes relevant expressions of the liquid crystal theory, such as

$$h(\boldsymbol{x}, Q) = \mathrm{tr}(Q - Q_0)^2, \tag{3.23}$$

with $Q_0 \in \mathcal{Q}$ prescribed.

In the case that $\boldsymbol{\varphi}$ does not satisfy Dirichlet boundary conditions on any part of $\partial\Omega$, we still allow for the modification of the energy as in (3.21), with $\Gamma \subseteq \partial\Omega$. We point out that the new energy integral is taken on the boundary of the reference domain and it involves the pull-back tensor $\tilde{Q}$. Additional regularity is required to pose that energy integral in the current domain; this issue will not be addressed in the current work.

The next two results will be employed in the proof of existence of energy minimizer. The first one establishes properties of weak limits of sequences of effective deformation tensors and their relation with those of the corresponding deformation gradient tensors. The second lemma refers to the preservation of relation (3.4) under weak convergence.

Lemma 3.4. *Let $L_k \in L^\infty(\Omega, \mathbb{S}^3_+)$ with $\|L_k\|_\infty \leq C$. Let $G_k = L_k^{-1/2} F_k$. Suppose $G_k \rightharpoonup \bar{G}$, $F_k \rightharpoonup \bar{F}$ in $L^p(\Omega, \mathbb{M}^3)$, where $p > 3$. Then, via a subsequence, $\mathrm{adj}\, G_k \rightharpoonup \bar{H}$, $\mathrm{adj}\, F_k \rightharpoonup \bar{K}$ in $L^{p/2}(\Omega, \mathbb{M}^3)$ and $\det G_k \rightharpoonup \bar{g}$, $\det F_k \rightharpoonup \bar{f}$ in $L^{p/3}(\Omega)$. Moreover, if $L_k(\boldsymbol{x}) \to \bar{L}(\boldsymbol{x})$ for a.e. $\boldsymbol{x} \in \Omega$, then*

$$\bar{L}^{1/2}\bar{G} = \bar{F}, \quad \bar{K} = \bar{H}\,\mathrm{adj}(\bar{L})^{1/2}, \quad (\det \bar{L}^{1/2})\,\bar{g} = \bar{f} \quad a.e. \ \Omega.$$

Proof. Clearly, if $\{G_k\}$ is bounded in $L^p(\Omega)$, then $\{\det G_k\}$ and $\{\mathrm{adj}\, G_k\}$ are bounded in $L^{p/3}(\Omega)$ and $L^{p/2}(\Omega)$, respectively. Hence the weak convergence of a further subsequence of both sequences follows as $p > 3$. By the bounded convergence theorem, our assumption implies that $g(L_k) \to g(\bar{L})$ strongly in $L^q(\Omega)$, for all $q \geq 1$ and for all continuous functions g. Therefore, $F_k = L_k^{1/2} G_k \rightharpoonup \bar{L}^{1/2}\bar{G}$ in $L^1(\Omega)$, and $\bar{L}^{1/2}\bar{G} = \bar{F}$. The two remaining statements follow from the elementary matrix identities: $\det(AB) = \det A \det B$ and $\mathrm{adj}(AB) = \mathrm{adj}(B)\,\mathrm{adj}(A)$. $\qquad\square$

Lemma 3.5. *Let $\boldsymbol{\varphi}_k, \boldsymbol{\varphi} \colon \bar{\Omega} \to \mathbb{R}^3$ be continuous. Suppose $|\boldsymbol{\varphi}(\partial\Omega)| = 0$ and $\boldsymbol{\varphi}_k \to \boldsymbol{\varphi}$ uniformly on Ω as $k \to \infty$. Then*

$$\limsup_{k\to\infty} |\boldsymbol{\varphi}_k(\Omega)| \leq |\boldsymbol{\varphi}(\Omega)|. \tag{3.24}$$

Furthermore, relation (3.4) remains invariant under weak convergence in $W^{1,p}(\Omega, \mathbb{R}^3)$, for $p > 3$.

Proof. Without loss of generality, let us assume that $\lim_{k\to\infty} |\boldsymbol{\varphi}_k(\Omega)|$ exists. So, for each $\epsilon > 0$, there exists a positive integer N such that

$$|\boldsymbol{\varphi}_k(\boldsymbol{x}) - \boldsymbol{\varphi}(\boldsymbol{x})| < \epsilon, \quad \forall\, k \geq N, \quad \forall\, \boldsymbol{x} \in \bar{\Omega}.$$

Let us denote $S = \boldsymbol{\varphi}(\Omega)$. The previous inequality implies that $\boldsymbol{\varphi}_k(\Omega) \subseteq S_\epsilon$, for all $k \geq N$, where $S_\epsilon = \{\boldsymbol{y} \in \mathbb{R}^3 \colon \operatorname{dist}(\boldsymbol{y}, S) < \epsilon\}$. Hence $|\boldsymbol{\varphi}_k(\Omega)| \leq |S_\epsilon|$, for all $k \geq N$. So

$$\lim_{k\to\infty} |\boldsymbol{\varphi}_k(\Omega)| \leq |S_\epsilon|. \tag{3.25}$$

