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New variational models for nematic elastomers

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Contents

Notation

- $\mathbb{N}, \mathbb{Z}, \mathbb{R}$. The sets of natural, integer, real numbers.
- $\mathbb{R}^n$. The space of real vectors, $\mathbb{N} \ni n \geq 2$.
- $\mathbb{M}^{n\times n}$. The space of square matrices of order $n \times n$, $\mathbb{N} \ni n \geq 2$.
- $\mathbb{M}^{n\times n}_{sym}$. The space of square and symmetric matrices of order $n \times n$, $\mathbb{N} \ni n \geq 2$.
- $\mathbb{M}^{n\times n}_0$. The space of traceless matrices of order $n \times n$, $\mathbb{N} \ni n \geq 2$.
- $\mathbb{M}^{n\times n}_{0sym}$. The space of square and symmetric and traceless (deviatoric) matrices of order $n \times n$, $\mathbb{N} \ni n \geq 2$.
- $\mathbb{E} : \mathbb{M}^{n\times n} \mapsto \mathbb{M}^{n\times n}_{sym}$. The symmetric part, $n \in \mathbb{N}$.
- $\mathbb{E}_0 : \mathbb{M}^{n\times n} \mapsto \mathbb{M}^{n\times n}_{0sym}$. The deviatoric part, $n \in \mathbb{N}$.
- $\mathbf{I}_n$. The identity in $\mathbb{M}^{n\times n}$ (we always omit the subscription $_n$).
- $\mathbb{S}^{k-1}$. The unit sphere in $\mathbb{R}^k$, $\mathbb{N} \ni k \geq 2$.
- $\mathbb{SO}(n)$. The group of rotations, i.e. $\{\mathbf{R} \in \mathbb{M}^{n\times n}, \det \mathbf{M} = 1, \mathbf{M}^{-1} = \mathbf{M}^T\}$.
- $C^i(\Omega), C^i(\Omega, \mathbb{R}^n), C^i(\Omega, \mathbb{M}^{n\times n})$. Spaces of continuous functions with continuous derivative up to order i, with $i \in \mathbb{N} \cup \{0, \infty\}$.
- $C^i_c(\Omega), C^i_c(\Omega, \mathbb{R}^n), C^i_c(\Omega, \mathbb{M}^{n\times n})$. Spaces of continuous functions with compact support in Ω with continuous derivative up to order i, with $i \in \mathbb{N} \cup \{0, \infty\}$.
- $L^p(\Omega), L^p(\Omega, \mathbb{R}^n), L^p(\Omega, \mathbb{M}^{n\times n})$. Spaces of Lebesgue functions, $p \in \mathbb{N} \cup \{\infty\}$.
- $H^{i,p}(\Omega), H^{i,p}(\Omega, \mathbb{R}^n), H^{i,p}(\Omega, \mathbb{M}^{n\times n})$. Spaces of Sobolev functions. $n \in \mathbb{N}$, $p \in \mathbb{N} \cup \{\infty\}$, $i \in \mathbb{N}$.
- $H^{i,p}_o(\Omega), H^{i,p}_o(\Omega, \mathbb{R}^n), H^{i,p}_o(\Omega, \mathbb{M}^{n\times n})$. The closure of $C^\infty_c(\Omega), C^\infty_c(\Omega, \mathbb{R}^n), C^\infty_c(\Omega, \mathbb{M}^{n\times n})$ in $H^{1,p}$, $p \in [1, \infty)$.
- $H^1(\Omega), H^1(\Omega, \mathbb{R}^n), H^1(\Omega, \mathbb{M}^{n\times n})$, $H^1_o(\Omega), H^1_o(\Omega, \mathbb{R}^n), H^1_o(\Omega, \mathbb{M}^{n\times n})$. As above, in the case $p = 2$, $n \in \mathbb{N}$.
- $H^{1,\infty}_o(\Omega)$. The intersection of $H^{1,\infty}(\Omega)$ with $H^{1,1}_o(\Omega)$ (and similarly for $H^{1,\infty}_o(\Omega, \mathbb{R}^n), H^{1,\infty}_o(\Omega, \mathbb{M}^{n\times n})$).
- $H^{1/2}(\partial\Omega), H^{1/2}(\partial\Omega, \mathbb{R}^n), H^{1/2}(\partial\Omega, \mathbb{M}^{n\times n})$. Spaces of traces, $n \in \mathbb{N}$.
- $\tau : H^1(\Omega) \to H^{1/2}(\partial\Omega)$, $H^1(\Omega, \mathbb{R}^3) \to H^{1/2}(\partial\Omega, \mathbb{R}^3)$, $H^1(\Omega, \mathbb{M}^{3\times 3}) \to H^{1/2}(\partial\Omega, \mathbb{M}^{3\times 3})$ the trace.
- $\mathcal{H}^n$. The Hausdorff measure.

0.1 Introduction

Studying the microstructure of complex materials is one of the most interesting problems in modern applied mathematics and statistical mechanics. A paradigmatic case is represented by nematic liquid crystal elastomers (LCEs). Nematic liquid crystal elastomers are a class of materials which associate a liquid crystalline microstructure composed of rigid rod-like molecules (nematic mesogens) with an elastic continuum matrix made of crosslinked polymeric chains. Their interesting properties stem from the interaction between liquid crystalline order and the elastic response of the substrate. One of the most interesting properties is the large spontaneous deformation accompanying a temperature-induced phase transformation from the isotropic to the nematic state. This spontaneous deformation can reach 400% with respect to the reference configuration. LCEs can also deform and bend under UV-light excitation or in the presence of electric or magnetic fields. These properties make them extremely interesting for applications in bioengineering and robotics (e.g. artificial muscles).

Understanding the complex behavior of LCEs requires some familiarity with liquid crystal modelling and with the theory of elasticity. We refer to [24], [49], and [50] for a physical and mathematical introduction to liquid crystals and liquid crystal elastomers. To sketch the internal organization of such materials, consider that nematic molecules are linked to long polymeric chains, forming an anisotropic solid structure which has extraordinary properties of deformability. Rods can be directly attached to the backbone being part of the chain (main-chain polymers) or simply be pendant to it (side-chain polymers). This is a fascinating example of a multi-scale material, that is a substance whose macroscopic behavior depends on the average properties of its microscopic structure.

Nowadays, the mathematical investigation on nematic elastomers focuses essentially on modelling the interaction between the liquid crystal and applied electro-magneto-mechanical fields which act also on the elastic substrate. The choice of the variable which describes the microscopic structure is crucial since it must satisfy some theoretical requirements in statistical mechanics and, on the other hand, must justify the observed microstructure in elastomeric samples. To model the nematic molecules, a possibility is to recover the theories which are available in the literature on liquid crystals and which are characterized through a symmetric 3×3 tensor field which ranges in $\mathcal{Q}_{Fr}$ (Frank tensor model), $\mathcal{Q}_U$ (Ericksen uniaxial tensor model), $\mathcal{Q}_B$ (de Gennes biaxial tensor model). The sets $\mathcal{Q}_{Fr}, \mathcal{Q}_U, \mathcal{Q}_B$ are defined later (see Section 0.1.1). For the sake of our discussion, it suffices to recall that $\mathcal{Q}_B$ is a compact and convex set, while $\mathcal{Q}_U$ and $\mathcal{Q}_{Fr}$ are non-convex and compact sets. The following inclusions hold

$$\mathcal{Q}_{Fr} \subset \mathcal{Q}_U \subset \mathcal{Q}_B$$

and only $\mathcal{Q}_B$ and $\mathcal{Q}_U$ contain the null matrix. Moreover, $\mathcal{Q}_B$ is the convex hull of $\mathcal{Q}_{Fr}$ and $\mathcal{Q}_U$. In brief, Frank set $\mathcal{Q}_{Fr}$ is that of matrices with eigenvalues identically equal to $\{2/3, -1/3, -1/3\}$. Frank theory consists in describing the local directions of the molecules through the eigenvectors of the tensor $\mathbf{Q}$ and hence this is suitable to describe an *ordered* system where the molecules are perfectly aligned along some direction $\mathbf{n} \in \mathbb{S}^2$, called the *director*. On the other hand, Ericksen and de Gennes models can be interpreted as a further development of Frank theory, in the sense that they also permit the description of *disordered* systems, that is when the eigenvalue of $\mathbf{Q}$ are allowed to be slightly different from $\{2/3, -1/3, -1/3\}$ (perfect order) and possibly close to $\{0, 0, 0\}$ (isotropy). The connection of Frank model to the one of de Gennes is that the director $\mathbf{n}$ represents one distinguished eigenvector of the order tensor $\mathbf{Q}$.

While all these models are perfectly legitimate to describe *liquid* crystal, it is a non-trivial problem to extend them to the case of liquid crystal *elastomers*. According to de Gennes model, equilibrium configurations of liquid crystals are obtained by minimizing a free-energy functional which depends on the pointwise values of the *order tensor* $\mathbf{Q}$. This state variable describes both the degree of nematic order, and the average direction of the nematic mesogens at each point of the sample. One of the main points in passing from liquid crystals to LCEs is to discuss how a macroscopic displacement can interact with the local direction and the local degree of order of the nematic mesogens embedded in a gel, which are encoded in $\mathbf{Q}$. One of the possibilities which we consider in this thesis is to model a coupling term which is minimized when the order tensor $\mathbf{Q} \in \mathcal{Q}_X$, where X stands either in Fr, U or B, is coaxial with the mechanical strain. In Frank scenario, the main effect of the coupling between liquid crystalline order and elasticity is the possibility of reorienting the common direction $\mathbf{n}$ of the nematic molecules through applied forces or imposed displacements. In the more general scenario of the order parameters, also the local degree of orientation may be affected by mechanical means and, depending on whether $\mathbf{Q}$ is constrained to be uniaxial or is allowed to be fully biaxial, one obtains the two different order-tensor models of Ericksen and de Gennes respectively.

The main results of this work are summarized below.

Part I: well-posed problems

We study well-posed optimization problems for systems of nematic elastomers in the presence of magnetic or electric fields and of boundary conditions which model traction on the boundary of the domain. In this part of the thesis, we describe the equilibrium of the systems in all the available models. The discussion of which model is the most satisfactory to describe the nematic molecules is postponed to Part II together with the analysis of ill-posed problems.

Here, let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain (an open, bounded, connected set with Lipschitz boundary). Under the hypothesis of the principle of superposition of effects in the linear theory of elasticity, the energy of the system in the presence of a magnetic field is written as the sum of some energetic contributions

$$\mathcal{E}(\mathbf{Q}, \mathbf{u}, \mathbf{h}) = \int_\Omega \Big\{ f_{nem}(\mathbf{Q}, \nabla\mathbf{Q}) + f_{mec}(\mathbf{Q}, \nabla\mathbf{u}) - f_{mag}(\mathbf{Q}, \mathbf{h}) \Big\} dx, \tag{0.1.1}$$

where $\mathbf{u} \in H^1(\Omega, \mathbb{R}^3)$, $\mathbf{Q} \in H^1(\Omega, \mathcal{Q}_X)$ (and X stands either for Fr, U or B), $\mathbf{h} \in L^2(\Omega, \mathbb{R}^3)$. The first term is classical in the literature on nematic liquid crystals (see [24], [49]). It penalizes spatial variations and deviations of the order tensor $\mathbf{Q}$ from some assigned tensor-shape $\mathbf{Q}_o$. Even though more general expressions are available for f_{nem}, we may assume

$$f_{nem}(\mathbf{Q}, \nabla\mathbf{Q}) = \frac{\kappa^2}{2}|\nabla\mathbf{Q}|^2 + \Psi_{LdG}(\mathbf{Q}),$$

where Ψ_{Ldg} is the Landau-de Gennes free-energy density, that is a multi-well potential whose shape depends on some external parameter, such as the temperature of the system (which we assume to be constant). It is enough to require that Ψ_{LdG} be lower semicontinuous, and in practical cases it is taken as a polynomial in $\mathbf{Q}$ with absolute minimum at $\mathbf{Q} = \mathbf{Q}_o$, so that this energy contribution is bounded below. We anticipate that the term Ψ_{LdG} will be neglected in Part 2. The material parameter κ^2, which is called the *curvature* constant, penalizes spatial variations of the tensor field $\mathbf{Q}$. The mechanical free-energy density $f_{mec}(\mathbf{Q}, \mathbf{F})$ is another multi-well function which couples the mechanical strain $\mathbb{E}(\mathbf{F}) = (\mathbf{F} + \mathbf{F}^T)/2$ to the order tensor $\mathbf{Q} \in \mathcal{Q}_X$

$$f_{mec}(\mathbf{Q}, \mathbf{F}) = \mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}|^2 + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2. \tag{0.1.2}$$

Here μ, λ, γ are positive constants, $\mathbf{F} \in \mathbb{M}^{3\times 3}$ and X stands either for Fr, U or B. The algebraic properties of this function are analyzed in Chapters 2 and 3. The last summand $f_{mag}(\mathbf{Q}, \mathbf{h})$ has to be interpreted as the density of the work executed by an external magnetic field onto the system (this is the reason for the minus sign in front of this energy contribution). We write

$$f_{mag}(\mathbf{Q}, \mathbf{h}) = \langle \mathbf{A}(\mathbf{Q})\mathbf{h}, \mathbf{h}\rangle \tag{0.1.3}$$

where $\mathbf{A} : \mathcal{Q}_X \mapsto \mathbb{M}^{3\times 3}_{sym}$ (here X stands either for Fr, U or B) is a linear map in $\mathbf{Q}$ such that

$$m|\mathbf{h}|^2 \le \langle \mathbf{A}(\mathbf{Q})\mathbf{h}, \mathbf{h}\rangle \le M|\mathbf{h}|^2 \quad \text{with} \quad 0 < m \le M < +\infty, \forall\, \mathbf{h} \in \mathbb{R}^3. \tag{0.1.4}$$

In all our models, polarization or internal magnetization phenomena are neglected, since they are not relevant at a first analysis for nematic elastomers. Furthermore, another typical simplification is to assume $\mathbf{h}$ as an assigned function in $L^2(\Omega, \mathbb{R}^3)$ and hence not subject to Maxwell laws [49, Chapter 4]. The functional (0.1.1) can be defined over some function space and minimized with the standard machinery of the calculus of variations.

Theorem 1 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain and $\Gamma_u \subseteq \partial\Omega$ an open subset with positive surface measure. Let $\mathbf{u}_o \in H^1(\Omega, \mathbb{R}^3)$ and $\mathbf{h} \in L^2(\Omega, \mathbb{R}^3)$. The problem*

$$\min_{\substack{H^1(\Omega, \mathcal{Q}_X)\times \\ H^1_{\Gamma_u}(\Omega, \mathbb{R}^3)+\mathbf{u}_o}} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \mathbf{h}), \tag{0.1.5}$$

where X stands either for Fr, U or B, admits solutions.

In the presence of an electric field the functional which describes the energy of the system reads

$$\mathcal{E}(\mathbf{Q},\mathbf{u},\phi)=\int_\Omega\Big\{f_{nem}(\mathbf{Q},\nabla\mathbf{Q})+f_{mec}(\mathbf{Q},\nabla\mathbf{u})-f_{ele}(\mathbf{Q},\nabla\phi)\Big\}dx, \tag{0.1.6}$$

where $\phi:\Omega\mapsto\mathbb{R}$ is the electric potential. The density f_{ele} has the same properties as the function f_{mag} (differing only in dimensional units) and with some abuse of notation we write

$$f_{ele}(\mathbf{Q},\mathbf{e})=\langle\mathbf{A}(\mathbf{Q})\mathbf{e},\mathbf{e}\rangle$$

where $\mathbf{A}:\mathcal{Q}_X\mapsto\mathbb{M}^{3\times3}_{sym}$ is the same linear map introduced in (0.1.3) such that

$$m|\mathbf{e}|^2\le\langle\mathbf{A}(\mathbf{Q})\mathbf{e},\mathbf{e}\rangle\le M|\mathbf{e}|^2\quad\text{with}\quad 0<m\le M<+\infty,\forall\,\mathbf{e}\in\mathbb{R}^3.$$

The analysis of the functional $\mathcal{E}(\mathbf{Q},\mathbf{u},\phi)$ is different from the one just seen for the case of an applied magnetic field. The potential ϕ is subject to Gauss-Maxwell law

$$\operatorname{div}\big(\mathbf{A}(\mathbf{Q})\nabla\phi\big)=0$$

which holds in weak sense (see below). Hence, the equilibrium of the system is determined by the minima of $(\mathbf{Q},\mathbf{u})\mapsto\mathcal{E}(\mathbf{Q},\mathbf{u},\phi)$ under the (non-local) differential constraint (0.1.7). It is important to notice that Gauss law arises from the first variation of

$$\phi\mapsto\int_\Omega\big\langle\mathbf{A}(\mathbf{Q})\nabla\phi,\nabla\phi\big\rangle dx. \tag{0.1.7}$$

The main consequence of this fact is that the minima of $(\mathbf{Q},\mathbf{u})\mapsto\mathcal{E}(\mathbf{Q},\mathbf{u},\phi)$ under Gauss law are in fact min-max points of $(\mathbf{Q},\mathbf{u},\phi)\mapsto\mathcal{E}(\mathbf{Q},\mathbf{u},\phi)$, and we have the following theorem.

Theorem 2 *Let $\Omega\subset\mathbb{R}^3$ be a Lipschitz domain and $\Gamma_u,\Gamma_\phi\subseteq\partial\Omega$ two open subsets with positive surface measure. Let $\mathbf{u}_o\in H^1(\Omega,\mathbb{R}^3)$, $\phi_o\in H^1(\Omega)$. Then, $(\overline{\mathbf{Q}},\overline{\mathbf{u}},\overline{\phi})$ is a min-max critical point of $\mathcal{E}$, i.e.*

$$\mathcal{E}(\overline{\mathbf{Q}},\overline{\mathbf{u}},\overline{\phi})=\min_{\substack{(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X)\\ \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o}}\ \max_{\phi\in H^1_{\Gamma_\phi}(\Omega)+\phi_o}\mathcal{E}(\mathbf{Q},\mathbf{u},\phi), \tag{0.1.8}$$

if and only if $(\overline{\mathbf{Q}},\overline{\mathbf{u}})$ is a solution to this problem

$$\min_{\substack{(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X)\\ \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o}}\mathcal{E}(\mathbf{Q},\mathbf{u},\Phi),\quad \textit{where } \Phi \textit{ is the solution to Gauss law,}$$

and where X stands either for Fr, U or B.

More in detail, the weak form of Gauss law (0.1.7) reads

$$\begin{cases} \text{Find } \phi \in H^1(\Omega) \text{ s.t.} \\ \int_\Omega \langle \mathbf{A}(\mathbf{Q})\nabla\phi, \nabla\varphi\rangle dx = 0 \\ \phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall \varphi \in H^1_{\Gamma_\phi}(\Omega), \end{cases} \tag{0.1.9}$$

and it is clear that it coincides with the first variation of (0.1.7) in $H^1_{\Gamma_\phi}(\Omega)+\phi_o$. Denoting with $\Phi = \Phi[\mathbf{Q}]$ the solution to Gauss equation, we can also define the new functional

$$\mathcal{E}^*(\mathbf{Q}, \mathbf{u}) := \mathcal{E}(\mathbf{Q}, \mathbf{u}, \Phi) = \max_{\phi \in H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi). \tag{0.1.10}$$

Then, the proof of Theorem 2 follows by applying standard techniques (Direct Method in the Calculus of Variations), since the min-max problem (0.1.8)-right can be written as

$$\min_{\substack{(\mathbf{Q},\mathbf{u}) \in H^1(\Omega, \mathcal{Q}_X) \\ \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o}} \mathcal{E}^*(\mathbf{Q}, \mathbf{u}). \tag{0.1.11}$$

This observation is fundamental also in order to treat the asymptotic case of small particles in the presence of Gauss law (Chapter 3), which is in fact another well-posed problem.