Since $S_\epsilon \subseteq S_\delta$ for all $0 < \epsilon < \delta$, and $\cap_{\epsilon>0} S_\epsilon = \bar{S}$, we have

$$\lim_{\epsilon\to^+} |S_\epsilon| = |\cap_{\epsilon>0} S_\epsilon| = |\bar{S}| = |S| + |\partial S \setminus S|.$$

Since $S = \boldsymbol{\varphi}(\Omega)$, we easily verify that $\partial S \setminus S \subseteq \boldsymbol{\varphi}(\partial\Omega)$ and hence $|\partial S \setminus S| = 0$. This proves that $\lim_{\epsilon\to 0^+} |S_\epsilon| = |S|$, and thus (3.24) follows from (3.25). To show that condition (3.4) holds under weak convergence in $W^{1,p}(\Omega, \mathbb{R}^3)$, let us assume that $\boldsymbol{\varphi}_k \rightharpoonup \boldsymbol{\varphi} \in W^{1,p}(\Omega, \mathbb{R}^3)$ and also that

$$\int_\Omega \det \nabla\boldsymbol{\varphi}_k \, d\boldsymbol{x} \leq |\boldsymbol{\varphi}_k(\Omega)| \quad \forall\, k = 1, 2, \cdots.$$

A classical weak continuity theorem on determinants [3] asserts that $\det \nabla\boldsymbol{\varphi}_k \rightharpoonup \det \nabla\boldsymbol{\varphi}$ in $L^{p/3}(\Omega)$ as $p > 3$. Also, by the compact embedding of $W^{1,p}(\Omega) \to C(\bar{\Omega})$, it follows that $\boldsymbol{\varphi}_k \to \boldsymbol{\varphi}$ uniformly on Ω. Taking limits as $k \to \infty$ in the above inequality and applying (3.24), we obtain relation (3.4) for $\boldsymbol{\varphi}$. This concludes the proof of the lemma. $\square$

4. **Energy minimization.** The following theorem establishes the existence of minimizer of the energy $\mathcal{E}$ in the admissible class $\mathcal{A}$ defined above.

Theorem 4.1. *Let the admissible set $\mathcal{A}$ be defined as in (3.12). Suppose there exists a pair $(\boldsymbol{\varphi}, Q) \in \mathcal{A}$ such that $\mathcal{E}(\boldsymbol{\varphi}, Q) < \infty$. Then, there exists at least one pair $(\boldsymbol{\varphi}^*, Q^*) \in \mathcal{A}$ such that*

$$\mathcal{E}(\boldsymbol{\varphi}^*, Q^*) = \inf_{(\boldsymbol{\varphi}, Q)\in\mathcal{A}} \mathcal{E}(\boldsymbol{\varphi}, Q). \tag{4.1}$$

Proof. By assumption, there exists a constant $K_1 > 0$ such that

$$0 \leq \inf_{(\boldsymbol{\varphi}, Q)\in\mathcal{A}} \mathcal{E}(\boldsymbol{\varphi}, Q) < K_1. \tag{4.2}$$

Let $(\boldsymbol{\varphi}_k, Q_k) \in \mathcal{A}$ be a minimizing sequence for $\mathcal{E}$, that is

$$\lim_{k\to\infty} \mathcal{E}(\boldsymbol{\varphi}_k, Q_k) = \inf_{(\boldsymbol{\varphi}, Q)\in\mathcal{A}} \mathcal{E}(\boldsymbol{\varphi}, Q) < K_1. \tag{4.3}$$

Denote $F_k, G_k, L_k, \tilde{Q}_k, \tilde{L}_k$ the corresponding quantities defined from $(\boldsymbol{\varphi}_k, Q_k)$ as above.

Step 1. Coercivity. Given any $(\boldsymbol{\varphi}, Q) \in \mathcal{A}$, since $0 < \lambda_{\max}(\tilde{L}(\boldsymbol{x})) \leq a_0$, we easily see that

$$|\nabla\boldsymbol{\varphi}| \leq \sqrt{a_0}\, |\tilde{L}^{-1/2}\nabla\boldsymbol{\varphi}| = \sqrt{a_0}\, |G|. \tag{4.4}$$

By the coercivity assumptions,

$$\mathcal{E}(\boldsymbol{\varphi}, Q) \geq \alpha \int_\Omega |G|^p \, d\boldsymbol{x} + \int_{\boldsymbol{\varphi}(\Omega)} \big(f(Q) + \kappa|\nabla_{\boldsymbol{y}} Q|^r\big) \, d\boldsymbol{y}. \tag{4.5}$$

By (4.4), we have

$$\int_{\varphi(\Omega)} |\nabla_{\boldsymbol{y}} Q|^r \, d\boldsymbol{y} + \int_{\Omega} |\nabla \varphi|^p \, d\boldsymbol{x} \le C \, \mathcal{E}(\varphi, Q).$$

Since $\varphi \in \mathcal{D}_{S,\beta}(\Omega)$ (as defined in (3.8)), applying (3.7) and (3.17) yields

$$\|G\|_{L^p(\Omega)} + \|\varphi\|_{W^{1,p}(\Omega)} + \|\tilde{Q}\|_{W^{1,q}(\Omega)} \le C(\mathcal{E}(\varphi, Q)), \tag{4.6}$$

where $C(M)$ is a constant depending on $M > 0$ that remains bounded for M in a bounded set.