All the theorems above hold also in the presence of slightly different boundary conditions which are used to model some traction experiments of interest in engineering and for incompressible nematic elastomers (for which the divergence of $\mathbf{u}$ is constrained to be zero).

The same results may also be obtained by a different argument based on a more explicit parameterization of the tensor field $\mathbf{Q}$. For instance, in the uniaxial case which corresponds to taking $X = U$ in the previous theorems, we write[31]

$$\mathbf{Q} = s\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big) \tag{0.1.12}$$

and we take $(s, \mathbf{n})$ in the set

$$\mathrm{D}_s := \{(s, \mathbf{n}) : \Omega \mapsto [-0.5, 1] \times \mathbb{S}^2 : s \in H^1(\Omega), \mathbf{v} := s\mathbf{n} \in H^1(\Omega, \mathbb{R}^3)\}, \tag{0.1.13}$$

which has been introduced by Ambrosio[3] in order to study equilibrium configurations of nematic liquid crystals. Substituting (0.1.12) in $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \mathbf{h})$ and $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$ we obtain new functionals $\mathcal{E}(s, \mathbf{n}, \mathbf{u}, \mathbf{h})$ and $\mathcal{E}(s, \mathbf{n}, \mathbf{u}, \phi)$ and the techniques used to prove Theorems 1 and 2 are easily adapted to the new set of variables. Analogously, in order to treat the Frank model it is enough to set $s \equiv 1$ in (0.1.12) and to take $\mathbf{n} \in H^1(\Omega, \mathbb{S}^2)$. This last case is particularly interesting in view of some other recent results in the literature on nematics. Using the language of J. Ball, A. Zarnescu[4], if we write

$$\mathbf{Q} = \mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I} \tag{0.1.14}$$

with $\mathbf{n} \in H^1(\Omega, \mathbb{S}^2)$, then we restrict the class of $H^1(\Omega, \mathcal{Q}_{Fr})$ tensors to the subset of the *orientable* ones. The consequence of this fact is interesting because our energies depend now on the variable $\mathbf{n} \in \mathbb{S}^2$ which can be directly measured and is the one used by experimentalists and engineers.

In the last part of this chapter we apply Theorem 2 in order to find particular solutions of

$$\min_{\substack{(\mathbf{Q},\mathbf{u}) \in H^1(\Omega, \mathcal{Q}_X) \times \\ H^1_o(\Omega, \mathbb{R}^3) + \mathbf{F}(x-O)}} \ \max_{\phi \in H^1_{\Gamma_\phi}(\Omega) + \phi_o} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi), \tag{0.1.15}$$

with constant $\mathbf{Q}$, affine $\mathbf{u}$ and $\phi \equiv 0$, and where X stands either for Fr, U or B. These special solutions are relevant in the engineering literature as they capture the essential features of the minimizers of the energy also in the presence of more general boundary conditions, but sufficiently far away from the boundary of the sample. The pictorial representation of the minimizer $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ is the *phase diagram* of f_{mec} and corresponds to Figures 1.2, 1.3.

Part II: ill-posed problems

The second part of the thesis is devoted to the analysis of minima and minimizers of the energies introduced in Part I in the asymptotic cases of large bodies and small particles, to the discussion of some of their physical implications (Chapters 2, 3), and to the presentation of a new anisotropic model (Chapter 4). In particular, we focus our attention on the analysis of ill-posed minimization problems for not semicontinuous energies (or for functionals defined over non-closed function spaces), even though several well-posed optimization problems are also discussed.

Figure 1: Stripe-domain formation in nematic elastomers under stretch. The length of the sample is of the order of 10 mm, the thickness is 0.3 mm and the width of the stripes is about 1 to 10 μm. The different colors correspond to different director orientations. Courtesy of Prof. H. Finkelmann. More information is available on-line at *http://people.sissa.it/~desimone/Nematic/experiment.html*.

We recall that the theories based on the tensor $\mathbf{Q}$ offer a more detailed description of nematic order with respect to director $\mathbf{n}$. It is important to observe that $\mathcal{Q}_{Fr} \subset \mathcal{Q}_U \subset \mathcal{Q}_B$ and that the set $\mathcal{Q}_{Fr}$ does not contain the trivial tensor $\mathbf{Q} \equiv 0$. In particular, according to formula (0.1.12), *loss of local order* (that is $s < 1$) and *isotropy* (also known as *melting*), can be obtained in Ericksen (and de Gennes) model, since $\mathbf{Q} = 0 \Longleftrightarrow s = 0$.

On the other hand, the direct coupling between order tensor and strain imposed by equation (0.1.2) may be accepted if $\mathbf{Q} \in \mathcal{Q}_{Fr}$, while it may seem too simplistic if $\mathbf{Q} \in \mathcal{Q}_U$ or $\mathcal{Q}_B$. While a direct experimental justification of Frank model (a uniaxial stretch aligns the molecules along the axis of the largest eigenvalue of the stretch) is available, a direct experimental confirmation of the possibility of affecting s or inducing biaxial states by applying mechanical stresses are not available.

The considerations above pertain the microscopic description of order in nematic elastomers. In stretching experiments of sufficiently large samples, loss of local order and melting can be observed even though in a *macroscopic scale*. The former is the formation of stripe-domains (see Figure 1), the second is blurring near the clamps. These phenomena can be modelled by functionals defined in the scenario of Frank tensor and analyzed in the context of the relaxation theory for not lower semicontinuous energies. More precisely, all these material instabilities are described by low energy minimizing sequences for functionals defined over non-closed sets of functions.

The functionals describing such phenomena arise by the asymptotic analysis for large bodies. A by-product of the analysis contained in Part I is that the following problem

$$\mathcal{P}_\Lambda : \qquad \text{Minimize} \quad (\mathbf{Q}, \mathbf{u}) \mapsto \int_\Omega \Big(\frac{\kappa^2}{2\Lambda^2} |\nabla \mathbf{Q}|^2 + f_{mec}(\mathbf{Q}, \nabla \mathbf{u}) \Big) dx, \qquad (0.1.16)$$
$$\text{with } \mathbf{Q} \in H^1(\Omega, \mathcal{Q}_{Fr}), \mathbf{u} \in H^1(\Omega, \mathbb{R}^3), \mathbf{u}|_{\partial\Omega} \text{ assigned,}$$

where Ω is a Lipschitz domain and Λ is a given positive constant, admits solutions. The functional appearing in (0.1.16) is obtained when we operate a re-scaling of domain and variables in the energies introduced in Part I (this justifies the presence of the factor Λ^2 in front of $|\nabla \mathbf{Q}|^2$). This procedure is explained in Paragraph 3.1.2. The limit case as $\Lambda \to +\infty$, which describes the asymptotics of large bodies, is very relevant for our discussion. Our results regard the explicit characterization of minima and minimizers of $\mathcal{P}_\Lambda$ in a suitable topology, as $\Lambda \to +\infty$. We present two equivalent strategies to discuss this problem.

First strategy. We start with an heuristic argument. Let us consider the problem formally obtained by setting $\Lambda = +\infty$ in (0.1.16), that is

$$\mathcal{P}_\infty : \qquad \text{Minimize} \quad (\mathbf{Q}, \mathbf{u}) \mapsto \int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u}) dx, \qquad (0.1.17)$$
$$\text{with } \mathbf{Q} \in L^2(\Omega, \mathcal{Q}_{Fr}), \mathbf{u} \in H^1(\Omega, \mathbb{R}^3), \mathbf{u}|_{\partial\Omega} \text{ assigned.}$$

In the absence of the penalization term for the gradient of $\mathbf{Q}$, we can take a minimizing sequence $\{\mathbf{Q}_k\}$ in the set $L^2(\Omega, \mathcal{Q}_{Fr})$ endowed with the weak topology. Since $\mathcal{Q}_{Fr}$ is not convex, then $L^2(\Omega, \mathcal{Q}_{Fr})$ is not weakly closed and the minimization problem (0.1.17) may be ill-posed. To overcome this degeneracy, we replace the original density $f_{mec}(\mathbf{Q}, \mathbf{F})$ with a *macroscopic* model defined as

$$f_X(\mathbf{F}) := \inf_{\mathbf{Q} \in \mathcal{Q}_X} f_{mec}(\mathbf{Q}, \mathbf{F}) \text{ where } X \text{ stands either for } Fr \text{ or } B, \qquad (0.1.18)$$

that is a new function obtained by taking the infimum over all possible tensors ranging in the available sets at any constant $\mathbf{F} \in \mathbb{M}^{3\times3}$. We also refer to [28] for an example of this approach. The properties of the function f_X are directly inherited from the algebraic properties of the set $\mathcal{Q}_X$. Since

$$\inf_{\mathbf{Q}\in\mathcal{Q}_X} f_{mec}(\mathbf{Q},\mathbf{F}) = \inf_{\mathbf{Q}\in\mathcal{Q}_X} \mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}|^2 + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2 = \mu\, dist^2\big(\mathbb{E}(\mathbf{F}), \gamma\mathcal{Q}_X\big) + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2,$$

it follows that f_X is (essentially) the square of the distance from the set $\gamma\mathcal{Q}_X$. Recalling that the distance from a convex set is a convex function, f_B is convex, while f_{Fr} is a non-convex function. Assuming that $\Omega \subset \mathbb{R}^3$ is a Lipschitz domain, we define the energies

$$\mathrm{J}_X^{\Gamma_u,g}(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_X(\nabla\mathbf{u})dx & \text{in } H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \\ +\infty & \text{otherwise in } H^1(\Omega,\mathbb{R}^3) \end{cases} \tag{0.1.19}$$

where X stands either for Fr or B, $\mathbf{g}(x) \in H^1(\Omega,\mathbb{R}^3)$ and $\Gamma_u \subseteq \partial\Omega$ with positive surface measure. We observe that in the case $X = B$, the functional is lower semicontinuous by convexity. Moreover, the observation that $\mathcal{Q}_B$ is the convex envelope of $\mathcal{Q}_{Fr}$ suggests a possible connection between the relaxation of $\mathrm{J}_{Fr}^{\Gamma_u,g}$ with $\mathrm{J}_B^{\Gamma_u,g}$. In fact, we prove that the quasiconvex envelope of f_{Fr} is f_B and that the relaxation of $\mathrm{J}_{Fr}^{\Gamma_u,g}$ is $\mathrm{J}_B^{\Gamma_u,g}$. An analogous result can be obtained also for models of incompressible elastomers, that is for functionals defined in the presence of a penalty function on the divergence of $\mathbf{u}$, as exposed in the next theorem.

Theorem 3 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain and denote with Γ_u an open subset of $\partial\Omega$ with positive surface measure. Let* $\mathbf{g}(x) \in H^1(\Omega,\mathbb{R}^3)$ *with* $\operatorname{div}\mathbf{g}(x) = 0$. *Let $f_X(\cdot)$ as in* (0.1.18) *(where X stands either for Fr or B) and define*

$$\mathcal{J}_X^{\Gamma_u,g}(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_X(\nabla\mathbf{u})dx & \text{on } H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \operatorname{div}\mathbf{u} = 0, \\ +\infty & \text{otherwise in } H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Then, the relaxation of $\mathcal{J}_{Fr}^{\Gamma_u,g}$ is $\mathcal{J}_B^{\Gamma_u,g}$.

The most difficult point in the proof is to treat the constraint on the divergence of $\mathbf{u}$. It is known that the relaxation of a functional in the presence of a linear (and constant-rank) constraint on the gradient (or, in general, on some weakly convergent variable), can be written as the integral of a new density energy, the so called $\mathcal{A}$-quasiconvex envelope of the original non convex function[10]. Moreover, in this case we obtain explicitly the relaxed energy density and show that it satisfies a solenoidal quasiconvexification formula, that is

$$|\omega| f_B(\mathbf{Z}) = \inf\Big\{\int_\omega f_X\big(\mathbf{Z} + \nabla\mathbf{w}\big)dx : \mathbf{w} \in C_c^\infty(\omega,\mathbb{R}^3), \operatorname{div}\mathbf{w} = 0\Big\} \forall\, \mathbf{Z} \in \mathbb{M}_0^{3\times3} \tag{0.1.20}$$

where $\omega \subset \mathbb{R}^3$ is any Lipschitz domain[1]. To prove this, we use an argument due to Braides[8]. Re-labelling the functional defined in (0.1.19) (X stands either for Fr or B) as

$$\mathrm{J}^{\Gamma_u,g}_{X,\lambda}(\mathbf{u}) := \begin{cases} \displaystyle\int_\Omega \Big\{\mu\, dist^2\big(\mathbb{E}(\nabla \mathbf{u}), \gamma \mathcal{Q}_X\big) + \frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2\Big\} dx & \text{on } H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \\ +\infty & \text{otherwise in } H^1(\Omega,\mathbb{R}^3), \end{cases}$$

(here $\operatorname{div}\mathbf{g} = 0$) we show that the relaxation of $\mathcal{J}^{\Gamma_u,g}_{Fr}$ coincides with the Gamma-limit of $\mathrm{J}^{\Gamma_u,g}_{Fr,\lambda}$ as $\lambda \to +\infty$. Thanks to a well-know property of the Gamma-convergence, we can write[2]

$$\Gamma\text{-}\lim_{\lambda\to+\infty} \mathrm{J}^{\Gamma_u,g}_{Fr,\lambda} = \Gamma\text{-}\lim_{\lambda\to+\infty} \overline{\mathrm{J}}^{\Gamma_u,g}_{Fr,\lambda} = \sup_\lambda \mathrm{J}^{\Gamma_u,g}_{B,\lambda}, \tag{0.1.21}$$

where the last equality is the crucial result obtained for models of compressible elastomers. Then, thanks to Beppo-Levi Theorem, we are left with taking the supremum of a scalar valued function. A direct corollary of Theorem 3 is that

$$\inf_{H^1(\Omega,\mathbb{R}^3)} \mathcal{J}^{\Gamma_u,g}_{Fr}(\mathbf{u}) = \min_{H^1(\Omega,\mathbb{R}^3)} \mathcal{J}^{\Gamma_u,g}_{B}(\mathbf{u}). \tag{0.1.22}$$

This last equality yields the interpretation of our relaxation result. In view of (0.1.22), the infima of the energy functionals defined in the scenario of Frank order tensor are described by minima of the model based on the biaxial tensor. The point is that the de Gennes model is not imposed as an *a-priori* assumption, but it is obtained effectively by relaxation. Hence, the biaxial energy density f_B (appearing as the integrand of $\mathcal{J}^{\Gamma_u,g}_B$) is not obtained as the pointwise minimization of f_{mec} over the set $\mathcal{Q}_B$ as in (0.1.18), but it is obtained thanks to the formation of a microstructure which arises at a different scale. Interestingly, we obtain the full information associated with the de Gennes theory, that is isotropy and low order phases, thus justifying the materials instabilities introduced in this section. Furthermore, our explicit constructions of the minimizing sequences for the Gamma-limit of the original non-convex functionals (see Chapter 3) give an explanation to the stripe-domains observed in experiments (Figure 1).

Second strategy. Chapter 3 is devoted to the analysis of minima and minimizers for problem $\mathcal{P}_\Lambda$ (0.1.16) in the limit as $\Lambda \to +\infty$ with the language of Gamma-convergence. Here we define $\varepsilon^2 := \kappa^2/2\Lambda^2$ and discuss the limit as $\varepsilon \to 0$. In what follows we denote with σ the product of the weak topology of $L^2(\Omega,\mathbb{M}^{3\times3})$ with the weak topology of $H^1(\Omega,\mathbb{R}^3)$.

Theorem 4 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, $\Gamma_u \subseteq \partial\Omega$ an open subset with positive surface measure and $\mathbf{g}(x) \in H^1(\Omega,\mathbb{R}^3)$ with* $\operatorname{div}\mathbf{g}(x) = 0$ *a.e. in Ω. Let f_{mec} as in*

[1] see Remark 15 in Paragraph 2.2.2 for an alternative characterization

[2] here and elsewhere we write for simplicity $\overline{\mathrm{J}}^{\Gamma_u,g}_{Fr,\lambda} \equiv \overline{\mathrm{J}^{\Gamma_u,g}_{Fr,\lambda}}$

(0.1.2), $X = Fr, B$, and

$$\mathcal{F}^{\Gamma_u,g}_{\varepsilon,Fr}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx \\ \qquad\qquad \text{on } H^1(\Omega,\mathcal{Q}_{Fr}) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}, \operatorname{div}\mathbf{u} = 0, \\ +\infty \qquad\qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Then

$$\Gamma(\sigma)\text{-}\lim_{\varepsilon\to0} \mathcal{F}^{\Gamma_u,g}_{\varepsilon,Fr} = \mathcal{F}^{\Gamma_u,g}_{mec,B}, \tag{0.1.23}$$

where

$$\mathcal{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } L^2(\Omega,\mathcal{Q}_B) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}, \operatorname{div}\mathbf{u} = 0, \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

The proof of the previous result is divided into two parts. The first one concerns the relaxation of the functional $\mathcal{F}^{\Gamma_u,g}_{mec,Fr}$ which is defined as

$$\mathcal{F}^{\Gamma_u,g}_{mec,Fr}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } L^2(\Omega,\mathcal{Q}_{Fr}) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}, \operatorname{div}\mathbf{u} = 0, \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

We show that (under the hypotheses of Theorem 4) the relaxation of $\mathcal{F}^{\Gamma_u,g}_{mec,Fr}$ in the sense of σ is $\mathcal{F}^{\Gamma_u,g}_{mec,B}$. Interestingly, the proof of the relaxation result for $\mathcal{F}^{\Gamma_u,g}_{mec,Fr}$ requires an intermediate step, that is the relaxation of a model for compressible elastomers defined as (here X stands either for Fr or B)

$$\mathrm{F}^{\lambda,\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\mu|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}|^2 + \frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2\Big)dx \\ \qquad\qquad \text{on } L^2(\Omega,\mathcal{Q}_X) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}, \\ +\infty \qquad\qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

We show that the relaxation of $\mathrm{F}^{\lambda,\Gamma_u,g}_{mec,Fr}$ is $\mathrm{F}^{\lambda,\Gamma_u,g}_{mec,B}$ by constructing a suitable recovery sequence. Then, exactly as in the paragraph above, we show that the relaxation of $\mathcal{F}^{\Gamma_u,g}_{mec,Fr}$ is the Gamma-limit of the sequence $\mathrm{F}^{\lambda,\Gamma_u,g}_{mec,Fr}$ as $\lambda \to +\infty$. Then, we have

$$\Gamma\text{-}\lim_{\lambda\to+\infty} \mathrm{F}^{\lambda,\Gamma_u,g}_{mec,Fr} = \Gamma\text{-}\lim_{\lambda\to+\infty} \overline{\mathrm{F}}^{\lambda,\Gamma_u,g}_{mec,Fr} = \sup_\lambda \overline{\mathrm{F}}^{\lambda,\Gamma_u,g}_{mec,B}, \tag{0.1.24}$$

and the last (elementary) computation yields $\mathcal{F}^{\Gamma_u,g}_{mec,B}$. Then, the second part of the proof of Theorem 4 contains the Gamma-convergence argument. As a corollary we have

$$\inf_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathcal{F}^{\Gamma_u,g}_{mec,Fr}(\mathbf{Q},\mathbf{u}) = \min_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathcal{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q},\mathbf{u}), \tag{0.1.25}$$

which is a result analogous to (0.1.22).

Equivalence between the first and the second strategy. The two strategies presented are not independent, in the sense that minima and minimizers of the macroscopic models are strictly related to those of the large-body Gamma-limit. By manipulating all the previous functionals and applying some well known properties of the distance function we show that

$$\min_{L^2(\Omega,\mathbb{M}^{3\times 3})\times H^1(\Omega,\mathbb{R}^3)} \mathcal{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q},\mathbf{u}) = \min_{H^1(\Omega,\mathbb{R}^3)} \mathcal{J}^{\Gamma_u,g}_{B}(\mathbf{u}). \tag{0.1.26}$$

This result allows us to calculate explicitly the minimizers of (0.1.26)-left by solving the minimization problem (0.1.26)-right in the presence of particular boundary conditions and is discussed in detail in Paragraph 3.3.2. We also believe that this result may be helpful in numerical simulations. Indeed, (0.1.26) shows that the full information on minima and minimizers of (0.1.26)-left may be obtained by approximating the solutions of problem (0.1.26)-right. However, a numerical code for (0.1.26)-left requires to parameterize the set $\mathcal{Q}_B$ of de Gennes order tensors. This is a non-trivial operation which is not required by (0.1.26)-right. All the Gamma-convergence results are also obtained for the case of compressible elastomers, that is if we remove the constraint on the divergence of $\mathbf{u}$ and replace it by a finite energy cost for volumetric changes and in the presence of slightly different boundary conditions.

Small particles: the phase diagrams and the presence of electric fields. After analyzing the asymptotic models of large bodies, we turn our attention to the analysis of minima and minimizers in the limit of small particles, that is for problem $\mathcal{P}_\Lambda$ (0.1.16) as $\Lambda \to 0^+$. In this case the curvature elasticity is predominant and, as a consequence, the nematic order variable is constant in the specimen. Denoting with σ' the product of the strong $L^2(\Omega,\mathbb{M}^{3\times 3})$-topology with the weak $H^1(\Omega,\mathbb{R}^3)$-topology, we obtain the following theorem.

Theorem 5 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, $\Gamma_u \subseteq \partial\Omega$ an open subset with positive surface measure and $\mathbf{g}(x) \in H^1(\Omega,\mathbb{R}^3)$ with $\operatorname{div}\mathbf{g} = 0$. Let f_{mec} as in* (0.1.2)*, $\mathcal{F}_{\varepsilon,X}$, $\mathcal{F}^{\Gamma_u,g}_{\varepsilon,X}$ as in Theorem* 4 *where X stands either for Fr or B. Then*

$$\mathcal{G}^{\Gamma_u,g}_{mec,X} = \Gamma(\sigma')\text{-}\lim_{\varepsilon\to+\infty} \mathcal{F}^{\Gamma_u,g}_{\varepsilon,X} \tag{0.1.27}$$

where

$$\mathcal{G}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx \\ \qquad \text{on } \{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X), \text{const.}\} \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}, \operatorname{div}\mathbf{u} = 0, \\ +\infty \qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times 3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

The predominance of the curvature term and the strong $L^2(\Omega,\mathbb{M}^{3\times 3})$-topology rule out any relaxation phenomenon. Hence, if we start with a Frank-like model ($\mathbf{Q} \in \mathcal{Q}_{Fr}$), then the small-particle limit remains of Frank type. This result sheds light on the interpretation of the particular solutions briefly discussed at the end of Part I (see (0.1.15)). We give an alternative explanation of the phase diagrams by proving that they represent the minimizers $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ of the Gamma-limit $\mathcal{G}^{\Gamma_u,g}_{mec,X}$ in the presence of affine boundary conditions on $\partial\Omega$.

Another interesting result is the characterization of the asymptotic behavior of the minima and minimizers in the presence of an electric field. Precisely, we want to study the behavior of minima and minimizers $(\mathbf{Q}, \mathbf{u})$ of the following problem

$$\min_{\substack{(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X)\times \\ H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o,\operatorname{div}\mathbf{u}=0}} \int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u}) - f_{ele}(\mathbf{Q},\nabla\phi)\Big)dx \qquad (0.1.28)$$

under Gauss law (0.1.9) (here X stands either for Fr or B), as $\varepsilon \to \infty$ and in the sense of σ'. This new problem is not trivial because Gauss law is a differential equation (hence non-local constraint), and, as already observed, the functional in (0.1.28) is not bounded below. In view of Theorem 2, we have a recipe to turn this problem into the following minimization problem

$$\min_{\substack{(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X)\times \\ H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o,\operatorname{div}\mathbf{u}=0}} \int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u}) - f_{ele}(\mathbf{Q},\nabla\Phi)\Big)dx, \qquad (0.1.29)$$

where $\Phi = \Phi[\mathbf{Q}]$ is the solution to Gauss law (0.1.9). We can attack the functional appearing in (0.1.29) by means of Gamma-convergence. In brief, it is possible to show that

$$\mathbf{Q} \mapsto \int_\Omega \Big(-f_{ele}(\mathbf{Q},\nabla\Phi[\mathbf{Q}])\Big)dx, \qquad (0.1.30)$$

is continuous in the strong topology of $L^2(\Omega, \mathbb{M}^{3\times3})$. As a corollary of Theorem 5, we obtain the following result. Let

$$\mathcal{E}^{*\Gamma_u,g}_{X,\varepsilon}(\mathbf{Q},\mathbf{u}) := \begin{cases} \int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx - \int_\Omega f_{ele}\big(\mathbf{Q},\nabla\Phi[\mathbf{Q}]\big)dx \\ \qquad\qquad \text{on } H^1(\Omega,\mathcal{Q}_X)\times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div}\mathbf{u}=0 \\ +\infty \qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3), \end{cases}$$

where X stands either for Fr or B and $\Phi[\mathbf{Q}]$ is the solution to Gauss law (0.1.9). Then

$$\Gamma(\sigma')\text{-}\lim_{\varepsilon\to+\infty} \mathcal{E}^{*\Gamma_u,g}_{X,\varepsilon} = \mathcal{E}^{*\Gamma_u,g}_{mec,X} \qquad (0.1.31)$$

where

$$\mathcal{E}^{*\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx - \int_\Omega f_{ele}\big(\mathbf{Q},\nabla\Phi[\mathbf{Q}]\big)dx \\ \qquad \text{on } \{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X), \text{const}\}\times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div}\mathbf{u}=0 \\ +\infty \qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

In view of Theorem 2 the previous Gamma-convergence result can be translated into a Gamma-convergence-like result for a min-max problem, that is the Gamma-convergence result under Gauss law. Let us define

$$\mathcal{E}^{\varepsilon}(\mathbf{Q},\mathbf{u},\phi) := \int_{\Omega}\Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u}) - f_{ele}(\mathbf{Q},\nabla\phi)\Big)dx, \tag{0.1.32}$$

$$\mathcal{E}_{mec}(\mathbf{Q},\mathbf{u},\phi) := \int_{\Omega}\Big(f_{mec}(\mathbf{Q},\nabla\mathbf{u}) - f_{ele}(\mathbf{Q},\nabla\phi)\Big)dx. \tag{0.1.33}$$

Then, we obtain the following characterization for the minima and minimizers of the asymptotic problem for small particles.

1. *Convergence of min-max values.*

$$\min_{\substack{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),const,\\ \mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0}} \Big\{\mathcal{E}_{mec}(\mathbf{Q},\mathbf{u},\phi) \textit{ sub Gauss law } (0.1.9)\Big\} \tag{0.1.34}$$

$$= \lim_{j\to+\infty}\left(\inf_{\substack{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),\\ \mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0}} \Big\{\mathcal{E}^{\varepsilon_j}(\mathbf{Q},\mathbf{u},\phi) \textit{ sub Gauss law } (0.1.9)\Big\}\right).$$

2. *Convergence of min-max points.*

Denote with $\Phi = \Phi[\mathbf{Q}]$ *the solution to Gauss equation* (0.1.9). *Let* $\{\mathbf{Q}_j,\mathbf{u}_j,\Phi_j\} \subset H^1(\Omega,\mathcal{Q}_X)\times\{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0\}\times H^1_{\Gamma_\phi}(\Omega)+\phi_o(x)$ *be a min-maximizing sequence for* $\{\mathcal{E}^{\varepsilon_j}\}$, *i.e.*

$$\lim_{j\to+\infty}\mathcal{E}^{\varepsilon_j}\big(\mathbf{Q}_j,\mathbf{u}_j,\Phi_j\big) = \tag{0.1.35}$$

$$\lim_{j\to+\infty}\inf_{\substack{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),\\ \mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0}} \Big\{\mathcal{E}^{\varepsilon_j}(\mathbf{Q},\mathbf{u},\phi) \textit{ sub Gauss law } (0.1.9)\textit{-right}\Big\}.$$

Then, up to subsequences, $\mathbf{Q}_{j_k} \to \overline{\mathbf{Q}}$, $\mathbf{u}_{j_k} \rightharpoonup \overline{\mathbf{u}}$ *in* $L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)$ *with* $\overline{\mathbf{Q}}$ *constant and* $\Phi[\mathbf{Q}_{j_k}] \to \Phi[\overline{\mathbf{Q}}]$ *s-*$H^1(\Omega)$. *Then, we have*

$$\mathcal{E}_{mec}\big(\overline{\mathbf{Q}},\overline{\mathbf{u}},\Phi[\overline{\mathbf{Q}}]\big) = \min_{\substack{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),const,\\ \mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0}} \Big\{\mathcal{E}_{mec}(\mathbf{Q},\mathbf{u},\phi) \textit{ sub Gauss law } (0.1.9)\Big\}.$$

The previous Gamma-convergence result may not hold for the case of large bodies. This is because the functional in (0.1.30) is not continuous in the sense of the weak topology of $L^2(\Omega,\mathbb{M}^{3\times3})$. To conclude this chapter, we also consider the Gamma-limit of the energy of the system $\mathcal{E}(\mathbf{Q},\mathbf{u},\mathbf{h})$ defined in (0.1.1). In this case the result is trivial both in the limit for small particles and in the limit for large bodies, since the energy $\int_{\Omega} f_{mag}(\mathbf{Q},\mathbf{h})dx$ is continuous both in the strong and weak topology of $L^2(\Omega,\mathbb{M}^{3\times3})$.

The anisotropic model. Chapter 4 is devoted to the analysis of another model which can be interpreted as the anisotropic version of the energy density f_X (introduced in (0.1.18)) and defined as

$$f^{\beta}_{Fr}(\mathbf{F}) := \mu\, dist^2\big(\mathbb{E}(\mathbf{F}), \gamma\mathcal{Q}_{Fr}\big) + \beta\mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}_o|^2 + \frac{\lambda}{2}(\mathrm{tr}\,\mathbf{F})^2. \qquad (0.1.36)$$

Here β is a positive parameter. In the limit case $\beta = 0$, then $f^0_{Fr} \equiv f_{Fr}$ and we are left with the isotropic energy density studied in the previous section. Then, if $\beta > 0$, $f^{\beta}_{Fr} = 0$ only if $\mathbb{E}(\mathbf{F}) = \gamma\mathbf{Q}_o$, in which case all the three summands in (0.1.36) are equal to zero. The constant tensor field $\mathbf{Q}_o$ represents the order tensor at the moment of the formation of the crosslinks. Letting $\mathbf{n}_o$ be the original direction of the molecules in the sample, then $\mathbf{Q}_o := \mathbf{n}_o \otimes \mathbf{n}_o - (1/3)\mathbf{I}$. Since in general $f^{\beta}_{Fr}(\mathbf{R}\mathbf{F}\mathbf{R}^T) \neq f^{\beta}_{Fr}(\mathbf{F})$, the function f^{β}_{Fr} is anisotropic. We calculate explicitly the relaxation of the functional obtained by integrating in a Lipschitz domain $S \subset \mathbb{R}^2$ the two-dimensional version of (0.1.36), that is (here $\mathbf{v} : S \mapsto \mathbb{R}^2$)

$$\mathcal{G}^{\beta}_X(\mathbf{v}) := \begin{cases} \displaystyle\int_S g^{\beta}_X(\nabla\mathbf{v})dx & \text{on } H^1(S,\mathbb{R}^2), \mathrm{div}\,\mathbf{v} = \gamma/3, \\ +\infty & \text{otherwise in } H^1(S,\mathbb{R}^2), \end{cases}$$

where $X = Fr, B$ and

$$g^{\beta}_X(\mathbf{F}) = \mu\, dist^2\big(\mathbb{E}(\mathbf{F}), \gamma\mathcal{Q}^{2dim}_X\big) + \beta\mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}_o|^2 + \frac{\lambda}{2}\Big(\mathrm{tr}\,\mathbf{F} - \frac{\gamma}{3}\Big)^2,$$

($\mathcal{Q}^{2dim}_{Fr}$ and $\mathcal{Q}^{2dim}_B$ are the two-dimensional version of the sets $\mathcal{Q}_{Fr}$ and $\mathcal{Q}_B$). In the case $X = B$, then $\mathcal{G}^{\beta}_B$ is convex and hence its relaxation is trivial, while the relaxation of $\mathcal{G}^{\beta}_{Fr}$ is the new energy

$$\mathcal{G}^{\beta}_A(\mathbf{v}) := \begin{cases} \displaystyle\int_S g^{\beta}_A(\nabla\mathbf{v})dx & \text{on } H^1(S,\mathbb{R}^2), \mathrm{div}\,\mathbf{v} = \gamma/3, \\ +\infty & \text{otherwise in } H^1(S,\mathbb{R}^2), \end{cases}$$

where (here $\mathbf{F} \in \mathbb{M}^{2\times 2}$ and $\mathbf{Q}_o = \mathrm{diag}\,(2/3, -1/3)$)

$$\begin{aligned} g^{\beta}_A(\mathbf{F}) = (\mu + \beta\mu) dist^2\Big(\mathbb{E}_0(\mathbf{F}), \frac{\gamma}{1+\beta}\mathbb{E}_0\big(\mathcal{Q}^{2dim}_B\big)\Big) + \\ \mu\frac{\gamma^2}{2}\Big(\frac{\beta^2 + 2\beta}{1+\beta}\Big) - 2\beta\mu\gamma\mathbb{E}_0(\mathbf{F}) : \mathbb{E}_0(\mathbf{Q}_o) + \Big(\frac{\lambda}{2} + \frac{\mu}{2} + \frac{\beta\mu}{2}\Big)\Big(\mathrm{tr}\,\mathbf{F} - \frac{\gamma}{3}\Big)^2. \end{aligned} \qquad (0.1.37)$$

We investigate some of the mathematical properties of this result, while the mechanical interpretation is still under investigation and is left to future works [14], [16].

0.1.1 Physical overview

Liquid crystals

Liquid crystals are *mesophases*, namely, intermediate states of matter, which inhabit the grey area between liquids and solids. At a macroscopic scale, they flow like nearly incompressible viscous fluids and yet retain some properties typical of solid crystals. Their discovery goes back to the pioneering work of Frederich Reinitzer (Austrian botanist, 1888) who observed phase transitions by heating some organic substances related to cholesterol which are solid at room temperature. Classical liquid crystals are typically fluids of relatively stiff rod-like molecules with long range orientational order. The simplest order is *nematic*, in which case the mean direction of the molecules, the *director* $\mathbf{n}$, is uniform. We summarize below the three theories which we follow in this thesis.

Order parameters

Let $\mathcal{B} \subset \mathbb{R}^3$ be the region occupied by the liquid crystal. We suppose that the orientation of the molecules is described in terms of probability measures. Let $(\mathbb{S}^2, \mathbb{F}, \mu)$ be a probability space modelled on the unit sphere, namely $0 \leq \mu(A) \leq 1 \; \forall A \in \mathbb{F}$ and $\mu(\mathbb{S}^2) = 1$. Moreover, in accordance with the nematic *mirror symmetry*, we require that $\mu(A) = \mu(-A) \; \forall A \in \mathbb{F}$, since a system of nematic molecules has the same properties if we replace the director field $\mathbf{n}(x)$ with $-\mathbf{n}(x)$. Hence, the probability of finding a certain amount of molecules in some cone of directions over the unit sphere (and in the cone which is symmetric with respect to the origin) is

$$\mathrm{P}(A) = \mathrm{P}(-A) = \int_A d\mu(\mathbf{n}).$$

When $\mathbf{n}$ is continuously distributed over the sphere, we introduce the probability density $f : \mathbb{S}^2 \mapsto \mathbb{R}^+$, such that

$$f(\mathbf{n}) = f(-\mathbf{n}) \; \forall \, \mathbf{n} \in \mathbb{S}^2, \quad \text{and} \quad d\mu(\mathbf{n}) = f(\mathbf{n})da, \quad \int_{\mathbb{S}^2} f(\mathbf{n})da = 1. \tag{0.1.38}$$

A straightforward consequence of the mirror symmetry is that the first moment is trivial

$$\int_{\mathbb{S}^2} \mathbf{n} d\mu(\mathbf{n}) = 0, \tag{0.1.39}$$

and the same holds for all the moments of odd order. Hence, the first non-trivial information on μ is encoded in the second order moment

$$\mathbf{M} := \int_{\mathbb{S}^2} \mathbf{n} \otimes \mathbf{n} d\mu(\mathbf{n}). \tag{0.1.40}$$

Clearly, $\mathbf{M}$ is a symmetric tensor field with $\operatorname{tr} \mathbf{M} = 1$. Also, since

$$\langle \mathbf{M}\mathbf{i}, \mathbf{i} \rangle = \int_{\mathbb{S}^2} (\mathbf{n} \cdot \mathbf{i})^2 d\mu(\mathbf{n}) \geq 0 \quad \forall \, \mathbf{i} \in \mathbb{S}^2, \tag{0.1.41}$$

then $\mathbf{M}$ is positive semi-definite. The *de Gennes (biaxial) order tensor* (1974, [24]) measures the deviation of the second moment from the reference case in which $\mathbf{M}$ is equal to $\frac{1}{3}\mathbf{I}$ and is defined as

$$\mathbf{Q} := \mathbf{M} - \frac{1}{3}\mathbf{I}.$$

In brief, $\mathbf{Q}$ is a 3×3 symmetric matrix with trace equal to 0 and whose eigenvalues are constrained in the compact set $[-1/3, 2/3]$. We define the set of such tensors

$$\mathcal{Q}_B := \Big\{ \mathbf{Q} \in \mathbb{M}^{3\times 3}_{0sym}, \text{ s.t. spectrum}(\mathbf{Q}) \in \Big[-\frac{1}{3}, \frac{2}{3}\Big] \Big\}. \tag{0.1.42}$$

If we label λ_{max} and λ_{min} the largest and the smallest eigenvalue of a symmetric (and traceless) matrix, it follows that $\lambda_{max} \leq -2\lambda_{min}$ and

$$\mathcal{Q}_B = \Big\{ \mathbf{Q} \in \mathbb{M}^{3\times 3}_{0sym}, \text{ s.t. } \lambda_{min}(\mathbf{Q}) \geq -\frac{1}{3} \Big\}. \tag{0.1.43}$$

Since the de Gennes tensors are defined as convex combinations of diads (see (0.1.40)), it follows that $\mathcal{Q}_B$ is a convex and compact set. We can prove this property directly by (0.1.42). To this aim, we recall the following characterization for the smallest eigenvalue of a symmetric matrix[39]

$$\lambda_{min}(\mathbf{Q}) = \inf_{\mathbf{n}\in\mathbb{S}^2} \langle \mathbf{Q}\mathbf{n}, \mathbf{n} \rangle. \tag{0.1.44}$$