Step 2. Convergence and compactness. Let $(\varphi_k, Q_k) \in \mathcal{A}$ be the minimizing sequence above. By (4.6), we obtain that

$$\{(G_k, \varphi_k, \tilde{Q}_k)\} \text{ is bounded in } L^p(\Omega) \times W^{1,p}(\Omega) \times W^{1,q}(\Omega). \tag{4.7}$$

Hence, there exists a subsequence (labeled also by k) such that

$$G_k \rightharpoonup G^* \text{ in } L^p(\Omega), \quad \varphi_k \rightharpoonup \varphi^* \text{ in } W^{1,p}(\Omega), \quad \tilde{Q}_k \rightharpoonup \tilde{Q}^* \text{ in } W^{1,q}(\Omega), \tag{4.8}$$

$$g_k \equiv \det G_k \rightharpoonup g^* \text{ in } L^{p/3}(\Omega), \quad H_k \equiv \mathrm{adj}(G_k) \rightharpoonup H^* \text{ in } L^{p/2}(\Omega), \tag{4.9}$$

$$\det \nabla \varphi_k \rightharpoonup \det \nabla \varphi^* \text{ in } L^{p/3}(\Omega), \quad \mathrm{adj} \, \nabla \varphi_k \rightharpoonup \mathrm{adj} \, \nabla \varphi^* \text{ in } L^{p/2}(\Omega). \tag{4.10}$$

Since $p > 3$, the convergence statements in (4.10) follow from the classical weak continuity theorem of null-Lagrangians [3].

We first prove the following result on compensated compactness.

Lemma 4.2. *Let $p > 3$ and $q \in \mathbf{R}$ be as in (2.19), and define $m = \frac{pq}{p+2q}$. Then $m > 1$ and*

$$\nabla_{\boldsymbol{x}} \tilde{Q}_k \, \mathrm{adj} \, \nabla \varphi_k \rightharpoonup \nabla_{\boldsymbol{x}} \tilde{Q}^* \, \mathrm{adj} \, \nabla \varphi^* \quad \text{in } L^m(\Omega). \tag{4.11}$$

Proof. Since $\{\nabla_{\boldsymbol{x}} \tilde{Q}_k\}$ is bounded in $L^q(\Omega)$ and $\{\mathrm{adj} \, \nabla \varphi_k\}$ is bounded in $L^{p/2}(\Omega)$, we have that $\{\nabla_{\boldsymbol{x}} \tilde{Q}_k \, \mathrm{adj} \, \nabla \varphi_k\}$ is bounded in $L^m(\Omega)$, with m as above. It follows from (]refq) that $m > 1$. Therefore, we only need to show the convergence (4.11) in the distribution sense. Component-wise, such a convergence follows from the classical div-curl lemma, or from the representation

$$\left((\nabla_{\boldsymbol{x}} \tilde{Q})(\mathrm{adj} \, \nabla \varphi) \right)_{isj} = \sum_{m=1}^{3} \frac{\partial \tilde{Q}_{is}}{\partial x_m} (\mathrm{adj} \, \nabla \varphi)_{mj} = \det(\nabla \mathbf{u}), \tag{4.12}$$

where, for fixed $i, j, s = 1, 2, 3$, the vector-field $\mathbf{u} : \Omega \to \mathbb{R}^3$ is defined with components u_1, u_2, u_3 given by $u_j = \tilde{Q}_{is}$ and $u_k = \varphi \cdot \mathbf{e}_k, \, \forall k \ne j$. $\qquad \square$

Since $\|\varphi_k\|_{W^{1,p}(\Omega)}$ and $\|Q_k\|_{W^{1,r}(\varphi_k(\Omega))}$ are bounded and p, r are both greater than 3, we have by Morrey's inequality,

$$|\varphi_k(\boldsymbol{x}) - \varphi_k(\boldsymbol{x}')| \le C_1 |\boldsymbol{x} - \boldsymbol{x}'|^{1 - \frac{3}{p}}, \quad \forall \, \boldsymbol{x}, \, \boldsymbol{x}' \in \bar{\Omega},$$

$$|Q_k(\boldsymbol{y}) - Q_k(\boldsymbol{y}')| \le C_2 |\boldsymbol{y} - \boldsymbol{y}'|^{1 - \frac{3}{r}}, \quad \forall \, \boldsymbol{y}, \, \boldsymbol{y}' \in \overline{\varphi_k(\Omega)}.$$

Hence

$$|\tilde{Q}_k(\boldsymbol{x}) - \tilde{Q}_k(\boldsymbol{x}')| \le C_3 |\boldsymbol{x} - \boldsymbol{x}'|^{\gamma}, \quad \forall \, \boldsymbol{x}, \, \boldsymbol{x}' \in \bar{\Omega},$$

where $\gamma = (1 - \frac{3}{p})(1 - \frac{3}{r}) \in (0, 1)$. This shows that both (φ_k) and $(\tilde{Q}_k)$ are uniformly bounded and equi-continuous on $\bar{\Omega}$; hence, by Arzela-Ascoli theorem, it follows that, via another subsequence,

$$\varphi_k \to \varphi_* \quad \text{and} \quad \tilde{Q}_k(\boldsymbol{x}) \to \tilde{Q}_*(\boldsymbol{x}),$$

uniformly on $\bar{\Omega}$. Moreover, by uniqueness of weak limit, $\boldsymbol{\varphi}_* = \boldsymbol{\varphi}^*$ and $\tilde{Q}_* = \tilde{Q}^*$; that is, $\boldsymbol{\varphi}_k \to \boldsymbol{\varphi}^*$ and $\tilde{Q}_k = Q_k(\boldsymbol{\varphi}_k) \to \tilde{Q}^*$ uniformly on $\bar{\Omega}$. This imply that $\tilde{L}_k(\boldsymbol{x}) \to a_0(\tilde{Q}^*(\boldsymbol{x}) + \frac{1}{3}I) \equiv \tilde{L}^*(\boldsymbol{x})$ uniformly on Ω. Hence, by Lemma 3.4, for a.e. $\boldsymbol{x} \in \Omega$,

$$\tilde{L}^*(\boldsymbol{x})^{1/2} G^*(\boldsymbol{x}) = \nabla \boldsymbol{\varphi}^*(\boldsymbol{x}), \tag{4.13}$$

$$\mathrm{adj}\, \nabla \boldsymbol{\varphi}^*(\boldsymbol{x}) = H^*(\boldsymbol{x}) \, \mathrm{adj}(\tilde{L}^*(\boldsymbol{x}))^{1/2}, \tag{4.14}$$

$$\det \nabla \boldsymbol{\varphi}^*(\boldsymbol{x}) = g^*(\boldsymbol{x}) \det(\tilde{L}^*(\boldsymbol{x}))^{1/2}. \tag{4.15}$$

Step 3. Definition and properties of Q^*. By the weak convergence property $\det \nabla \boldsymbol{\varphi}_k \rightharpoonup \det \nabla \boldsymbol{\varphi}^*$, Lemma 3.5 and the weak closedness of $\mathcal{B}(\Omega)$, we have that $\boldsymbol{\varphi}^* \in \mathcal{B}(\Omega)$ and it satisfies (2.7) and (3.4). Hence, by Lemma 3.2, there exists an inverse map

$$\boldsymbol{\psi}^* = (\boldsymbol{\varphi}^*)^{-1} \in W^{1,p/2}(\boldsymbol{\varphi}^*(\Omega) \setminus Z, \Omega \setminus N).$$

This allows us to define the tensor map

$$Q^*(\boldsymbol{y}) = \tilde{Q}^*(\boldsymbol{\psi}^*(\boldsymbol{y})), \quad \boldsymbol{y} \in \boldsymbol{\varphi}^*(\Omega) \setminus Z. \tag{4.16}$$

From (3.1), it follows that $|(\boldsymbol{\psi}^*)^{-1}(N_j)| = |\boldsymbol{\varphi}^*(N_j)| \to 0$ if $N_j \subset \boldsymbol{\varphi}^*(\Omega) \setminus Z$ and $|N_j| \to 0$. Therefore, we follow the same lines of proof as in Lemma 3.3 to conclude that Q^* is weakly differentiable and

$$\nabla_{\boldsymbol{y}} Q^*(\boldsymbol{y}) = \nabla_{\boldsymbol{x}} \tilde{Q}^*(\boldsymbol{\psi}^*(\boldsymbol{y}))(\nabla_{\boldsymbol{x}} \boldsymbol{\varphi}^*(\boldsymbol{\psi}^*(\boldsymbol{y})))^{-1} \quad a.e.\ \boldsymbol{y} \in \boldsymbol{\varphi}^*(\Omega) \setminus Z. \tag{4.17}$$

This, together with the fact that $\nabla \tilde{Q}^* \in L^q$ and $(\nabla \boldsymbol{\varphi}^*)^{-1} = \frac{\mathrm{adj}\, \nabla \boldsymbol{\varphi}^*}{\det \nabla \boldsymbol{\varphi}^*} \in L^{p/2}$ give

$$Q^* \in W^{1,m}(\boldsymbol{\varphi}^*(\Omega) \setminus Z), \tag{4.18}$$

with m as in Lemma 4.2.

We next show that $\tilde{Q}^*(\boldsymbol{x}) \in \mathcal{Q}$ and thus $Q^*(\boldsymbol{y}) \in \mathcal{Q}$, by studying the properties of the minimizing sequence $\{\tilde{Q}_k\}$. We may assume $\tilde{Q}_k(\boldsymbol{x}) \to \tilde{Q}^*(\boldsymbol{x})$ for a.e. $\boldsymbol{x} \in \Omega$. Since $\tilde{Q}_k(\boldsymbol{x}) \in \mathcal{Q}$, it follows that

$$\tilde{Q}^*(\boldsymbol{x}) \in \mathcal{Q} \quad \forall \boldsymbol{x} \in \Omega. \tag{4.19}$$