We have

$$\begin{aligned} \lambda_{min}\big(t\mathbf{Q}_1 + (1-t)\mathbf{Q}_2\big) &= \inf_{\mathbf{n}\in\mathbb{S}^2} \big\langle \big(t\mathbf{Q}_1 + (1-t)\mathbf{Q}_2\big)\mathbf{n}, \mathbf{n} \big\rangle \geq \\ t \inf_{\mathbf{n}\in\mathbb{S}^2} \langle \mathbf{Q}_1\mathbf{n}, \mathbf{n}\rangle + (1-t) \inf_{\mathbf{n}\in\mathbb{S}^2} &\langle \mathbf{Q}_2\mathbf{n}, \mathbf{n}\rangle = t\lambda_{min}\big(\mathbf{Q}_1\big) + (1-t)\lambda_{min}\big(\mathbf{Q}_2\big), \end{aligned} \tag{0.1.45}$$

for any $t \in [0,1]$. Therefore $\lambda_{min} : \mathbb{M}^{3\times 3}_{sym} \mapsto \mathbb{R}$ is a concave and a locally Lipschitz continuous function [39, Theorem 3.1.1], and a convex combination of two elements of $\mathcal{Q}_B$ remains in $\mathcal{Q}_B$. Moreover, $\mathcal{Q}_B$ is compact. Analogously, $\lambda_{max} : \mathbb{M}^{3\times 3}_{sym} \mapsto \mathbb{R}$ is a convex and locally Lipschitz function. By the spectral theorem it is possible to write $\mathbf{Q}$ in diagonal form

$$\mathbf{Q} = \lambda_1 \mathbf{i}_1 \otimes \mathbf{i}_1 + \lambda_2 \mathbf{i}_2 \otimes \mathbf{i}_2 + \lambda_3 \mathbf{i}_3 \otimes \mathbf{i}_3, \tag{0.1.46}$$

where $\{\lambda_i\}$ are the eigenvalues of $\mathbf{Q}$,

$$\lambda_1, \lambda_2, \lambda_3 \in \Big[-\frac{1}{3}, \frac{2}{3}\Big], \qquad \lambda_1 + \lambda_2 + \lambda_3 = 0, \tag{0.1.47}$$

and $\{\mathbf{i}_i\}$ is an orthonormal basis of eigenvectors (we present a different parameterization of the de Gennes tensor in Chapter 1). Suppose that two of the eigenvalues coincide, say $\lambda_1 = \lambda_2$. Writing $\mathbf{I} = \mathbf{i}_1 \otimes \mathbf{i}_1 + \mathbf{i}_2 \otimes \mathbf{i}_2 + \mathbf{i}_3 \otimes \mathbf{i}_3$, we can then write (0.1.46) in the equivalent form[31]

$$\mathbf{Q} = s\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big), \tag{0.1.48}$$

with $s = -3\lambda_1$ and $\mathbf{n} = \mathbf{e}_3$ yielding the *Ericksen (uniaxial) order tensor*. We define $\mathcal{Q}_U$ as the set of all the tensors in the form (0.1.48), that is the set of all matrices in $\mathcal{Q}_B$ such that two eigenvalues coincide

$$\mathcal{Q}_U := \left\{ \mathbf{Q} \in \mathcal{Q}_B, \text{ s.t. } \lambda_{max}(\mathbf{Q}) = -2\lambda_{min}(\mathbf{Q}) \text{ or } \lambda_{min}(\mathbf{Q}) = -2\lambda_{max}(\mathbf{Q}) \right\}. \quad (0.1.49)$$

We give a physical meaning to the variables appearing in (0.1.48). The vector $\mathbf{n}$ is associated with a common orientation of the molecules and the scalar parameter $s \in [-1/2, 1]$ with the degree of orientation of the molecules. The case $s = 0$ ($\mathbf{Q} = 0$) corresponds to isotropy, that is when the molecules are spread with equal probability along the three directions in $\mathbb{R}^3$ and it is impossible to identify a common direction. This is a phase of both the de Gennes and Ericksen tensor. If $s = -1/2$, then all the molecules lie with equal probability in the two directions in the place orthogonal to $\mathbf{n}$. In the limit case $s = 1$, $\mathbf{Q}$ can be written as

$$\mathbf{Q} = \mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}, \quad (0.1.50)$$

where we recognize the director $\mathbf{n} \in \mathbb{S}^2$, which represents the direction common to all the molecules[3]. This last case corresponds to Frank theory [33], [49, Chapter 3]. The set of Frank tensors is defined as

$$\mathcal{Q}_{Fr} := \left\{ \mathbf{Q} \in \mathcal{Q}_U, \text{ s.t. spectrum}(\mathbf{Q}) = \left\{ \frac{2}{3}, -\frac{1}{3}, -\frac{1}{3} \right\} \right\}. \quad (0.1.51)$$

It is easy to prove that any tensor in $\mathcal{Q}_{Fr}$ can be written in the form (0.1.50) (this is explicitly done also in the proof of Lemma 3, Chapter 3). It is remarkable that if we plug $\mathbf{n}$ and $-\mathbf{n}$ in (0.1.50) we obtain the same tensor field, and hence the information on the orientation of $\mathbf{n}$ is left out of picture. For the readers' convenience we recall the important chain of inclusions

$$\mathcal{Q}_{Fr} \subset \mathcal{Q}_U \subset \mathcal{Q}_B$$

and that $\mathcal{Q}_B$ is compact and convex, while $\mathcal{Q}_{Fr}$ and $\mathcal{Q}_U$ are compact and non-convex sets.

To conclude our overview on liquid crystals, we comment that the expressions *isotropic*, *uniaxial* and *biaxial* are borrowed from optics (see for instance [2]). It suffices to recall that in an optically isotropic material, light can propagate in all directions without suffering any change in its polarization. In optically anisotropic materials there exists at least one direction of propagation such that every polarization orthogonal to it would travel undistorted, if excited.

Nematic elastomers

Nematic liquid crystal elastomers are solid materials made of long polymeric chains with incorporated rigid anisotropic units. When these rigid units orient, thus assuming a uniaxial order, the chains stretch along the common direction of alignment. Nematic

[3] intermediate situations are obtained for $s \in (-1/2, 1) \backslash \{0\}$

elastomers usually exhibit a high temperature isotropic phase and undergo an isotropic-to-nematic transformation after cooling. Linking the polymer chains together into a gel network fixes their topology, and the melt is transformed into an elastic solid (a rubber). Rods can be directly attached to the backbone being part of the chain (main-chain polymers) or simply be pendant to it (side-chain polymers). It is well known ([15], [19], [20], [25], [27], [28]) that mechanical fields can deform the chains and re-arrange the local orientation of the mesogenic groups, modifying the optical properties of the material as well.

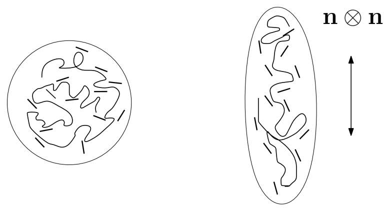

Figure 2: LEFT: high temperature (isotropic phase in elastomers). RIGHT: low temperature (nematic phase) with spontaneous alignment along the nematic director $\mathbf{n}$.

In rubber, monomers remain highly mobile. Thermal fluctuations move the chains as rapidly as in the melt, but only as far as their topological crosslinking constraints allow. These loose constraints make the polymeric liquid into a weak, highly extensible material. Rubber is a solid in that an energy input is required to change its macroscopic shape (in contrast to a liquid, which flows in response to shears) and recovers its original state when external influences are removed. New properties can now arise from the interaction between rubber elasticity, and nematic order. There is a debate on how to model this interaction (see [6], [19], [20], [23], [28], [34], [44]), and the many possible answers lead to interesting new effects such as shape changes without energy cost and strain-order coupling. In this dissertation we decribe a mathematical approach to such problems, showing that our results can be used to explain many of these phenomena.

0.1.2 Mathematical tools

Basic linear algebra. Let $\mathbf{F} \in \mathbb{M}^{n\times n}$. We recall the orthogonal decomposition

$$\mathbf{F} = \mathbb{E}(\mathbf{F}) + \mathbf{F}^{sk} = \mathbb{E}_0(\mathbf{F}) + \mathbf{F}^{sk} + \frac{(\operatorname{tr}\mathbf{F})}{n}\mathbf{I}, \tag{0.1.52}$$

where $\mathbf{F}^{sk} := (\mathbf{F} - \mathbf{F}^T)/2$, $\mathbb{E}(\mathbf{F}) := (\mathbf{F} + \mathbf{F}^T)/2$, $\mathbb{E}_0(\mathbf{F}) = \mathbb{E}(\mathbf{F}) - ((\operatorname{tr}\mathbf{F})/n)\mathbf{I}$. In this last definition we can consider the trace of $\mathbb{E}(\mathbf{F})$ as well, since $\operatorname{tr}\mathbf{F} = \operatorname{tr}\mathbb{E}(\mathbf{F})$. This fact will be widely used.

We write $\langle \mathbf{A}\xi, \eta\rangle = \sum_{ij} A_{ij}\xi_j\eta_i$ for the scalar product of a matrix $\mathbf{A}$ in $\mathbb{M}^{n\times n}$ with two vectors ξ, η in $\mathbb{R}^n$. Here A_{ij}, and ξ_i, η_j are the cartesian components of the respective matrices and vectors.

As already explained in the Introduction, by *domain* we mean an open, bounded and connected subset of $\mathbb{R}^n$ (with $n = 2, 3$). Moreover, by *Lipschitz domain* we mean an open, bounded and connected subset of $\mathbb{R}^n$ with Lipschitz boundary.

Korn's inequalities [17, Thms 6.3-3,6.3-4]. Let $\Omega \subset \mathbb{R}^n$ $(n = 2, 3)$ be a Lipschitz domain. Let $\mathbf{z} \in H^1(\Omega, \mathbb{R}^n)$. Then, there exists a positive constant $K_1 = K_1(\Omega, n)$ s.t.

$$\|\nabla \mathbf{z}\|^2_{L^2(\Omega,\mathbb{M}^{n\times n})} \leq K_1(\Omega, n)\Big(\|\mathbf{z}\|^2_{L^2(\Omega,\mathbb{R}^n)} + \|\mathbb{E}(\nabla \mathbf{z})\|^2_{L^2(\Omega,\mathbb{M}^{n\times n})}\Big). \tag{0.1.53}$$

Let now $\mathbf{z} \in H^1_{\Gamma_u}(\Omega, \mathbb{R}^n)$. Then, there exists a positive constant $K_2 = K_2(\Omega, n)$ s.t.

$$\|\nabla \mathbf{z}\|^2_{L^2(\Omega,\mathbb{M}^{n\times n})} \leq K_2(\Omega, n)\Big(\|\mathbb{E}(\nabla \mathbf{z})\|^2_{L^2(\Omega,\mathbb{M}^{n\times n})}\Big). \tag{0.1.54}$$

We introduce some notions on semi-convex functions and laminations. For this subject our main references are [21], [45]. We recall that $f : \mathbb{M}^{n\times n} \mapsto \mathbb{R} \cup \{+\infty\}$ is rank-1 convex if by definition $f(r\xi_1 + (1-r)\xi_2) \leq rf(\xi_1) + (1-r)f(\xi_2)$ for every $r \in [0, 1]$, $\xi_1, \xi_2 \in \mathbb{M}^{3\times 3}$ with $rank(\xi_1 - \xi_2) \leq 1$. A function $f : \mathbb{M}^{n\times n} \mapsto \mathbb{R} \cup \{+\infty\}$ is said to be polyconvex, if there exists a convex function h such that $f(\mathbf{F}) = h(M(\mathbf{F}))$, where $M(\mathbf{F})$ is the vector of all the minors of $\mathbf{F}$. We give the definition of quasiconvexity[1].

Definition 1 *A continuous function $f : \mathbb{M}^{n\times n} \mapsto \mathbb{R}$ is quasiconvex if and only if for every $\mathbf{Z} \in \mathbb{M}^{n\times n}$, ω open, bounded subset of $\mathbb{R}^n$, $\mathbf{w} \in C^1_o(\omega, \mathbb{R}^n)$, we have*

$$f(\mathbf{Z}) \leq |\omega|^{-1} \int_\omega f\big(\mathbf{Z} + \nabla \mathbf{w}(y)\big)dy. \tag{0.1.55}$$

Remark 1 *We can take $\mathbf{w} \in C^\infty_c(\omega, \mathbb{R}^n)$ in* (0.1.55) *(see [1, Def. I.2] and comment below). If f is quasiconvex and satisfies growth conditions as* (2.2.27)*, then* (0.1.55) *is true also for any $\mathbf{w} \in H^1_o(\omega, \mathbb{R}^n)$ (see [8, comment after Def. 2.2]) and in particular for any $\mathbf{w} \in H^{1,\infty}_o(\omega, \mathbb{R}^n)$.*

We define the convex envelope of a function f as $f^c(\xi) := \sup\{g(\xi) : g \leq f, g\,\text{convex}\}$. In the same way we define the poly-, quasi- and rank-one- convex envelopes, by requiring that the function g satisfies the corresponding requirement of partial convexity. In order to give a characterization for f^{rc}, which is crucial to our developments, we follow [21, Sect. 6.4]. To start, we need some preliminary definitions (see [21, Sect. 5.2.5]).

Definition 2 *Let us write for any integer K*

$$\Lambda_K := \Big\{\overline{\lambda} = (\lambda_1, \ldots, \lambda_K) : \lambda_i \geq 0, \sum_i^K \lambda_i = 1\Big\}. \tag{0.1.56}$$

Consider $\overline{\lambda} \in \Lambda_K$ and let $\xi_i \in \mathbb{M}^{n\times n}$, $1 \leq i \leq K$. We say that $\{\lambda_i, \xi_i\}_{i=1}^K$ satisfy (H_K) if (by induction on the index i)

- *when $K = 2$, then $rank(\xi_1 - \xi_2) \leq 1$;*
- *when $K > 2$, then, up to a permutation, $rank(\xi_1 - \xi_2) \leq 1$ and if, for every $2 \leq i \leq K - 1$, we define*

$$\begin{cases} \mu_1 = \lambda_1 + \lambda_2 & \eta_1 = \dfrac{\lambda_1\xi_1 + \lambda_2\xi_2}{\lambda_1 + \lambda_2} \\ \mu_i = \lambda_{i+1} & \eta_i = \xi_{i+1} \end{cases}$$

  then $\{\mu_i, \eta_i\}_{i=1}^K$ satisfy (H_{K-1}).

Remark 2 *When* $K = 4, \overline{\lambda} \in \Lambda_4$, *then* $\{\lambda_i, \xi_i\}_{i=1}^4$ *satisfy* H_4 *if, up to a permutation*

$$\begin{cases} rank(\xi_1 - \xi_2) \leq 1, \quad rank(\xi_3 - \xi_4) \leq 1 \\ rank(\eta_1 - \eta_2) \leq 1, \eta_1 := \dfrac{\lambda_1\xi_1 + \lambda_2\xi_2}{\lambda_1 + \lambda_2}, \eta_2 := \dfrac{\lambda_3\xi_3 + \lambda_4\xi_4}{\lambda_3 + \lambda_4} \end{cases}$$

holds.

For any $f : \mathbb{M}^{n\times n} \mapsto \mathbb{R} \cup \{+\infty\}$ one can characterize f^{rc} as [21, Thm 6.10]

$$f^{rc}(\xi) = \inf\Big\{\sum_i^K \lambda_i f(\xi_i) : \overline{\lambda} \in \Lambda_K, \sum_i^K \lambda_i\xi_i = \xi,\ \{\lambda_i, \xi_i\} \text{ satisfy } (H_K)\Big\}. \quad (0.1.57)$$

If we restrict our attention to the case of real valued functions, the following chain of inequalities follows by definition (see [21], page 265)

$$f^c \leq f^{pc} \leq f^{qc} \leq f^{rc}. \quad (0.1.58)$$

If $f : \mathbb{M}^{n\times n} \mapsto \mathbb{R} \cup \{+\infty\}$ the inequality $f^{qc} \leq f^{rc}$ needs not hold.

We define some semi-convex hulls of sets. Given any set (not necessarily compact) $E \subset \mathbb{M}^{n\times n}$ we define E^c the smallest convex set containing E. It can be proved that

$$E^c = \Big\{\xi \in \mathbb{M}^{n\times n} : \xi = \sum_i^K \lambda_i\xi_i : \xi_i \in E, \overline{\lambda} \in \Lambda_K, K = 1, 2, 3\ldots\Big\}. \quad (0.1.59)$$

We define by induction E^{lc}, the lamination-convex envelope of E as

$$E^{lc} = \bigcup_{i=0}^{\infty} E^{(i)}, \quad (0.1.60)$$

where $E^{(0)} = E$,

$$E^{(1)} = \big\{\xi = s\xi_1 + (1-s)\xi_2,\ \xi_1, \xi_2 \in E,\ \text{rank}(\xi_1 - \xi_2) \leq 1,\ s \in [0,1]\big\} \quad (0.1.61)$$

that is the set of first order laminates of E and

$$E^{(i+1)} = E^{(i)} \cup \big\{\xi = s\xi_1 + (1-s)\xi_2,\ \xi_1, \xi_2 \in E^{(i)},\ \text{rank}(\xi_1 - \xi_2) \leq 1,\ s \in [0,1]\big\} (0.1.62)$$

Coherently with our definitions, we have this chain of inequalities:

$$E \subseteq E^{lc} \subseteq E^c. \quad (0.1.63)$$

The following proposition, which is due to Bogovskiĭ (see [35, Thm 3.1]), has an important rôle in order to treat the case of the incompressible elastomers.

Proposition 1 *Consider* $\mathbb{N} \ni n \geq 2$ *and* $p \in (1, \infty)$. *Let* $\Omega \subset \mathbb{R}^n$ *be a Lipschitz domain. Assume* $\mathbf{z} \in H_o^{1,p}(\Omega, \mathbb{R}^n)$. *Then, there exists at least one solution to the problem*

$$\begin{cases} \mathbf{w} \in H_o^{1,p}(\Omega, \mathbb{R}^n), \\ \operatorname{div} \mathbf{w} = \operatorname{div} \mathbf{z}, \\ \|\mathbf{w}\|_{H^{1,p}(\Omega,\mathbb{R}^n)} \leq C_b(\Omega, n, p)\|\operatorname{div} \mathbf{z}\|_{L^p(\Omega)}, \end{cases}$$

where $C_b = C_b(\Omega, n, p) > 0$.

Gamma-convergence and relaxation

In this dissertation we will encounter several definitions of Gamma-convergence. We will use the Gamma-convergence in the product of the weak topology of L^2 with the weak topology of H^1, and the Gamma-convergence with respect to the product of the strong topology of L^2 with the weak topology of H^1. Here, as a paradigm, we give the definition of Gamma-convergence with respect to the weak topology of H^1, following the theory of Gamma-convergence in a topological space endowed with the weak topology. The general theory can be found in [22].

Definition 3 *Let $\mathcal{F}$ be a functional defined on $H^1(\Omega, \mathbb{R}^3)$. We define the relaxation of $\mathcal{F}$ in the weak topology of $H^1(\Omega, \mathbb{R}^3)$*

$$\overline{\mathcal{F}} = \sup\{\mathcal{G} : \mathcal{G} \text{ is } H^1(\Omega, \mathbb{R}^3) \text{ lower semicontinuous}, \mathcal{G} \leq \mathcal{F}\}. \tag{0.1.64}$$

Definition 4 *Let $\{\mathcal{F}_h\}$ be a sequence of functionals defined on $H^1(\Omega, \mathbb{R}^3)$. We define for $\mathbf{u} \in H^1(\Omega, \mathbb{R}^3)$*

$$\Gamma\text{-}\liminf_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) = \sup_{\mathcal{A}\in\mathcal{S}(\mathbf{u})} \liminf_{h\to+\infty} \inf\{\mathcal{F}_h(\mathbf{v}) : \mathbf{v} \in \mathcal{A}\},$$

$$\Gamma\text{-}\limsup_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) = \sup_{\mathcal{A}\in\mathcal{S}(\mathbf{u})} \limsup_{h\to+\infty} \inf\{\mathcal{F}_h(\mathbf{v}) : \mathbf{v} \in \mathcal{A}\},$$

where $\mathcal{S}(\mathbf{u})$ is the family of all the open sets in the weak topology of $H^1(\Omega, \mathbb{R}^3)$. If we have

$$\Gamma\text{-}\liminf_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) = \Gamma\text{-}\limsup_{h\to+\infty} \mathcal{F}_h(\mathbf{u}),$$

then the common value is said to be the $\Gamma\text{-}\lim_{h\to+\infty} \mathcal{F}_h(\mathbf{u})$.

In general we follow the sequential characterization of Gamma-convergence, which is equivalent to the abstract topological one [22, Chapt. 8] if $\mathcal{F}_h$ satisfy some coercivity condition uniformly in h (e.g. $\|\mathbf{u}_h\|^2_{H^1(\Omega,\mathbb{R}^3)} \leq \mathcal{F}_h(\mathbf{u}_h) \leq Const, \forall h \in \mathbb{N}$). We can thus write

$$\Gamma\text{-}\liminf_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) = \inf\big\{\liminf_{h\to+\infty} \mathcal{F}_h(\mathbf{u}_h), \mathbf{u}_h \rightharpoonup \mathbf{u}\big\},$$

$$\Gamma\text{-}\limsup_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) = \inf\big\{\limsup_{h\to+\infty} \mathcal{F}_h(\mathbf{u}_h), \mathbf{u}_h \rightharpoonup \mathbf{u}\big\}.$$

Also, we recall the useful characterization of the Gamma-limit which involves a lower and an upper bound.

- (*Liminf* inequality) $\forall\{\mathbf{u}_h\} \subset H^1(\Omega, \mathbb{R}^3)$, $\mathbf{u}_h \rightharpoonup \mathbf{u}$ in $H^1(\Omega, \mathbb{R}^3)$

$$\Gamma\text{-}\lim_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) \leq \liminf_{h\to+\infty} \mathcal{F}_h(\mathbf{u}_h),$$

- (*Limsup* inequality) there exists a sequence $\{\widetilde{\mathbf{u}}_h\} \subset H^1(\Omega, \mathbb{R}^3)$, $\widetilde{\mathbf{u}}_h \rightharpoonup \mathbf{u}$ in $H^1(\Omega, \mathbb{R}^3)$ such that

$$\Gamma\text{-}\lim_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) \geq \limsup_{h\to+\infty} \mathcal{F}_h(\widetilde{\mathbf{u}}_h).$$

Other equivalent characterization of the liminf and limsup inequalities are available in [7] and [22].

Fundamental Theorem of Gamma-convergence

Let $\{\mathcal{F}_h\}$ be a sequence of functionals defined on $H^1(\Omega, \mathbb{R}^3)$. Suppose that:

- $\forall \{\mathbf{u}_h\} \subset H^1(\Omega, \mathbb{R}^3)$ with $\sup_h \mathcal{F}_h(\mathbf{u}_h) < +\infty$, up to subsequences, we have $\mathbf{u}_h \rightharpoonup \overline{\mathbf{u}}$ to some $\overline{\mathbf{u}} \in H^1(\Omega, \mathbb{R}^3)$.
- $\forall \mathbf{u} \in H^1(\Omega, \mathbb{R}^3)$ there exits $\mathcal{F}(\mathbf{u}) = \Gamma\text{-}\lim_{h\to+\infty} \mathcal{F}_h(\mathbf{u})$.

Then, we have

- $\lim_{h\to+\infty}(\inf \mathcal{F}_h) = \min \mathcal{F}$ (convergence of minima).
- Let $\{\mathbf{u}_h\} \subset H^1(\Omega, \mathbb{R}^3)$ be a minimizing sequence for $\{\mathcal{F}_h\}$ (i.e. $\lim_h \mathcal{F}_h(\mathbf{u}_h) = \lim_h \inf \mathcal{F}_h$). Then, up to a subsequence, $\mathbf{u}_h \rightharpoonup \overline{\mathbf{u}}$ in H^1, where

$$\mathcal{F}(\overline{\mathbf{u}}) = \min \mathcal{F} \qquad \text{(convergence of minimum points).}$$

Proposition 2 *Let $\{\mathcal{F}_h\}$ be an increasing sequence of functionals defined on $H^1(\Omega, \mathbb{R}^3)$. Then, for every $\mathbf{u} \in H^1(\Omega, \mathbb{R}^3)$ there exists the*

$$\Gamma\text{-}\lim_{h\to+\infty} \mathcal{F}_h(\mathbf{u}) = \Gamma\text{-}\lim_{h\to+\infty} \overline{\mathcal{F}_h}(\mathbf{u}) = \sup_h \overline{\mathcal{F}_h}(\mathbf{u}),$$

where $\overline{\mathcal{F}_h}$ is the relaxation of $\mathcal{F}_h$.

Part I

Well-posed problems

Chapter 1

Strain-order coupling: equilibrium configurations

1.1 Introduction

We consider models that describe liquid crystal elastomers either in a biaxial or in a uniaxial phase and in the framework of Frank director theory. We prove existence of static equilibrium solutions in the presence of frustrations due to electro-mechanical boundary conditions and to applied loads and fields. We provide a mathematical framework for the study of equilibrium configurations of LCEs in the presence of external fields and boundary conditions.

The chapter is organized as follows. In Paragraph 1.1.1 we discuss the form of the energy functional in the most general of the theories, namely the biaxial (de Gennes) one. Section 1.2 is devoted to the proof of the existence result in this case. We introduce the functionals arising in the other two models (the uniaxial theory and the director theory) and present the corresponding existence results in Sections 1.3 and 1.4. In Section 1.5 we discuss some special equilibrium configurations, leading to phase diagrams relating order to imposed boundary displacements which may be significant in understanding experimental observations.

1.1.1 The functional $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$: equilibrium configurations

We introduce the functional

$$\begin{aligned}\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi) &:= \mathcal{F}_{nem}(\mathbf{Q}) + \mathcal{F}_{mec}(\mathbf{Q}, \mathbf{u}) - \mathcal{F}_{ele}(\mathbf{Q}, \phi) \qquad (1.1.1)\\ &= \int_\Omega f_{nem}(\mathbf{Q}, \nabla\mathbf{Q})dx + \int_\Omega f_{mec}(\mathbf{Q}, \nabla\mathbf{u})dx - \int_\Omega f_{ele}(\mathbf{Q}, \nabla\phi)dx.\end{aligned}$$

The energy densities appearing in (1.1.1) are defined below. The first term is classical in the theory of nematic liquid crystals (see [24],[49]):

$$f_{nem}(\mathbf{Q}, \nabla\mathbf{Q}) := \frac{L_1}{2} Q_{\alpha\beta,\gamma}Q_{\alpha\beta,\gamma} + \frac{L_2}{2} Q_{\alpha\beta,\beta}Q_{\alpha\gamma,\gamma} \frac{L_3}{2} Q_{\alpha\beta,\gamma}Q_{\alpha\gamma,\beta} + \Psi_{LdG}(\mathbf{Q}), \quad (1.1.2)$$

where L_i, $i = 1, 2, 3$ are the elastic constants, and $Q_{\alpha\beta,\gamma}$ is the $\alpha\beta$ cartesian component of the first derivative of $\mathbf{Q}$ with respect to x_γ ($\alpha, \beta, \gamma = 1, 2, 3$). Summation over repeated indices is understood. The constants L_i satisfy some constraints[43] in order to make (1.1.2) a positive definite expression of the first order derivatives of $\mathbf{Q}$. With no loss of generality, we assume $L_1 = \kappa^2, L_2 = L_3 = 0$ (well satisfying the constraints in [43]) in order to compare our results with those in [3]. Hence, (1.1.2) becomes:

$$f_{nem}(\mathbf{Q}, \nabla\mathbf{Q}) = \frac{\kappa^2}{2}|\nabla\mathbf{Q}|^2 + \Psi_{LdG}(\mathbf{Q}). \tag{1.1.3}$$

The term f_{nem} penalizes spatial variations of $\mathbf{Q}$ and introduces the Landau-de Gennes potential energy (LdG) $\Psi_{LdG}(\cdot) : \mathcal{Q}_B \mapsto \mathbb{R}$ which accounts for phase-transitions. It is usually given in the form of a truncated expansion of invariants of powers of $\mathbf{Q}$. The only technical assumption we need for Ψ_{LdG} is that it is lower semicontinuous.

One possible model for the mechanical coupling between nematic order and mechanical strain is given by

$$f_{mec}(\mathbf{Q}, \mathbf{F}) := \frac{1}{2}\mathbb{C}\big(\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}\big) : \big(\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}\big). \tag{1.1.4}$$

Here $\mathbf{F} \in \mathbb{M}^{3\times3}$, $\mathbb{E}(\mathbf{F}) = (\mathbf{F} + \mathbf{F}^T)/2$ is called the *strain tensor*, $\mathbb{C}$ is the fourth order tensor of elastic moduli (see [37, Section 29]), and γ is a positive constant that measures the interaction between $\mathbf{Q}$ and the strain. To explain our notation, we recall that, in cartesian components, $2E_{ij} = \partial u_i/\partial x_j + \partial u_j/\partial x_i$ and

$$\frac{1}{2}\mathbb{C}\mathbf{E} : \mathbf{E} = \frac{1}{2}\sum_{ijkl} C_{ijkl}E_{kl}E_{ij}.$$

We require that

$$-C_1 + C_2|\mathbb{E}(\mathbf{F})|^2 \leq \frac{1}{2}\mathbb{C}\big(\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}\big) : \big(\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}\big), \tag{1.1.5}$$

for some positive constants C_1, C_2. We take $\mathbb{C}(\mathbf{A}) = 2\mu\mathbf{A} + \lambda\,\mathrm{tr}\,(\mathbf{A})\mathbf{I}$, $\forall\mathbf{A} \in \mathbb{M}^{3\times3}_{sym}$, with μ, λ positive, hence satisfying (1.1.5). The parameter μ, λ are the classical Lamé constants of linearized isotropic elasticity. In this case, (1.1.4) becomes

$$f_{mec}(\mathbf{Q}, \mathbf{F}) = \mu\big(|\mathbb{E}(\mathbf{F})|^2 - 2\gamma\mathbb{E}(\mathbf{F}) : \mathbf{Q} + \gamma^2|\mathbf{Q}|^2\big) + \frac{\lambda}{2}(\mathrm{tr}\,\mathbf{F})^2. \tag{1.1.6}$$

We remark that accepting equations (1.1.4)-(1.1.6) has non-trivial physical implications. In particular, (1.1.6) states that the coupling energy vanishes if and only if the order tensor can *reproduce* the mechanical strain ($\mathbf{Q} = \frac{1}{\gamma}\mathbb{E}(\mathbf{u})$), and that when $\mathbf{Q}$ differs from $\frac{1}{\gamma}\mathbb{E}(\mathbf{u})$, there is a finite energetic penalty for any value of $\mathbf{Q}$ within the admissible set $\mathcal{Q}_B$. This is consistent with [23, 44], but other scenarios are possible. Indeed, by constraining the admissible $\mathbf{Q}$ to be uniaxial, or in the framework of Frank director theory, we will instead accept that certain changes in the state of order of the system (those violating the constraints) are not achievable by means of mechanical stresses, see also [18]-[20], [23]-[28]. We refer to [6, 30, 34, 50] for more discussions on this topic, both in the framework of linear and of nonlinear kinematics.

Finally, we introduce the electric displacement $\mathbf{d}$ (see [24], [46]) related to the electric field $\mathbf{e}$ in this way

$$\mathbf{d} = \epsilon_o(\bar{\epsilon}\mathbf{I} + \epsilon_a\mathbf{Q})\mathbf{e}, \tag{1.1.7}$$

and the electric energy density (see [5])

$$f_{ele}(\mathbf{Q},\mathbf{e}) := \frac{1}{2}\mathbf{d}\cdot\mathbf{e} = \frac{\epsilon_o}{2}\Big(\bar{\epsilon}|\mathbf{e}|^2 + \epsilon_a\langle\mathbf{Q}\mathbf{e},\mathbf{e}\rangle\Big). \tag{1.1.8}$$

The minus sign in front of $\mathcal{F}_{ele}$ in (1.1.1) arises because this term represents the work done by an external field on the system. Here ϵ_o, $\bar{\epsilon}$, ϵ_a are dielectric constants, see Table 1.1. For definiteness, we assume $\epsilon_a > 0$, in which case the electric field aligns the mesogens along itself. In the case $\epsilon_a < 0$ the molecules have a tendency to spread in a plane orthogonal to the direction of the vector $\mathbf{e}$.

$\epsilon_o > 0$	Dielectric constant in vacuum
$\epsilon_\parallel > 0$	(Relative) parallel dielectric constant
$\epsilon_\perp > 0$	(Relative) perpendicular dielectric constant
$\epsilon_a := \epsilon_\parallel - \epsilon_\perp$	(Relative) dielectric anisotropy constant
$\bar{\epsilon} := (2\epsilon_\perp + \epsilon_\parallel)/3$	(Relative) average dielectric constant

Table 1.1: Dielectric constants.

We find it convenient to introduce the map $\mathbf{A}(\cdot) : \mathcal{Q}_X \longrightarrow \mathbb{M}^{3\times3}_{sym}$ defined as

$$\mathbf{A}(\mathbf{Q}) := \frac{\epsilon_o}{2}\Big(\bar{\epsilon}\mathbf{I} + \epsilon_a\mathbf{Q}\Big), \tag{1.1.9}$$

where X stands either for Fr, U or B. Letting $\mathbf{e} = -\nabla\phi$ (see Paragraph 1.2.1), we can write

$$\mathcal{F}_{ele}(\mathbf{Q},\phi) = \int_\Omega \big\langle\mathbf{A}(\mathbf{Q})\nabla\phi, \nabla\phi\big\rangle dx. \tag{1.1.10}$$

We recall that $\epsilon_\perp, \epsilon_\parallel$ are assumed to be strictly positive. Suppose for a moment $\epsilon_a > 0$. Trivially we have

$$\frac{\epsilon_o}{2}\epsilon_\perp|\xi|^2 \le \big\langle\mathbf{A}(\mathbf{Q})\xi,\xi\big\rangle \le \frac{\epsilon_o}{2}\epsilon_\parallel|\xi|^2, \quad \forall\,\mathbf{Q}\in\mathcal{Q}_B, \forall\xi\in\mathbb{R}^3, \tag{1.1.11}$$

(and hence for any $\mathbf{Q} \in \mathcal{Q}_{Fr}$ and $\mathcal{Q}_U$). Suppose now $\epsilon_a < 0$. By elementary manipulations we can write (1.1.9) as $\mathbf{A}(\mathbf{Q}) = \frac{\epsilon_o}{2}\big(\epsilon_\parallel\mathbf{I} + (-\epsilon_a)\big(\frac{2}{3}\mathbf{I} - \mathbf{Q}\big)\big)$. It then follows

$$\frac{\epsilon_o}{2}\epsilon_\parallel|\xi|^2 \le \big\langle\mathbf{A}(\mathbf{Q})\xi,\xi\big\rangle \le \frac{\epsilon_o}{2}\epsilon_\perp|\xi|^2, \quad \forall\,\mathbf{Q}\in\mathcal{Q}_B, \forall\xi\in\mathbb{R}^3. \tag{1.1.12}$$

Considering (1.1.11) and (1.1.12), we can write

$$m\int_{\Omega}|\nabla\phi|^2dx \leq \mathcal{F}_{ele}(\mathbf{Q},\phi) \leq M\int_{\Omega}|\nabla\phi|^2dx, \tag{1.1.13}$$

having introduced positive constants

$$m := \min\Big\{\frac{\epsilon_o}{2}\epsilon_{\|}, \frac{\epsilon_o}{2}\epsilon_{\perp}\Big\}, \quad M := \max\Big\{\frac{\epsilon_o}{2}\epsilon_{\|}, \frac{\epsilon_o}{2}\epsilon_{\perp}\Big\}. \tag{1.1.14}$$

We note that, since $\mathbf{A}$ is positive definite and symmetric, $\mathcal{F}_{ele}$ is a uniformly elliptic integral. When $\epsilon_a = 0$, $\mathcal{F}_{ele}$ is independent of $\mathbf{Q}$. Correctly, the lower and upper bound coincide.

1.2 The biaxial theory

Setting of the problem. We introduce subsets of $L^2(\Omega, \mathbb{M}^{3\times3})$ and of $H^1(\Omega, \mathbb{M}^{3\times3})$

$$L^2(\Omega, \mathcal{Q}_X) := \{\mathbf{Q} \in L^2(\Omega, \mathbb{M}^{3\times3}) \text{ s.t. } \mathbf{Q}(x) \in \mathcal{Q}_X \text{ a.e.}\}, \tag{1.2.1}$$

$$H^1(\Omega, \mathcal{Q}_X) := \{\mathbf{Q} \in H^1(\Omega, \mathbb{M}^{3\times3}) \text{ s.t. } \mathbf{Q}(x) \in \mathcal{Q}_X \text{ a.e.}\}, \tag{1.2.2}$$

where X stands either for Fr, U or B. We assume Ω a Lipschitz domain in $\mathbb{R}^3$ (so that we can apply Rellich Theorem [17, Theorem 6.1-5]). We discuss some properties of the set $H^1(\Omega, \mathcal{Q}_B)$. Let us start proving that it is closed in the strong $H^1(\Omega, \mathbb{M}^{3\times3})$-topology. Let us take a sequence $\{\mathbf{Q}_k\}$ in $H^1(\Omega, \mathcal{Q}_B)$ strongly converging to $\mathbf{Q}$. Up to a subsequence (not re-labelled), we have $\mathbf{Q}_k \to \mathbf{Q}$ a.e. in Ω. Since $\lambda_{min}(\cdot)$ is a continuous function, it follows that $\lambda_{min}(\mathbf{Q}_k) \to \lambda_{min}(\mathbf{Q})$ a.e. in Ω. Therefore, if $\lambda_{min}(\mathbf{Q}_k) \geq -1/3$, then $\lambda_{min}(\mathbf{Q}) \geq -1/3$ a.e. in Ω and $H^1(\Omega, \mathcal{Q}_B)$ is strongly closed. Now, from the convexity of $\mathcal{Q}_B$, we have that $H^1(\Omega, \mathcal{Q}_B)$ is convex, and hence closed in the weak topology of $H^1(\Omega, \mathbb{M}^{3\times3})$. Analogously, the subset $L^2(\Omega, \mathcal{Q}_B)$ is strongly and weakly closed in $L^2(\Omega, \mathbb{M}^{3\times3})$. Now we consider $H^1(\Omega, \mathcal{Q}_U)$ and $H^1(\Omega, \mathcal{Q}_{Fr})$. Thanks to the continuity properties of λ_{min} and λ_{max}, it is straightforward to verify that they are strongly closed and weakly sequentially closed. Furthermore, $L^2(\Omega, \mathcal{Q}_X)$ (where X stands either for Fr or U) is strongly closed but not weakly closed (the consequence of this fact are crucial to the analysis of Chapter 3).

In order to take into account the presence of boundary conditions, in what follows we deal with the subspaces $H^1_{\Gamma_\phi}(\Omega)$ and $H^1_{\Gamma_u}(\Omega, \mathbb{R}^3)$, that is the set of H^1-functions which vanish (in the sense of traces) on Γ_ϕ, Γ_u. Similarly, we define $H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_B)$ the (non-empty) set of de Gennes tensors with components in H^1 and which vanish on Γ_Q. Letting $\mathbf{Q}_o \in H^1(\Omega, \mathcal{Q}_X)$, where X stands either for U or Fr, we denote with $H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_X) + \mathbf{Q}_o$ two subsets of H^1-tensors with assigned trace on Γ_Q. As above, they are strongly and weakly closed in $H^1(\Omega, \mathbb{M}^{3\times3})$.