It remains to show that $\det(\tilde{Q}^*(\boldsymbol{x}) + \frac{1}{3}) > 0$ a.e. on Ω. For this, let us denote $q_k := \det(\tilde{Q}_k + \frac{1}{3}I)$. Hence, the sequence $\{q_k\}$ is bounded and

$$q_k(\boldsymbol{x}) \to q^*(\boldsymbol{x}) = \det(\tilde{Q}^*(\boldsymbol{x}) + \frac{1}{3}),$$

a.e. $\boldsymbol{x} \in \Omega$. Now, we want to prove that $q^* > 0$ a.e. Ω. For this, we argue by contradiction and supposes that $q^* = 0$ on a set $A \subset \Omega$, with $|A| > 0$. Note that

$$\int_A \det(\tilde{Q}_k + \frac{1}{3}I)\, d\boldsymbol{x} \to \int_A \det(\tilde{Q}^* + \frac{1}{3}I)\, d\boldsymbol{x} = 0.$$

Consider now the sequence $f_k(\boldsymbol{x}) := f(\tilde{Q}_k(\boldsymbol{x}))$. Since $f_k \geq 0$, it follows from Fatou's theorem that,

$$\int_A \liminf_{k \to \infty} f_k(\boldsymbol{x})\, d\boldsymbol{x} \leq \liminf_{k \to \infty} \int_A f_k(\boldsymbol{x})\, d\boldsymbol{x}.$$

By the blow-up assumption (2.18) on f, for $\boldsymbol{x} \in A$,

$$\liminf_{k \to \infty} f_k(\boldsymbol{x}) = \lim_{\det(Q + \frac{1}{3}I) \to 0} f(Q) = +\infty,$$

and consequently $\lim_{k\to\infty} \int_A f(\tilde{Q}_k(\boldsymbol{x}))\, d\boldsymbol{x} = +\infty$. This contradicts the fact that

$$\int_\Omega f(\tilde{Q}_k(\boldsymbol{x}))d\boldsymbol{x} \leq C\mathcal{E}(\boldsymbol{\varphi}_k, Q_k) < CK_1.$$

Hence, $\tilde{Q}^*(\boldsymbol{x}) \in \mathcal{Q}$ a.e. $\boldsymbol{x} \in \Omega$. So $Q^*(\boldsymbol{y}) \in \mathcal{Q}$ for a.e. $\boldsymbol{y} \in \boldsymbol{\varphi}^*(\Omega)$.

Finally, we define

$$L^*(\boldsymbol{y}) = a_0\left(Q^*(\boldsymbol{y}) + \frac{1}{3}I\right). \tag{4.20}$$

Then $\det L^*(\boldsymbol{y}) > 0$; hence $L^*(\boldsymbol{y}) = a_0(Q^*(\boldsymbol{y}) + \frac{1}{3}I)$ is invertible a.e. $\boldsymbol{y} \in \boldsymbol{\varphi}^*(\Omega)$.

By (4.13) and (4.14), we have

$$G^* = (\tilde{L}^*)^{-1/2}\nabla\boldsymbol{\varphi}^*,\ \ H^* = \operatorname{adj} G^*,\ \ g^* = \det G^* \quad a.e.\ \Omega.$$

Therefore, $\mathcal{E}(\boldsymbol{\varphi}^*, Q^*) = E_1^* + E_2^* + E_3^*$, where

$$E_1^* = \int_\Omega \Psi(G^*, H^*, g^*)\, d\boldsymbol{x}, \quad E_2^* = \int_\Omega f(\tilde{Q}^*) \det \nabla\boldsymbol{\varphi}^* d\boldsymbol{x},$$

$$E_3^* = \int_\Omega \mathcal{L}(\nabla\tilde{Q}^*(\nabla\boldsymbol{\varphi}^*)^{-1}, \tilde{Q}^*) \det \nabla\boldsymbol{\varphi}^* d\boldsymbol{x}. \tag{4.21}$$

Step 4. Weak lower semicontinuity of the energy. As in (4.21), we write

$$\mathcal{E}(\boldsymbol{\varphi}_k, Q_k) = E_1^k + E_2^k + E_3^k,$$

where

$$E_1^k = \int_\Omega \Psi(G_k, H_k, g_k)\, d\boldsymbol{x}, \quad E_2^k = \int_\Omega f(\tilde{Q}_k) \det \nabla\boldsymbol{\varphi}_k d\boldsymbol{x},$$

$$E_3^k = \int_\Omega \mathcal{L}(\nabla\tilde{Q}_k(\nabla\boldsymbol{\varphi}_k)^{-1}, \tilde{Q}_k) \det \nabla\boldsymbol{\varphi}_k d\boldsymbol{x}. \tag{4.22}$$

The weak lower semicontinuity of $\mathcal{E}$ along $(\boldsymbol{\varphi}_k, Q_k)$ follows from that of each integral functional of (4.22). Specifically,

1. The weak lower semicontinuity of E_1^k follows from the convexity of $\Psi(G, H, g)$ on (G, H, g) and the weak convergence $G_k \rightharpoonup G^*$, $H_k \rightharpoonup H^*$ and $g_k \rightharpoonup g^*$ established above.

2. The weak lower semicontinuity of E_2^k follows from the weak convergence of $\det \nabla\boldsymbol{\varphi}_k \rightharpoonup \det \nabla\boldsymbol{\varphi}^*$ and the pointwise convergence of $f(\tilde{Q}_k(\boldsymbol{x})) \to f(\tilde{Q}^*(\boldsymbol{x}))$, which is uniform on sets where $\lambda_{\min}(\tilde{Q}^*(\boldsymbol{x})) \geq -\frac{1}{3} + \tau$ for any given $\tau > 0$.