1.2.1 Study of the functional $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$

Consider the functional (1.1.1) defined on $H^1(\Omega, \mathcal{Q}_B) \times H^1(\Omega, \mathbb{R}^3) \times H^1(\Omega)$ and accompanied by some boundary conditions (which we omit here for brevity). It is not a priori clear whether $\mathcal{E}$ is bounded below or above. The physical properties of the system suggest what kind of analysis to perform. It is well known (see [41, Chapter 2]) that an electric field induces a polarization field in dielectric materials. In the absence of free ions and in static conditions, the system is governed by Maxwell-Faraday's law $\operatorname{curl} \mathbf{e} = 0$ and Maxwell-Gauss law $\operatorname{div} \mathbf{d} = 0$. We notice that Faraday's law is solved by setting $\mathbf{e} = -\nabla\phi$ if we assume Ω simply connected. In principle, this hypothesis is not required to analyze the critical points of $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$, and has only this physical justification. Coherently, in Theorems 2 and 5 in the Introduction to the thesis, Ω is any Lipschitz domain, since this is enough to describe the critical points of $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$ (see also [38]). Then, we minimize $\mathcal{E}(\cdot, \cdot, \phi)$ in the first two variables imposing Gauss law $\operatorname{div} \mathbf{d} = 0$ as a constraint. We find a non-local dependence of the solution to Gauss equation that we describe as $\phi = \Psi[\mathbf{Q}]$. Our main result is the following.

Theorem 6 *Let $\Omega \subset \mathbb{R}^3$ be a simply connected and Lipschitz domain, let $\Gamma_Q, \Gamma_u, \Gamma_\phi \subseteq \partial\Omega$ be open subsets with positive surface measure, let $\mathbf{Q}_o \in H^1(\Omega, \mathcal{Q}_B), \mathbf{u}_o \in H^1(\Omega, \mathbb{R}^3), \phi_o \in H^1(\Omega)$. Let $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$ as in* (1.1.1)*, where $f_{nem}, f_{mec}, f_{ele}$ are given as in* (1.1.3), (1.1.6), (1.1.8)*. Then, $(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \overline{\phi})$ is a min-max critical point of $\mathcal{E}$, i.e.:*

$$\mathcal{E}(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \overline{\phi}) = \min_{\substack{\{H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_B) + \mathbf{Q}_o\} \\ \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}}} \max_{H^1_{\Gamma_\phi}(\Omega) + \phi_o} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi), \tag{1.2.3}$$

if and only if $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ is a solution to this problem:

$$\min_{\substack{\{H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_B) + \mathbf{Q}_o\} \\ \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}}} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi), \quad \text{sub Gauss law}, \tag{1.2.4}$$

with $\overline{\phi} = \Psi[\overline{\mathbf{Q}}]$.

Outline of the proof of Theorem 6. We write Gauss equation in weak form

$$\begin{cases} \text{Find } \phi \in H^1(\Omega) \text{ s.t.} \\ \displaystyle\int_\Omega \big\langle \epsilon_o \big(\bar{\epsilon}\mathbf{I} + \epsilon_a \mathbf{Q}\big) \nabla\phi, \nabla\varphi \big\rangle dx = 0 \\ \phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \varphi \in H^1_{\Gamma_\phi}(\Omega). \end{cases} \tag{1.2.5}$$

Let us attack problem (1.2.4). Suppose that for any given $\mathbf{Q} \in H^1(\Omega, \mathcal{Q}_B)$ we find a unique function which solves Gauss equation. We indicate it with $\Psi[\mathbf{Q}]$. We can thus plug $\Psi[\mathbf{Q}]$ in $\mathcal{F}_{ele}(\mathbf{Q},\cdot), \mathcal{E}(\mathbf{Q},\mathbf{u},\cdot)$ yielding

$$\mathcal{F}^*_{ele}(\mathbf{Q}) := \mathcal{F}_{ele}(\mathbf{Q},\Psi[\mathbf{Q}]), \quad \mathcal{E}^*(\mathbf{Q},\mathbf{u}) := \mathcal{E}(\mathbf{Q},\mathbf{u},\Psi[\mathbf{Q}]), \tag{1.2.6}$$
$$\mathcal{E}^*(\mathbf{Q},\mathbf{u}) = \int_\Omega \Big(f_{nem}(\mathbf{Q},\nabla\mathbf{Q}) + f_{mec}(\mathbf{Q},\nabla\mathbf{u}) - f_{ele}\big(\mathbf{Q},\nabla\Psi[\mathbf{Q}]\big)\Big) dx,$$

and start the minimization procedure for $\mathcal{E}^*(\mathbf{Q},\mathbf{u})$. On the other hand, consider now problem (1.2.3). We first maximize $\mathcal{E}(\mathbf{Q},\mathbf{u},\phi)$ in ϕ for any given $(\mathbf{Q},\mathbf{u}) \in H^1(\Omega,\mathcal{Q}_B) \times H^1(\Omega,\mathbb{R}^3)$, and then minimize in the first two variables. Actually, due to the structure of the functional, we observe that

$$\min_{\substack{\{H^1_{\Gamma_Q}(\Omega,\mathcal{Q}_B)+\mathbf{Q}_o\} \\ \times\{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}}} \ \max_{H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}(\mathbf{Q},\mathbf{u},\phi) = \tag{1.2.7}$$

$$\min_{\substack{\{H^1_{\Gamma_Q}(\Omega,\mathcal{Q}_B)+\mathbf{Q}_o\} \\ \times\{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}}} \left(\int_\Omega \big(f_{nem}(\mathbf{Q},\nabla\mathbf{Q}) + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\big) dx - \min_{H^1_{\Gamma_\phi}(\Omega)+\phi_o} \int_\Omega f_{ele}(\mathbf{Q},\nabla\phi) dx \right).$$

Suppose we can find a unique solution to the *inner* minimization problem for $\mathcal{F}_{ele}$

$$\min_{H^1_{\Gamma_\phi}(\Omega)+\phi_o} \int_\Omega f_{ele}(\mathbf{Q},\nabla\phi) dx, \quad \forall\, \mathbf{Q} \in H^1(\Omega,\mathcal{Q}_B). \tag{1.2.8}$$

We characterize it as $\Phi[\mathbf{Q}]$. By a direct inspection we observe that Gauss equation coincides with Euler-Lagrange equation associated with (1.2.8), so that $\Psi[\mathbf{Q}] \equiv \Phi[\mathbf{Q}], \forall\, \mathbf{Q} \in H^1(\Omega,\mathcal{Q}_B)$ and problems (1.2.3), (1.2.4) are exactly equivalent. Hence, if we plug $\Phi[\mathbf{Q}]$ in $\mathcal{E}(\mathbf{Q},\mathbf{u},\cdot)$ we obtain $\mathcal{F}^*_{ele}(\mathbf{Q}) = \mathcal{F}_{ele}(\mathbf{Q},\Phi[\mathbf{Q}])$, $\mathcal{E}^*(\mathbf{Q},\mathbf{u}) = \mathcal{E}(\mathbf{Q},\mathbf{u},\Phi[\mathbf{Q}])$. We are left with

$$\min_{\substack{\{H^1_{\Gamma_Q}(\Omega,\mathcal{Q}_B)+\mathbf{Q}_o\} \\ \times\{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}}} \mathcal{E}^*(\mathbf{Q},\mathbf{u}). \tag{1.2.9}$$

This is solved in Paragraph 1.2.3. In Paragraph 1.2.2 we show that Φ and Ψ exist and are unique and can be identified. First, we need to investigate some properties of $\mathcal{F}_{ele}$.

1.2.2 Minimizer $\Phi[\mathbf{Q}]$ of $\mathcal{F}_{ele}(\mathbf{Q},\phi)$

In this section we study the well-posedness of problem (1.2.8). We show that a solution to (1.2.8) exists and is unique yielding a coherent definition of $\Phi[\mathbf{Q}]$. For this purpose, we need to verify the hypotheses of the Direct Method in the Calculus of Variations (see [36] as general reference). This is done in Proposition 3. In brief, we recall that the existence of solutions of minimum problems follows from a version of Weiestrass Theorem for infinite dimensional function spaces. Two are the main ingredients. First, we require the boundedness of minimizing sequences so that we may extract subsequences converging in the weak topology. Secondly, we need the sequential lower semicontinuity of the functional with respect to the same topology. In Proposition 4 we discuss the continuity of $\Phi[\mathbf{Q}]$ in a sense to be specified. This is of fundamental importance in order to solve (1.2.9).

Existence and Uniqueness of $\Phi[\mathbf{Q}]$

Proposition 3 *For every given* $\mathbf{Q}$ *in* $H^1(\Omega, \mathcal{Q}_B)$ *there exists a unique* $\Phi[\mathbf{Q}]$ *which solves* (1.2.8).

Proof. We prove relative compactness of the minimizing sequence, and the weak sequential lower semicontinuity (in brief w.s.l.s.c.) of $\mathcal{F}_{ele}$. Uniqueness follows from the strict convexity. Let $\{\phi_k\} \subset \{H^1_{\Gamma_\phi}(\Omega) + \phi_o\}$ be a minimizing sequence of $\mathcal{F}_{ele}$. For any $\mathbf{Q} \in H^1(\Omega, \mathcal{Q}_B)$, by (1.1.13) we have

$$m \int_\Omega |\nabla \phi_k|^2 dx \leq \mathcal{F}_{ele}(\mathbf{Q}, \phi_k) \leq Const < +\infty. \tag{1.2.10}$$

By Poincaré inequality [17, Theorem 6.1-8], $\{\phi_k\}$ is bounded in $H^1(\Omega)$. From the reflexivity of $H^1(\Omega)$ and the continuity property of the trace we can extract a subsequence weakly convergent to some ϕ in $H^1_{\Gamma_\phi}(\Omega) + \phi_o$. Then, that

$$\int_\Omega f_{ele}(\mathbf{Q}, \nabla\phi)dx \leq \liminf_{k\to+\infty} \int_\Omega f_{ele}(\mathbf{Q}, \nabla\phi_k)dx, \quad \forall\, \mathbf{Q} \in H^1(\Omega, \mathcal{Q}_B) \tag{1.2.11}$$

when $\phi_k \rightharpoonup \phi$ w-$H^1(\Omega)$, follows by the convexity of $\mathcal{F}_{ele}(\mathbf{Q}, \cdot)$. □

We can characterize the solution to (1.2.8) as the unique solution to the associated Euler-Lagrange equation. In particular, Proposition 1.2.2 allows to identify Φ and Ψ. In the following we do not make any distinction between them. From now on, we focus our attention on $\mathcal{E}^*(\mathbf{Q}, \mathbf{u})$ as defined in (1.2.6) and on problem (1.2.9). Our first task is studying the non-local dependence of Φ on $\mathbf{Q}$.

Continuity properties of $\Phi[\mathbf{Q}]$

Proposition 4 *Assume that*

$$\lim_{k\to+\infty} \int_\Omega |\mathbf{Q}_k - \mathbf{Q}|^2 dx = 0, \tag{1.2.12}$$

where $\mathbf{Q}_k, \mathbf{Q} \in L^2(\Omega, \mathcal{Q}_X)$ $\forall\, k \in \mathbb{N}$ *and where* X *stands either for* Fr, U *or* B. *Then* $\Phi[\mathbf{Q}_k] \to \Phi[\mathbf{Q}]$ s-$H^1(\Omega)$.

Proof. Let us define the tensor field $\mathbf{B} : \Omega \mapsto \mathbb{M}^{3\times3}$ as follows

$$\mathbf{B}(x) := \mathbf{A}(\mathbf{Q})(x). \tag{1.2.13}$$

For a.e. x in Ω, $\mathbf{B}$ is a symmetric, positive definite matrix with bounded components (see (1.1.11)). It represents the matrix of the coefficients of the Euler-Lagrange equation for $\mathcal{F}_{ele}$ in the unknown variable $\phi \in H^1(\Omega)$ at a given $\mathbf{Q}$ in $L^2(\Omega, \mathcal{Q}_X)$:

$$\begin{cases} \int_\Omega \langle \mathbf{B}(x)\nabla\phi, \nabla\varphi \rangle dx = 0 \\ \phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \varphi \in H^1_{\Gamma_\phi}(\Omega). \end{cases}$$

We denote its unique solution with Φ. For every $k \in \mathbb{N}$ denote $\mathbf{B}_k(x) = \mathbf{A}(\mathbf{Q}_k)(x)$ and consider the problem

$$\begin{cases} \text{Find } \phi \in H^1(\Omega) \text{ s.t.} \\ \int_\Omega \langle \mathbf{B}_k(x)\nabla\phi, \nabla\varphi \rangle dx = 0 \\ \phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \varphi \in H^1_{\Gamma_\phi}(\Omega). \end{cases}$$

whose unique solution is Φ_k. From (1.2.13) it follows that $\mathbf{B}_k \to \mathbf{B}$ s-$L^2(\Omega, \mathbb{M}^{3\times3})$. Hence, the properties of ellipticity yield $\Phi_k \to \Phi$ s-$H^1(\Omega)$. A proof is given in Appendix 1.6.1 for the readers' convenience. We obtain the claim by noticing that $\Phi = \Phi[\mathbf{Q}]$, $\Phi_k = \Phi[\mathbf{Q}_k]$. □

In what follows we frequently indicate Φ instead of $\Phi[\mathbf{Q}]$ and Φ_k instead of $\Phi[\mathbf{Q}_k]$.

Remark 3 A consequence of Proposition 4 is that

$$\langle \mathbf{A}(\mathbf{Q}_k)\nabla\Phi_k, \nabla\Phi_k \rangle \to \langle \mathbf{A}(\mathbf{Q})\nabla\Phi, \nabla\Phi \rangle \quad s\text{-}L^1(\Omega). \tag{1.2.14}$$

Indeed, the convergence in (1.2.14) holds pointwise almost everywhere. Moreover, we have the uniform bound $0 \leq \langle \mathbf{A}(\mathbf{Q}_k)\nabla\Phi_k, \nabla\Phi_k \rangle \leq M|\nabla\Phi_k|^2$. We can then apply a generalized version of Lebesgue Dominated Convergence Theorem, and

$$\lim_{k\to+\infty} \int_\Omega \langle \mathbf{A}(\mathbf{Q}_k)\nabla\Phi_k, \nabla\Phi_k \rangle dx = \int_\Omega \langle \mathbf{A}(\mathbf{Q})\nabla\Phi, \nabla\Phi \rangle dx. \tag{1.2.15}$$

We are now ready to study the minimization problem in (1.2.9).

1.2.3 Minimization of $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \Phi[\mathbf{Q}])$ with respect to $(\mathbf{Q}, \mathbf{u})$

Proposition 5 *Let $\mathbf{Q}_o$, $\mathbf{u}_o$, ϕ_o, $\Omega, \Gamma_Q, \Gamma_u, \Gamma_\phi$ as in Theorem 6 and $\mathcal{E}^*$ defined as in (1.2.6). The problem*

$$\min_{\substack{\{H^1_{\Gamma_Q}(\Omega,\mathcal{Q}_B)+\mathbf{Q}_o\} \\ \times\{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}}} \mathcal{E}^*(\mathbf{Q}, \mathbf{u}) \tag{1.2.16}$$

admits solutions.

Proof. A first step (Step 1.2.3.(1)) consists in proving relative compactness of the minimizing sequence. Then, we prove the w.s.l.s.c. of the functional (Step 1.2.3.(2)).

Step 1.2.3.(1). Let $\{\mathbf{Q}_k, \mathbf{u}_k\} \subset \{H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_B) + \mathbf{Q}_o\} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$ be a minimizing sequence for $\mathcal{E}^*$. It is straightforward to obtain a uniform bound for some positive constant (in what follows, the constants may change from line to line while we maintain the same name):

$$\int_\Omega \Big\{ f_{nem}(\mathbf{Q}_k, \nabla \mathbf{Q}_k) + f_{mec}(\mathbf{Q}_k, \nabla \mathbf{u}_k) - f_{ele}\big(\mathbf{Q}_k, \nabla \Phi[\mathbf{Q}_k]\big) \Big\} dx \le Const < +\infty \tag{1.2.17}$$

In addition, we have a uniform bound for $\mathcal{F}_{ele}(\mathbf{Q}_k, \Phi[\mathbf{Q}_k])$. In fact, by the minimality of Φ, we know that $\mathcal{F}_{ele}(\mathbf{Q}, \Phi[\mathbf{Q}]) \le \mathcal{F}_{ele}(\mathbf{Q}, \phi_o)$. We obtain this chain of inequalities:

$$\begin{aligned} \int_\Omega \Big\{ f_{nem}(\mathbf{Q}_k, \nabla \mathbf{Q}_k) + f_{mec}(\mathbf{Q}_k, \nabla \mathbf{u}_k) \Big\} dx &\le Const + \int_\Omega f_{ele}(\mathbf{Q}_k, \nabla \Phi[\mathbf{Q}_k]) dx \\ \le Const + \int_\Omega f_{ele}(\mathbf{Q}_k, \nabla \phi_o) dx &\le Const + M \int_\Omega |\nabla \phi_o|^2 dx. \end{aligned} \tag{1.2.18}$$

Neglecting terms which are bounded from below in (1.2.18), we can find a uniform control of the sequence $\{\mathbf{u}_k\}$. In fact

$$0 \le \mu \int_\Omega \Big\{ |\mathbb{E}(\nabla \mathbf{u}_k)|^2 + \gamma^2 |\mathbf{Q}_k|^2 - 2\gamma \mathbb{E}(\nabla \mathbf{u}_k) : \mathbf{Q}_k \Big\} dx \le Const < +\infty. \tag{1.2.19}$$

Recalling that $\mathbf{Q}_k$ has almost everywhere bounded components uniformly in $k \in \mathbb{N}$, we easily get that

$$\mu \int_\Omega \Big\{ |\mathbb{E}(\nabla \mathbf{u}_k)|^2 - 2\gamma \mathbb{E}(\nabla \mathbf{u}_k) : \mathbf{Q}_k \Big\} dx \tag{1.2.20}$$

is bounded below and above. It is straightforward to see that $\mathbb{E}(\nabla \mathbf{u}_k)$ is uniformly bounded in $L^2(\Omega, \mathbb{M}^{3\times 3})$. Korn's inequality (0.1.54) yields boundedness of $\{\mathbf{u}_k\}$ in $H^1(\Omega, \mathbb{R}^3)$. Recalling that (1.2.20) is bounded from below, and neglecting other terms which are also bounded from below, (1.2.18) yields

$$0 \le \int_\Omega \Big(\frac{\kappa^2}{2} |\nabla \mathbf{Q}_k|^2 + \mu \gamma^2 |\mathbf{Q}_k|^2 \Big) dx \le Const < +\infty. \tag{1.2.21}$$

This guarantees the boundedness of $\{\mathbf{Q}_k\}$ in $H^1(\Omega, \mathbb{M}^{3\times 3})$ (notice that we do not need to invoke Poincaré inequality). By the reflexivity of the function spaces, we have that up to subsequences (not relabelled)

$$\mathbf{Q}_k \rightharpoonup \mathbf{Q} \quad w\text{-}H^1(\Omega, \mathbb{M}^{3\times 3}), \quad \mathbf{u}_k \rightharpoonup \mathbf{u} \quad w\text{-}H^1(\Omega, \mathbb{R}^3) \tag{1.2.22}$$

to some pair $(\mathbf{Q}, \mathbf{u}) \in \{H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_B) + \mathbf{Q}_o\} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$. This is true because of the continuity properties of the trace operator.