3. Let us now prove the weak lower semicontinuity of E_3^k. First, we note that

$$\mathcal{L}(AB^{-1}, Q) \det B = \mathcal{F}(A \operatorname{adj} B, \det B, Q),$$

where $\mathcal{F}(A, t, Q) = t\mathcal{L}(A/t, Q)$. Elementary calculations show that $\mathcal{F}(A, t, Q)$ is convex in (A, t), for $t > 0$, provided $\mathcal{L}(A, Q)$ is convex in A. Let us write

$$E_3^k = \int_\Omega \mathcal{F}(\nabla\tilde{Q}_k \operatorname{adj} \nabla\boldsymbol{\varphi}_k, \det \nabla\boldsymbol{\varphi}_k, \tilde{Q}_k)\, d\boldsymbol{x}. \tag{4.23}$$

The weak lower semicontinuity of E_3^k follows from the convexity of $\mathcal{F}(A, t, Q)$ with respect to (A, t), the weak convergences of $\nabla\tilde{Q}_k \operatorname{adj} \nabla\boldsymbol{\varphi}_k \rightharpoonup \nabla\tilde{Q}^* \operatorname{adj} \nabla\boldsymbol{\varphi}^*$ and $\det \nabla\boldsymbol{\varphi}_k \rightharpoonup \det \nabla\boldsymbol{\varphi}^*$, and the uniform convergence of $\tilde{Q}_k \to \tilde{Q}^*$.

So, the combination of these three steps establishes the weak lower semicontinuity of $\mathcal{E}$ on $\mathcal{A}$. Hence,

$$\mathcal{E}(\boldsymbol{\varphi}^*, Q^*) \leq \lim_{k\to\infty} \mathcal{E}(\boldsymbol{\varphi}_k, Q_k) < K_1 < \infty.$$

This, in turn, shows that

$$\int_{\boldsymbol{\varphi}^*(\Omega)} |\nabla_{\boldsymbol{y}} Q^*(\boldsymbol{y})|^r \, d\boldsymbol{y} < \infty.$$

Consequently, $Q^* \in W^{1,r}(\boldsymbol{\varphi}^*(\Omega), \mathcal{Q})$, and hence $(\boldsymbol{\varphi}^*, Q^*) \in \mathcal{A}$ is a minimizer of $\mathcal{E}$ on $\mathcal{A}$. This completes the proof of Theorem 4.1. □

In the last part of this section, we will address boundary conditions on Q, in cases compatible with the type of regularity assumed so far. Straightforward modifications of the above proof, allow us to establish the following results.

Corollary 1. *Let $p > 3$, and $\sigma \geq 0$. Suppose that $\boldsymbol{\varphi}_0 \in W^{1,p}(\partial\Omega, \mathbb{R}^3)$, injective, and $Q^0 \in W^{1,2}(\partial\Omega, \mathcal{Q})$ are prescribed. Let $\mathcal{E}$ and $\mathcal{E}_S$ be as in (2.9) and (3.23), respectively, and define*

$$\mathcal{E}_{total} = \mathcal{E} + \sigma \mathcal{E}_S. \tag{4.24}$$

Suppose that $\mathcal{A}$ is as in (3.12) with $r \geq 2$ and $\mathcal{B} = \mathcal{B}_1$. Then, there exists a minimizer of the energy (4.24), in each of the following cases:

1. $\sigma = 0$ and Q satisfies the boundary conditions (3.19).
2. $\sigma \neq 0$ and $\Gamma \subseteq \partial\Omega$.

This corollary establishes existence of minimizer, even in the case that the Landau-de Gennes energy is quadratic on gradient of Q, as for standard nematic liquid crystals.

Corollary 2. *Suppose that $\Gamma \subset \partial\Omega$, with $\Gamma \neq \partial\Omega$. Let p, σ, Q_0, $\mathcal{E}$ and $\mathcal{E}_S$ be as in Corollary 1. Suppose that $\boldsymbol{\varphi}_0 \in W^{1,p}(\Gamma, \mathbb{R}^3)$ is injective and (3.20) holds. Suppose that $\mathcal{A}$ is as in (3.12) with $\mathcal{B} = \mathcal{B}_3$. Then, there exists a minimizer of the energy (4.24), in each of the following cases:*

1. $\sigma = 0$ and Q satisfies the boundary conditions (3.19).
2. $\sigma \neq 0$.

Next, we give an example of a family of plane deformations in the framework of Corollary 2 and that are relevant to experimental settings of liquid crystal elastomers [31], [44], [40] and [41]. For prescribed constants $a > 0, b > 0, c > 0$, and denoting $\mathcal{D} = \{(x_1, x_2) : -a < x_1 < a, \ -b < x_2 < b\}$, we define the domain and boundary, respectively,

$$\Omega = \{\boldsymbol{x} : (x_1, x_2) \in \mathcal{D}, \ -c < x_3 < c\},$$
$$\Gamma_{\pm} = \{\boldsymbol{x} : -a < x_1 < a, \ x_2 = \pm b, \ -c < x_3 < c\}.$$

Suppose that $Q_0 \in W^{1,2}(\Gamma, \mathcal{Q})$, $\lambda \geq 1$ and $\delta > 0$ are also prescribed. Letting $\boldsymbol{x} = (x_1, x_2, x_3) \in \Omega$, we consider the family of plane deformations,

$$y_1 = \varphi_1(x_1, x_2),$$
$$y_2 = \varphi_2(x_1, x_2),$$
$$y_3 = x_3, \tag{4.25}$$

subject to the constraint $\det[\varphi_1, \varphi_2] \geq \delta$, and boundary conditions,

$$\varphi_2(x_1, \pm b) = \pm\lambda b,$$
$$Q(x_1, \pm b) = Q_0.$$

The following observations apply:

1. The deformations in (4.25) contain extensions, uniaxial and biaxial, and shear. A modification of the third equation to the form $y_3 = \alpha(x_1, x_2) + \beta(x_1, x_2)x_3$, with appropriate choices of the continuous coefficients α and β, also allows to include extension or compression along x_3.

2. The two-dimensional deformation map (φ_1, φ_2) belongs to the family of Lipschitz continuous functions in $\mathcal{D}$. This implies the absence of cavities in the deformed configuration, and it also guarantees injectivity of the map.

3. A class of critical points of the energy of the form (4.25) are the stripped domains occurring as $\lambda > 1$ reaches a critical value. These are domains parallel to the x_1-direction, with alternating positive and negative values of the shear rate. An analysis of the length scales of these patterns is carried out in [10].

5. **Conclusion.** [1] In this article, we study existence of minimizers of a Landau-de Gennes liquid crystal elastomer. Special features of the work include the modeling of the liquid crystal behavior with the nematic order tensor Q, defined in the current configuration, rather than the customary uniaxial director field $\boldsymbol{n}$. Also, the Landau-de Gennes energy is taken in the Eulerian frame of the liquid crystal. The passing between the Lagrangian frame of the elastic energy and the Eulerian one of the liquid crystal carries analytical difficulties due to the need to ensure invertibility of the deformation map. This is achieved for an appropriate class of class of Dirichlet boundary conditions. However, the analysis does not cover the case that an anchoring energy is prescribed on the deformed boundary of the domain. This requires a higher regularity of the order tensor to ensure that boundary integrals of the trace of Q^2 are well defined. This is the subject of current analysis.

REFERENCES

[1] V. Agostiniani and A. DeSimone, Ogden-type energies for nematic elastomers, *Int J. Nonlinear Mechanics*, **47** (2012), 402–412.

[2] D. Anderson, D. Carlson and E. Fried, A continuum-mechanical theory for nematic elastomers, *J. Elasticity*, **56** (1999), 33–58.

[3] J. M. Ball, Convexity conditions and existence theorems in nonlinear elasticity, *Archive for Rational Mechanics and Analysis*, **63** (1977), 337–403.

[4] J. M. Ball, Global invertibility of sobolev functions and the interpenetration of matter, *Proceedings Royal Soc. Edinburgh A*, **88** (1981), 315–328.

[5] J. M. Ball and A. Majumdar, Nematic liquid crystals: From maier-saupe to a continuum theory, *Molecular Crystals and Liquid Crystals,* **525** (2010), 1–11.

[6] M. Barchiesi and A. DeSimone, Frank energy for nematic elastomers. A nonlinear model, Preprint, 2013.

[7] M. C. Calderer and B. Mukherjee, Chevron patterns in liquid crystal flows, *Physica D*, **98** (1996), 201–224.

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[1]At the time of completion of this article, the authors became aware of a recent preprint studying a model of liquid crystal elastomer with director field gradients [6]. The model studied here and the methods of proof show fundamental differences with the aforementioned work, resulting in two independent articles, with different scope and research points of view.

[8] M. C. Calderer and B. Mukherjee, On poiseuille flow of liquid crystals, *Liquid Crystals*, **22** (1997), 121–135.

[9] M. C. Calderer and B. Mukherjee, Mathematical issues in the modeling of flow behavior of polymeric liquid crystals, *J. Rheol.*, **42** (1998), 1519–1536.

[10] M. C. Calderer, Critical size of stripe patterns in liquid crystal elastomers under extension, Preprint, 2013.

[11] M. C. Calderer, C. A. Garavito and C. Luo, *Liquid Crystal Elastomers and Phase Transitions in Rod Networks*, Technical Report, arXiv:1303.6548, 2013.

[12] M. C. Calderer and C. Liu, Liquid crystal flow: dynamic and static configurations, *SIAM Journal on Applied Mathematics*, **20** (2000), 1225–1249.

[13] M. C. Calderer, C. Liu and B. Yan, A mathematical theory for nematic elastomers with non-uniform prolate spheroids, in *Advances in Applied and Computational Mathematics* (eds. F. Liu, Z. Nashed, G.M. Guerekata, D. Pokrajac, Z. Qiao, X. Shi, and X. Xia), 2006, 245–259.

[14] M. C. Calderer and C. Luo, Numerical study of liquid crystal elastomers by a mixed finite element method, *European J. Appl. Math.*, **23** (2012), 121–154.