Step 1.2.3.(2). We prove that

$$\int_\Omega \Big(f_{nem}(\mathbf{Q}, \nabla\mathbf{Q}) + f_{mec}(\mathbf{Q}, \nabla\mathbf{u}) - f^*_{ele}(\mathbf{Q}) \Big) dx \leq \tag{1.2.23}$$

$$\liminf_{k\to+\infty} \int_\Omega \Big(f_{nem}(\mathbf{Q}_k, \nabla\mathbf{Q}_k) + f_{mec}(\mathbf{Q}_k, \nabla\mathbf{u}_k) - f^*_{ele}(\mathbf{Q}_k) \Big) dx,$$

with respect to the convergence in (1.2.22). In Proposition 4 we have already proved that $\mathcal{F}^*_{ele}(\mathbf{Q})$ is indeed continuous in the sense of (1.2.12), and hence of (1.2.22), thanks to Rellich's Theorem. Below, we show the w.s.l.s.c. of the first two terms separately. This is a sufficient condition in order to derive the w.s.l.s.c. of the whole functional $\mathcal{E}^*$. Having assumed $\Psi_{LdG}(\cdot)$ lower semicontinuous yields

$$\int_\Omega \Big(\frac{\kappa^2}{2} |\nabla\mathbf{Q}|^2 + \Psi_{LdG}(\mathbf{Q}) \Big) dx \leq \liminf_{k\to+\infty} \int_\Omega \Big(\frac{\kappa^2}{2} |\nabla\mathbf{Q}_k|^2 + \Psi_{LdG}(\mathbf{Q}_k) \Big) dx \tag{1.2.24}$$

with respect to the convergence (1.2.22), from standard facts in functional analysis (see [36, Chapter 4]). Since each single summand in (1.1.6) is w.s.l.s.c., we have

$$\int_\Omega f_{mec}(\mathbf{Q}, \nabla\mathbf{u}) dx \leq \liminf_{k\to+\infty} \int_\Omega f_{mec}(\mathbf{Q}_k, \nabla\mathbf{u}_k) dx, \tag{1.2.25}$$

where the convergence is as in (1.2.22). □

Remark 4 The previous result contains, in particular, the proof of the w.s.l.s.c. of

$$\mathcal{F}_{mec}(\mathbf{Q}, \mathbf{u}) = \int_\Omega \mu \Big(|\mathbb{E}(\nabla\mathbf{u})|^2 - \gamma \mathbb{E}(\nabla\mathbf{u}) : \mathbf{Q} \Big) dx. \tag{1.2.26}$$

This functional has been considered in other theories on nematic liquid crystal elastomers [44]. Repeating the proof from (1.2.20) on, we obtain the boundedness of the minimizing sequence $\{\mathbf{Q}_k, \mathbf{u}_k\}$ in $\{H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_B) + \mathbf{Q}_o\} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$. Then, the proof proceeds exactly as in our main case.

As a by-product of the previous analysis, we obtain the following result.

Theorem 7 *Let $\Omega \subset \mathbb{R}^3$ be a simply connected and Lipschitz domain, let $\Gamma_\phi \subseteq \partial\Omega$ be an open subset with positive surface measure, let $\phi_o \in H^1(\Omega)$. Let $\mathcal{E}$ as in* (1.1.1)*, where $f_{nem}, f_{mec}, f_{ele}$ are given as in* (1.1.3), (1.1.6), (1.1.8)*. Then $(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \overline{\phi})$ is a min-max critical point of $\mathcal{E}$, i.e.:*

$$\mathcal{E}(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \overline{\phi}) = \min_{\substack{H^1(\Omega,\mathcal{Q}_B)\times \\ \{H^1_o(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}}} \max_{H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi), \tag{1.2.27}$$

if and only if $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ is a solution to this problem:

$$\min_{\substack{H^1(\Omega,\mathcal{Q}_B)\times \\ \{H^1_o(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}}} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi), \quad \text{sub Gauss law}, \tag{1.2.28}$$

with $\overline{\phi} = \Psi[\overline{\mathbf{Q}}]$.

Proof. We only sketch the proof of this Theorem. Details can be worked out easily. The argument in Step 1.2.3.(1) shows that we may consider to take a minimizing sequence $\{\mathbf{Q}_k, \mathbf{u}_k\} \subset H^1(\Omega, \mathcal{Q}_B) \times \{H^1_o(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$. We can prove its boundedness exactly as above and extract a subsequence weakly convergent to some $(\mathbf{Q}, \mathbf{u}) \subset H^1(\Omega, \mathcal{Q}_B) \times \{H^1_o(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$. Then, the argument of Step 1.2.3.(2) yields the w.s.l.s.c. of $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$. □

Theorem 7 is relevant for the discussion of the phase diagrams (see Section 1.5). It is possible to modify slightly our results in order to treat other boundary conditions.

Remark 5 As already noticed in the comment below (1.1.14), when ϵ_a is zero, then $\mathcal{F}_{ele}$ is independent of $\mathbf{Q}$. As a consequence, the analysis is even more transparent. Maximization of $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$ in ϕ and minimization in $(\mathbf{Q}, \mathbf{u})$ are independent problems.

1.2.4 The model with the magnetic energy

We write the energy of the system in the presence of a magnetic field $\mathbf{h}$:

$$\mathcal{E}(\mathbf{Q}, \mathbf{u}, \mathbf{h}) = \mathcal{F}_{nem}(\mathbf{Q}) + \mathcal{F}_{mec}(\mathbf{Q}, \mathbf{u}) - \mathcal{F}_{mag}(\mathbf{Q}, \mathbf{h}), \tag{1.2.29}$$

where the density of $\mathcal{F}_{mag}$ is:

$$f_{mag}(\mathbf{Q}, \mathbf{h}) := \frac{\chi_o}{2}\big\langle(\overline{\chi}\mathbf{I} + \chi_a\mathbf{Q})\mathbf{h}, \mathbf{h}\big\rangle. \tag{1.2.30}$$

Here χ_o, $\overline{\chi}$, χ_a are the magnetic susceptibilities. Together with $\chi_\parallel$ and $\chi_\perp$, they can be defined as done in Table 1.1 for the dielectric constants. The only difference is that we do not require $\chi_\parallel$ and $\chi_\perp$ to be positive. We assume that the magnetic field $\mathbf{h}$ is imposed from an external source [49, Chapter 4], so that $\mathcal{E}$ is not subject to optimization in $\mathbf{h}$.

Theorem 8 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, let $\Gamma_Q, \Gamma_u \subseteq \partial\Omega$ be open subsets with positive surface measure. Let $\mathbf{Q}_o \in H^1(\Omega, \mathcal{Q}_B)$, $\mathbf{u}_o \in H^1(\Omega, \mathbb{R}^3)$. Let $\mathcal{E}$ as in* (1.2.29)*, where $f_{nem}, f_{mec}, f_{mag}$ are given as in* (1.1.3), (1.1.6), (1.2.30)*. Let $\mathbf{h} \in L^2(\Omega, \mathbb{R}^3)$. The problem*

$$\min_{\substack{\{H^1_{\Gamma_Q}(\Omega,\mathcal{Q}_B)+\mathbf{Q}_o\}\times \\ \{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}}} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \mathbf{h}) \tag{1.2.31}$$

admits solutions.

Proof. Since $\mathbf{h}$ is given in $L^2(\Omega, \mathbb{R}^3)$, $\mathcal{F}_{mag}(\mathbf{Q}, \mathbf{h})$ is linear in $\mathbf{Q}$. Hence, we can neglect this contribution and obtain the boundedness of a minimizing sequence $\{\mathbf{Q}_k, \mathbf{u}_k\}$ in $\{H^1_{\Gamma_Q}(\Omega, \mathcal{Q}_B) + \mathbf{Q}_o\} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$ as in Step 1.2.3.(1). By observing that $\mathbf{Q} \mapsto \mathcal{F}_{mag}(\mathbf{Q}, \mathbf{h})$ is continuous in the strong $L^2(\Omega, \mathbb{M}^{3\times3})$-topology, we obtain the w.s.l.s.c. of $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \mathbf{h})$ similarly as in Step 1.2.3.(2). □

Remark 6 The theorem above holds when $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \mathbf{h})$ is defined over $H^1(\Omega, \mathcal{Q}_B) \times \{H^1_o(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$. As hinted in the proof of Theorem 7, we obtain the boundedness of a minimizing sequence in $\{\mathbf{Q}_k, \mathbf{u}_k\} \subset H^1(\Omega, \mathcal{Q}_B) \times \{H^1_o(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$ and w.s.l.s.c. of the functional.

Remark 7 It is known that liquid crystals are diamagnetic, hence $\chi_{\|}$ and $\chi_{\perp}$ are negative [24, Section 3.2.1]. In any case, if we perform the substitution $\mathbf{h} \longrightarrow \mathbf{e}$, $\chi_{\|} \longrightarrow \epsilon_{\|}$, $\chi_{\perp} \longrightarrow \epsilon_{\perp}$ and so on, the result of this paragraph can be regarded as the case when an electric field is independent of the orientation of the nematic molecules.

1.3 The uniaxial theory

We turn to the analysis of equilibrium configurations in the framework of the uniaxial model. In brief, we constrain two of the eigenvalues of $\mathbf{Q}$ to be equal. We follow two alternative approaches. In the first one, we show that it is possible to modify slightly the argument used for the biaxial case. In the second one, we adapt to LCEs a technique developed by Ambrosio for Ericksen's theory of liquid nematics with variable degree of orientation. The two approaches are not exactly equivalent, see Remark 8.

First strategy

We recall the definition of the set

$$H^1(\Omega, \mathcal{Q}_U) := \{\mathbf{Q} \in H^1(\Omega, \mathbb{M}^{3\times3}) \text{ s.t. } \mathbf{Q}(x) \in \mathcal{Q}_U \text{ a.e.}\}, \tag{1.3.1}$$

which is strongly and w.s. closed in $H^1(\Omega, \mathbb{M}^{3\times3})$. Here, for completeness, we give an alternative characterization of $H^1(\Omega, \mathcal{Q}_U)$. Easy computations based on the Cayley-Hamilton Theorem [37, page 16] ensure that the constraint

$$|\mathbf{Q}|^6 = 54(\det \mathbf{Q})^2 \tag{1.3.2}$$

is a necessary and sufficient condition for a symmetric and traceless matrix in $\mathbb{M}^{3\times3}$ to be uniaxial and hence

$$\mathcal{Q}_U = \left\{\mathbf{Q} \in \mathbb{M}^{3\times3}_{0sym} \text{ s.t. } |\mathbf{Q}|^6 = 54(\det \mathbf{Q})^2\right\}, \tag{1.3.3}$$

$$H^1(\Omega, \mathcal{Q}_U) = \{\mathbf{Q} \in H^1(\Omega, \mathbb{M}^{3\times3}) \text{ s.t. } |\mathbf{Q}(x)|^6 = 54(\det \mathbf{Q}(x))^2 \text{ a.e.}\}. \tag{1.3.4}$$

It is straightforward to prove that the constraint in (1.3.2) is weakly sequentially closed. Indeed, suppose we have a sequence $\{\mathbf{Q}_k\}$ in $H^1(\Omega, \mathbb{M}^{3\times3})$ weakly convergent to some $\mathbf{Q}$. By standard arguments the convergence holds pointwise a.e. in Ω up to a subsequence. Now, (1.3.2) is closed for the pointwise convergence and the claim is proved.

With this argument, we can modify the procedure explained in the previous section, adding the constraint (1.3.2), provided that the uniform bound in (1.2.17) still holds. This is true if we assume that the boundary datum $\mathbf{Q}_o$ is given in $H^1(\Omega, \mathcal{Q}_U)$, so that the set of admissible functions is not empty. Thus, Theorems 6, 7 and 8 apply, provided that $H^1(\Omega, \mathcal{Q}_B)$ is replaced by $H^1(\Omega, \mathcal{Q}_U)$.

Second strategy

Following Ericksen's theory[31], we redefine $\mathbf{Q}$ as

$$\mathbf{Q} := s\Big(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\Big). \tag{1.3.5}$$

We redefine all the energy contributions previously introduced. With some abuse of notation, we do not introduce any new symbol. Having plugged (1.3.5) in (1.1.1), we label:

$$\begin{gathered}\mathcal{E}(s,\mathbf{n},\mathbf{u},\phi) := \mathcal{F}_{nem}(s,\mathbf{n}) + \mathcal{F}_{mec}(s,\mathbf{n},\mathbf{u}) - \mathcal{F}_{ele}(s,\mathbf{n},\phi) = \qquad (1.3.6)\\ \int_\Omega f_{nem}(s,\nabla s,\nabla\mathbf{n})dx + \int_\Omega f_{mec}(s,\mathbf{n},\nabla\mathbf{u})dx - \int_\Omega f_{ele}(s,\mathbf{n},\nabla\phi)dx.\end{gathered}$$

In order to define the summands in (1.3.6), we plug (1.3.5) in (1.1.3) and (1.1.6). We report some results of the computation:

$$|\mathbf{Q}|^2 = \frac{2}{3}s^2, \quad |\nabla\mathbf{Q}|^2 = \Big(\frac{2}{3}|\nabla s|^2 + 2s^2|\nabla\mathbf{n}|^2\Big), \tag{1.3.7}$$

$$\begin{gathered}\mu\Big(|\mathbb{E}(\nabla\mathbf{u})|^2 + \gamma^2|\mathbf{Q}|^2 - 2\gamma\mathbb{E}(\nabla\mathbf{u}):\mathbf{Q}\Big) + \frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2 = \qquad (1.3.8)\\ \mu\Big(|\mathbb{E}(\nabla\mathbf{u})|^2 + \frac{2}{3}\gamma^2 s^2 - 2\gamma\mathbb{E}(\nabla\mathbf{u}) : s\mathbf{n}\otimes\mathbf{n} + \frac{2}{3}\gamma s\operatorname{div}\mathbf{u}\Big) + \frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2.\end{gathered}$$

Since for physical reasons the LdG potential energy depends merely on the eigenvalues of $\mathbf{Q}$, we define $\Psi_{LdG}(s) := \Psi_{LdG}(\mathbf{Q})$. Furthermore, (1.1.9) becomes

$$\mathbf{A}(s,\mathbf{n}) := \frac{\epsilon_o}{2}\Big(\bar{\epsilon}\mathbf{I} + \epsilon_a s\Big(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\Big)\Big). \tag{1.3.9}$$

As before, we discuss equilibrium configurations represented by min-max critical points of the functional $\mathcal{E}(s,\mathbf{n},\mathbf{u},\phi)$. We follow Ambrosio's development in the study of a mathematical problem which is closely related to ours (see [3] and for further observations also [49, Chapter 6]). We introduce

$$\mathrm{D}_s := \{(s,\mathbf{n}) : \Omega \mapsto [-0.5, 1]\times\mathbb{S}^2 : s\in H^1(\Omega), \mathbf{v} := s\mathbf{n} \in H^1(\Omega,\mathbb{R}^3)\}, \tag{1.3.10}$$

and we assign $\widehat{s}_o \in H^{1/2}(\partial\Omega), \widehat{\mathbf{n}}_o : \partial\Omega \mapsto \mathbb{S}^2$, such that $\widehat{\mathbf{v}}_o := \widehat{s}_o\widehat{\mathbf{n}}_o \in H^{1/2}(\partial\Omega,\mathbb{R}^3)$. We recall Ambrosio's convergence in D_s [3, Formula (1.4)]: a sequence $\{s_k,\mathbf{n}_k\}\subset\mathrm{D}_s$ is said to converge to $(s,\mathbf{n})\in\mathrm{D}_s$ if

$$\lim_{k\to+\infty}\int_\Omega\big(|s_k - s|^2 + |s_k\mathbf{n}_k - s\mathbf{n}|^2\big)dx = 0. \tag{1.3.11}$$

Then (see also [3, Theorem 1.1])), by the continuity property of the trace operator (denoted by $\tau : H^1(\Omega)\to H^{1/2}(\partial\Omega)$), if $\{s_k,\mathbf{n}_k\}\subset\mathrm{D}_s$ with $\{\tau(s_k),\tau(\mathbf{v}_k)\} = (\widehat{s}_o,\widehat{\mathbf{v}}_o)$ on $\partial\Omega$, then $(s,\mathbf{n})\in\mathrm{D}_s$ and $\tau(s) = \widehat{s}_o, \tau(\mathbf{v}) = \widehat{\mathbf{v}}_o$. Therefore, the set defined as

$$\mathcal{D}_s^{\Gamma_s} := \{(s,\mathbf{n})\in\mathrm{D}_s,\ \text{s.t. } \tau(s) = \widehat{s}_o, \tau(s\mathbf{n}) = \widehat{\mathbf{v}}_o \text{ on } \Gamma_S\}, \tag{1.3.12}$$

is closed and nonempty (this last property is proved in [42]). In brief, we show that results analogous to those in Section 1.2 can be obtained following Ambrosio's approach. For the following result, only a sketch of proof is given below.

Theorem 9 *Let $\Omega \subset \mathbb{R}^3$ be a simply connected and Lipschitz domain. let $\Gamma_s, \Gamma_u, \Gamma_\phi \subseteq \partial\Omega$ be opens subsets with positive surface measure. Let $\mathcal{D}_s^{\Gamma_s}$ defined as in* (1.3.12) *with $\widehat{s}_o \in H^{1/2}(\partial\Omega)$, $\widehat{\mathbf{v}}_o \in H^{1/2}(\partial\Omega, \mathbb{R}^3)$, $\mathbf{u}_o \in H^1(\Omega, \mathbb{R}^3)$, $\phi_o \in H^1(\Omega)$. Let $\mathcal{E}$ as in* (1.3.6). *Then, $((\overline{s}, \overline{\mathbf{n}}), \overline{\mathbf{u}}, \overline{\phi})$ is a min-max critical point of $\mathcal{E}$, i.e.:*

$$\mathcal{E}(\overline{s}, \overline{\mathbf{n}}, \overline{\mathbf{u}}, \overline{\phi}) = \min_{\mathcal{D}_s^{\Gamma_s} \times \{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}} \max_{H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}(s, \mathbf{n}, \mathbf{u}, \phi), \tag{1.3.13}$$

if and only if $((\overline{s}, \overline{\mathbf{n}}), \overline{\mathbf{u}})$ is a solution to this problem:

$$\min_{\mathcal{D}_s^{\Gamma_s} \times \{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}} \mathcal{E}(s, \mathbf{n}, \mathbf{u}, \phi), \quad \text{sub Gauss law}, \tag{1.3.14}$$

with $\overline{\phi} = \Psi[\overline{s}, \overline{\mathbf{n}}]$.

Here $\Psi[s, \mathbf{n}]$ is the solution to Gauss equation in dependence of a given pair $(s, \mathbf{n}) \in \mathrm{D}_s$. In order to prove this assertion, we need the following result.