[15] P. Cesana and A. DeSimone, Strain-order coupling in nematic elastomers: Equilibrium configurations, *Math. Models Methods Appl. Sci*, **19** (2009), 601–630.

[16] P. Cesana and A. DeSimone, Quasiconvex envelopes of energies for nematic elastomers in the small strain regime and applications, *J. Mech. Phys. Solids*, **59** (2011), 787–803.

[17] P-G. Ciarlet and J. Nečas, Injectivity and self-contact in nonlinear elasticity, *Arch. Rational Mech. Anal.*, **97** (1987), 171–188.

[18] S. Conti, A. DeSimone and G. Dolzmann, Soft elastic response of stretched sheets of nematic elastomers: A numerical study, *Journal of the Mechanics and Physics of Solids*, **50** (2002), 1431–1451.

[19] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals*, Oxford University Press, USA, 1995.

[20] A. DeSimone and G. Dolzmann, Material instabilities in nematic elastomers, *Physica D*, **136** (2000), 175–191.

[21] A. DeSimone and G. Dolzmann, Macroscopic response of nematic elastomers via relaxation of a class of $SO(3)$-invariant energies, *Arch. Rat. Mech. Anal.*, **161** (2002), 181–204.

[22] A. DeSimone and L. Teresi, Elastic energies for nematic elastomers, *The European Physical Journal E: Soft Matter and Biological Physics*, **29** (2009), 191–204.

[23] J. L. Ericksen, Liquid crystals with variable degree of orientation, *Archive for Rational Mechanics and Analysis*, **113** (1991), 97–120.

[24] I. Fonseca and W. Gangbo, Local invertibility of sobolev functions, *SIAM J. Math. Anal.*, **26** (1995), 280–304.

[25] G. Forest, Q. Wang and R. Zhou, A kinetic theory for solutions of nonhomogeneous nematic liquid crystalline polymers with density variations, *J.Fluid Engineering*, **126** (2004), 180–188.

[26] E. Fried and S. Sellers, Free-energy density functions for nematic elastomers, *J. Mech. Phys. Solids*, **52** (1999), 1671–1689.

[27] E. Fried and S. Sellers, Soft elasticity is not necessary for striping in nematic elastomers, *Journal of Applied Physics*, **100** (2006), 043521–043325.

[28] M. Gardel, J. H. Shin, L. Mahadevan, F. C. MacKintosh, P. Matsudaira and D. A. Weitz, Elastic behavior of cross-linked and bundled actin networks, *Science*, **304** (2004), 1301–1305.

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

[30] P. Hajlasz, Sobolev mappings, co-area formula, and related topics, *Proceedings on Analysis and Geometry*, (2000), 227–254.

[31] I. Kundler and H. Finkelmann, Strain-induced director reorientation in nematic liquid single crystal elastomers, *Macromolecular Rapid Communications*, **16** (1995), 679–686.

[32] C Luo, *Modeling, Analysis and Numerical Simulations of Liquid Crystal Elastomers*, Ph.D dissertation, University of Minnesota, 2010.

[33] W. Maier and A. Saupe, A simple molecular statistical theory of the nematic liquid crystalline-liquid phase, *I Z Naturf. a*, **14** (1959), 882–889.

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

[35] A. Majumdar, The landau–de gennes theory of nematic liquid crystals: Uniaxiality versus biaxiality, *Communications on Pure and Applied Analysis*, **11** (2012), 1303–1337.

[36] A. Majumdar and A. Zarnescu, Landau–de gennes theory of nematic liquid crystals: The oseen–frank limit and beyond, *Archive for rational mechanics and analysis*, **196** (2010), 227–280.

[37] M. Marcus and V. J. Mizel, Transformations by functions in sobolev spaces and lower semicontinuity for parametric variational problems, *Bulletin of the American Mathematical Society*, **79** (1973), 790–795.

[38] N. J. Mottram and C. Newton, *Introduction to Q-Tensor Theory*, in Research Report no. 10, 2004.

[39] A. Rapini and M. Papoular, Surface anchoring of nematic liqud crystals, *J. Physique Coll*, **30** (1969), 54–66.

[40] A. Sanchez-Ferrer and H. Finkelmann, Uniaxial and shear deformation in smectic-c main-chain liquid-crystalline elastomers, *Macromolecules*, **41** (2008), 970–980.

[41] A. Sanchez-Ferrer and H. Finkelmann, Mechanical properties of new main-chain liquid-crystalline elastomers, *Mol. Cryst. Liq. Cryst.*, **508** (2009), 348–356.

[42] B. Wagner, R. Tharmann, I. Haase, M. Fischer and A. R. Bausch, Cytoskeletal polymer networks: The molecule structure of cross-linkers determines macroscopic properties of cochlear outer hair-cells, *Proc.Natl. Acad. Sci USA*, **103** (2006), 13974–13978.

[43] M. Warner and E. M. Terentjev, *Liquid Crystal Elastomers*, Oxford University Press, USA, 2007.

[44] E. R. Zubarev, S. A. Kuptsov, T. I. Yuranova, R. V. Talroze and H. Finkelmann, Monodomain liquid crystalline networks: Reorientation mechanism from uniform to stripe domains, *Liquid crystals*, **26** (1999), 1531–1540.

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