Lemma 1 *Let $\{s_k, \mathbf{n}_k\} \subset D_s, (s, \mathbf{n}) \in D_s$ s.t.*

$$\lim_{k \to +\infty} \int_\Omega (|s_k - s|^2 + |s_k \mathbf{n}_k - s\mathbf{n}|^2) dx = 0.$$

Then

$$\lim_{k \to +\infty} \int_\Omega |s_k \mathbf{n}_k \otimes \mathbf{n}_k - s\mathbf{n} \otimes \mathbf{n}|^2 dx = 0, \tag{1.3.15}$$

$$\mathbf{Q}_k = s_k\Big(\mathbf{n}_k \otimes \mathbf{n}_k - \frac{1}{3}\mathbf{I}\Big) \to s\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big) = \mathbf{Q} \quad s\text{-}L^2(\Omega, \mathbb{M}^{3\times 3}), \tag{1.3.16}$$

and

$$\mathbf{A}(s_k, \mathbf{n}_k) = \frac{\epsilon_o}{2}\Big(\overline{\epsilon}\mathbf{I} + \epsilon_a \mathbf{Q}_k\Big) \to \frac{\epsilon_o}{2}\Big(\overline{\epsilon}\mathbf{I} + \epsilon_a \mathbf{Q}\Big) = \mathbf{A}(s, \mathbf{n}) \quad s\text{-}L^2(\Omega, \mathbb{M}^{3\times 3}). \tag{1.3.17}$$

Proof. Notice that these results are not obvious because we do not assume a convergence directly for $\mathbf{n}$. We add and subtract terms in the integral in (1.3.15):

$$\int_\Omega |s_k \mathbf{n}_k \otimes \mathbf{n}_k - s\mathbf{n} \otimes \mathbf{n}|^2 dx = \int_\Omega |s_k \mathbf{n}_k \otimes \mathbf{n}_k \pm s\mathbf{n}_k \otimes \mathbf{n} \pm s_k \mathbf{n}_k \otimes \mathbf{n} - s\mathbf{n} \otimes \mathbf{n}|^2 dx. \tag{1.3.18}$$

We can estimate the right hand side in (1.3.18) for some positive constant C

$$\int_\Omega |\mathbf{n}_k \otimes s_k \mathbf{n}_k - \mathbf{n}_k \otimes s\mathbf{n} + s\mathbf{n}_k \otimes \mathbf{n} - s_k \mathbf{n}_k \otimes \mathbf{n} + s_k \mathbf{n}_k \otimes \mathbf{n} - s\mathbf{n} \otimes \mathbf{n}|^2 dx \leq \tag{1.3.19}$$
$$C \int_\Omega \Big(|\mathbf{n}_k \otimes s_k \mathbf{n}_k - \mathbf{n}_k \otimes s\mathbf{n}|^2 + |s\mathbf{n}_k \otimes \mathbf{n} - s_k \mathbf{n}_k \otimes \mathbf{n}|^2 + |(s_k \mathbf{n}_k - s\mathbf{n}) \otimes \mathbf{n}|^2\Big) dx.$$

Estimating the right-hand side in (1.3.19) yields

$$\int_\Omega |s_k \mathbf{n}_k \otimes \mathbf{n}_k - s\mathbf{n} \otimes \mathbf{n}|^2 dx \leq C \int_\Omega \Big(|s_k \mathbf{n}_k - s\mathbf{n}|^2 + |s - s_k|^2 + |s_k \mathbf{n}_k - s\mathbf{n}|^2 \Big) dx. \quad (1.3.20)$$

In the limit $k \to +\infty$, the right hand side in (1.3.20) vanishes, proving (1.3.15). Now (1.3.16) and (1.3.17) follow trivially. □

Outline of the proof of Theorem 9. For any given $(s, \mathbf{n}) \in \mathrm{D}_s$, the Euler-Lagrange equation for the problem

$$\min_{\phi \in H^1_{\Gamma_\phi}(\Omega) + \phi_o} \int_\Omega f_{ele}(s, \mathbf{n}, \nabla\phi) dx \quad (1.3.21)$$

coincides with Gauss equation

$$\begin{cases} \text{Find } \phi \in H^1(\Omega) \text{ s.t.} \\ \displaystyle\int_\Omega \langle \mathbf{A}(s, \mathbf{n}) \nabla\phi, \nabla\varphi \rangle dx = 0 \\ \phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall \varphi \in H^1_{\Gamma_\phi}(\Omega). \end{cases}$$

Therefore, equivalence of problems (1.3.13) and (1.3.14) follows exactly as in the previous section. Problem (1.3.21) has a unique solution for any given $(s, \mathbf{n}) \in \mathrm{D}_s$. In fact, exactly as in Step 1.2.2.(1) and Step 1.2.2.(2), we have boundedness of a minimizing sequence $\{\phi_k\}$ taken in $\{H^1_{\Gamma_\phi}(\Omega) + \phi_o\}$ and w.s.l.s.c. of $\mathcal{F}_{ele}(s, \mathbf{n}, \cdot)$ in the weak topology of $H^1(\Omega)$. Notice that the upper and lower bounds for $\mathcal{F}_{ele}(s, \mathbf{n}, \phi)$ (which is strictly convex in $\nabla\phi$) are the same as in (1.1.14). We label $\Phi[s, \mathbf{n}]$ the solution of (1.3.21). Again, we identify $\Phi[s, \mathbf{n}]$ with $\Psi[s, \mathbf{n}]$. We define

$$f^*_{ele}(s, \mathbf{n}) := f_{ele}\big(s, \mathbf{n}, \nabla\Phi[s, \mathbf{n}]\big), \quad f^*(s, \mathbf{n}, \mathbf{u}) := f\big(s, \mathbf{n}, \mathbf{u}, \Phi[s, \mathbf{n}]\big), \quad (1.3.22)$$

$$\mathcal{E}^*(s, \mathbf{n}, \mathbf{u}) := \int_\Omega \Big(f_{nem}(s, \nabla s, \nabla\mathbf{n}) + f_{mec}(s, \mathbf{n}, \nabla\mathbf{u}) - f^*_{ele}(s, \mathbf{n}) \Big) dx. \quad (1.3.23)$$

Now, the problem

$$\min_{\mathcal{D}_s^{\Gamma s} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}} \ \max_{H^1_{\Gamma_\phi}(\Omega) + \phi_o} \mathcal{E}(s, \mathbf{n}, \mathbf{u}, \phi) = \quad (1.3.24)$$

$$\min_{\mathcal{D}_s^{\Gamma s} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}} \Big\{ \int_\Omega \big(f_{nem}(s, \nabla s, \nabla\mathbf{n}) + f_{mec}(s, \mathbf{n}, \nabla\mathbf{u}) \big) dx - \min_{H^1_{\Gamma_\phi}(\Omega) + \phi_o} \int_\Omega f_{ele}(s, \mathbf{n}, \nabla\phi) dx \Big\}$$

becomes

$$\min_{\mathcal{D}_s^{\Gamma_s}\times\{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}} \mathcal{E}^*(s,\mathbf{n},\mathbf{u}). \tag{1.3.25}$$

Labelling $((\overline{s},\overline{\mathbf{n}}),\overline{\mathbf{u}})$ a solution to (1.3.25), an equilibrium configuration of the system is given by $((\overline{s},\overline{\mathbf{n}}),\overline{\mathbf{u}},\overline{\phi})$, where $\overline{\phi}=\Phi[\overline{s},\overline{\mathbf{n}}]$. Again, the proof follows by applying the Direct Method to problem (1.3.25). Existence of minimizers follows from boundedness of the minimizing sequence and s.l.s.c. of $\mathcal{E}^*(s,\mathbf{n},\mathbf{u})$. In particular, boundedness of $\{\mathbf{u}_k\}$ in $H^1(\Omega,\mathbb{R}^3)$ follows again from (1.2.19). Then, using (1.3.7) and $|s|^2=|s\mathbf{n}|^2=|\mathbf{v}|^2$, (1.2.21) becomes

$$\int_\Omega \kappa^2\Big(\frac{1}{3}|\nabla s_k|^2+s_k^2|\nabla\mathbf{n}_k|^2\Big)dx+\frac{\mu}{3}\gamma^2\int_\Omega\big(|s_k|^2+|\mathbf{v}_k|^2\big)dx\le Const. \tag{1.3.26}$$

This, together with the fact that $|\nabla\mathbf{v}|^2=|\nabla s|^2+s^2|\nabla\mathbf{n}|^2$ is sufficient to obtain the convergence of a minimizing sequence $\{s_k,\mathbf{n}_k\}\subset \mathrm{D}_s$ in the sense specified in (1.3.11), at least up to a subsequence [3, Theorem 1.1]. The continuity property of the trace operator ensures that if we take $\{s_k,\mathbf{n}_k\}$ in D_s with $(\tau(s_k),\tau(s_k\mathbf{n}_k))=(\widehat{s}_o,\widehat{\mathbf{v}}_o)$ converging to some $(s,\mathbf{n})$ in the sense of (1.3.11), then $(s,\mathbf{n})$ is in D_s with $(\tau(s),\tau(s\mathbf{n}))=(\widehat{s}_o,\widehat{\mathbf{v}}_o)$. Next, following Proposition 5 Step 1.2.3.(2), we prove the s.l.s.c. of $\mathcal{E}^*(s,\mathbf{n},\mathbf{u})$ with respect to the convergence defined in (1.3.11) for the variables $(s,\mathbf{n})$ and the weak convergence of $H^1(\Omega,\mathbb{R}^3)$ for the displacement $\mathbf{u}$. Invoking (1.3.9), we can prove the w.s.l.s.c. of $\mathcal{F}_{mec}(s,\mathbf{n},\mathbf{u})$ exactly as for the biaxial model. In fact, putting together (1.2.13) and (1.3.9), we define $\mathbf{B}(x):=\mathbf{A}(s,\mathbf{n})(x)$ and repeat the argument of Paragraph 1.2.2 in view of (1.3.16), yielding

$$\Phi[s_k,\mathbf{n}_k]\longrightarrow\Phi[s,\mathbf{n}]. \tag{1.3.27}$$

Now, thanks to (1.3.17), we are able to prove the continuity of $\mathcal{F}^*_{ele}(s,\mathbf{n})$ with respect to the convergence (1.3.11), exactly as in Remark 3. We are left to show the s.l.s.c. of $\mathcal{F}_{nem}(s,\mathbf{n})$ with respect to (1.3.11). The following result is contained in [3].

Theorem 10 ***(Ambrosio 1990, [3, Theorem 1.4])****.* *Let $c>0$, $\widehat{s}_o,\widehat{\mathbf{v}}_o$, be Borel functions defined on $\partial\Omega$, and let $\{s_k,\mathbf{n}_k\}\subset D_s$ be a sequence s.t.*

$$\sup_{k\in\mathbb{N}}\int_\Omega\Big(c|\nabla s_k|^2+s_k^2|\nabla\mathbf{n}_k|^2\Big)dx<+\infty, \tag{1.3.28}$$

$$\big(\tau(s_k)(x),\tau(s_k\mathbf{n}_k)(x)\big)=\big(\widehat{s}_o(x),\widehat{\mathbf{v}}_o(x)\big)\quad \mathcal{H}^2\text{-a.e.}\,\mathrm{in}\,\partial\Omega, \tag{1.3.29}$$

and assume that (1.3.11) *holds for some* $(s,\mathbf{n})\in D_s$*. Then*

$$\int_\Omega\Big(c|\nabla s|^2+s^2|\nabla\mathbf{n}|^2\Big)dx\le\liminf_{k\to+\infty}\int_\Omega\Big(c|\nabla s_k|^2|+s_k^2|\nabla\mathbf{n}_k|^2\Big)dx. \tag{1.3.30}$$

The Proof of s.w.l.s.c. of the first piece (the squared gradient of s) is trivial. By the slicing method, it is possible to prove the w.s.l.s.c. of the remaining part. We apply this theorem with $c=1/3$ and the requirement $\widehat{s}_o\in H^{1/2}(\partial\Omega),\widehat{s}_o\widehat{\mathbf{n}}_o=\widehat{\mathbf{v}}_o\in H^{1/2}(\partial\Omega,\mathbb{R}^3)$.

Remark 8 The two possible strategies presented for the uniaxial theory are not equivalent. There are examples where the minima of the free energy following strategies 1 or 2 are different. For simplicity we can consider the minimization of the nematic energy $\mathcal{F}_{nem}$ for $\Psi_{LdG} \equiv 0$:

$$\min_{H^1_{\Gamma_Q}(\Omega,\mathcal{Q}_U)+\mathbf{Q}_o} \int_\Omega \frac{\kappa^2}{2}|\nabla \mathbf{Q}|^2 dx, \tag{1.3.31}$$

$$\min_{\mathcal{D}_s^{\Gamma_s}} \int_\Omega \kappa^2\Big(\frac{1}{3}|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2\Big)dx. \tag{1.3.32}$$

Consider for instance Ω as a cube (see Figure 1.1). Let us assign boundary conditions

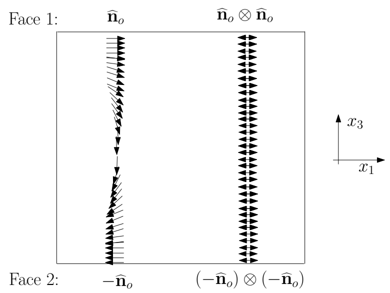

Figure 1.1: Geometry presented in Remark 8 (a section of Ω in the plane x_1, x_3).

for $(s, \mathbf{n})$ only on two parallel faces (labelled for convenience face 1 and face 2), leaving natural conditions on the remaining part of $\partial\Omega$. Assume $\widehat{s}_o = 1$ and some constant $\widehat{\mathbf{n}}_o \in \mathbb{S}^2$ on the face 1, and $-\widehat{\mathbf{n}}_o$ on the face 2. We impose the same boundary condition for $\mathbf{Q}$, which is $\widehat{\mathbf{Q}}_o = \widehat{s}_o(\widehat{\mathbf{n}}_o \otimes \widehat{\mathbf{n}}_o - \frac{1}{3}\mathbf{I})$ (that is $\widehat{\mathbf{Q}}_o = \tau(\mathbf{Q}_o)$, where $\mathbf{Q}_o = \mathbf{i}_1 \otimes \mathbf{i}_1 - \frac{1}{3}\mathbf{I}$, see Figure 1.1) both on face 1 and face 2. The absolute minimizer of (1.3.31) is $\mathbf{Q}(x)$ identically equivalent to $\mathbf{Q}_o$, while the solution to (1.3.32) is some couple $(s, \mathbf{n})$ that cannot be constant. In this case we have

$$\min_{\mathcal{D}_s^{\Gamma_s}} \int_\Omega \kappa^2\Big(\frac{1}{3}|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2\Big)dx > \min_{H^1_{\Gamma_Q}(\Omega,\mathcal{Q}_U)+\mathbf{Q}_o} \int_\Omega \frac{\kappa^2}{2}|\nabla \mathbf{Q}|^2 dx = 0,$$

and the physical solution is represented in (1.3.31). When (1.3.31) is equal to (1.3.32) then the two strategies are equivalent. In this case, the parameterization of $\mathbf{Q}$ as in (1.3.5) can be appealing, being based on the two variables $s, \mathbf{n}$ which are directly measurable in an experiment.

Remark 9 Trivial adjustments allow to extend our proof to a min-max problem in a space of functions with slightly different boundary conditions as done in Theorem 7. The case of a magnetic instead of an electric field can be considered as well. By plugging (1.3.5) in (1.2.30) we introduce $f_{mag}(s, \mathbf{n}, \mathbf{h})$. Then, we can also adapt Theorem 8 when $\mathcal{E}(s, \mathbf{n}, \mathbf{u}, \mathbf{h})$ is defined on $\mathcal{D}_s^{\Gamma_s} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\} \times L^2(\Omega, \mathbb{R}^3)$ or $\mathrm{D}_s \times \{H^1_o(\Omega, \mathbb{R}^3) + \mathbf{u}_o\} \times L^2(\Omega, \mathbb{R}^3)$.

1.4 The director theory

Specializing the model even further, one can describe the liquid crystal only in terms of the eigenspace of $\mathbf{Q}$. Even in this case we find two possible strategies. Again, the first one consists in studying the functional in the variable $\mathbf{Q}$ with some additional constraint. In the second one, we follow the classical Frank theory which is based on the formulation of the energy in terms of the director $\mathbf{n}$.

First strategy

We consider a uniaxial tensor field $\mathbf{Q}$ with eigenvalues $\{-1/3, -1/3, 2/3\}$. We recall the definition of the set

$$H^1(\Omega, \mathcal{Q}_{Fr}) := \{\mathbf{Q} \in H^1(\Omega, \mathbb{M}^{3\times3}) : \mathbf{Q}(x) \in \mathcal{Q}_{Fr} \text{ a.e.}\}. \tag{1.4.1}$$

We obtain results analogous to those of Theorems 6, 7, 8 with the obvious changes (e.g., to take $\mathbf{Q}_o \in H^1(\Omega, \mathcal{Q}_{Fr})$) by replacing $H^1(\Omega, \mathcal{Q}_B)$ with $H^1(\Omega, \mathcal{Q}_{Fr})$. The idea of the proof is the same as in Paragraph 1.3. The details can be worked out easily, and we omit them.

Second strategy

Setting $s \equiv 1$ in (1.3.5) – (1.3.9) we obtain a Frank-like model (see [49], [33])

$$\mathbf{Q} = \Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big), \tag{1.4.2}$$

$$\begin{gathered}\mathcal{E}(\mathbf{n}, \mathbf{u}, \phi) := \mathcal{F}_{nem}(\mathbf{n}) + \mathcal{F}_{mec}(\mathbf{n}, \mathbf{u}) - \mathcal{F}_{ele}(\mathbf{n}, \phi) = \\ \int_\Omega \kappa^2 |\nabla \mathbf{n}|^2 dx + \int_\Omega \Big\{\mu \Big|\mathbb{E}(\nabla \mathbf{u}) - \gamma\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big)\Big|^2 + \frac{\lambda}{2}(\operatorname{div} \mathbf{u})^2\Big\} dx - \\ \int_\Omega \frac{\epsilon_o}{2}\Big(\bar{\epsilon}|\nabla\phi|^2 + \epsilon_a \big\langle\big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\big)\nabla\phi, \nabla\phi\big\rangle\Big) dx,\end{gathered} \tag{1.4.3}$$

$$\mathbf{A}(\mathbf{n}) := \frac{\epsilon_o}{2}\Big(\bar{\epsilon}\mathbf{I} + \epsilon_a\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big)\Big). \tag{1.4.4}$$

Again, we keep for simplicity the notation of Section 1.2, even though the terms have now a different meaning. Notice that we neglect the LdG potential energy, since this reduces to a constant contribution. Let

$$H^1(\Omega, \mathbb{S}^2) := \{\mathbf{n} \in H^1(\Omega, \mathbb{R}^3) \text{ s.t. } \mathbf{n}(x) \in \mathbb{S}^2 \text{ a.e.}\}. \tag{1.4.5}$$

The space $H^1(\Omega, \mathbb{S}^2)$ is weakly sequentially closed. Let us take a sequence $\{\mathbf{n}_k\} \subset H^1(\Omega, \mathbb{S}^2)$ weakly convergent to some $\mathbf{n} \in H^1(\Omega, \mathbb{R}^3)$. By Rellich's theorem (in what follows Ω is a Lipschitz domain), we have that, up to subsequences, the convergence holds strongly in L^2 and hence $\mathbf{n} \in H^1(\Omega, \mathbb{S}^2)$. Analogously, letting $\mathbf{n}_o \in H^1(\Omega, \mathbb{S}^2)$, we have that

$$\mathcal{D}_n^{\Gamma_n} := \{\mathbf{n} \in H^1(\Omega, \mathbb{S}^2) \text{ s.t. } \tau(\mathbf{n}) = \tau(\mathbf{n}_o) \in \Gamma_n\}. \tag{1.4.6}$$

is w.s. closed.

Theorem 11 *Let* $\Omega \subset \mathbb{R}^3$ *be a simply connected and Lipschitz domain,* $\Gamma_n, \Gamma_u, \Gamma_\phi \subseteq \partial\Omega$ *be open subsets with positive surface measure. Let* $\mathcal{D}_n^{\Gamma_n}$ *as in* (1.4.6)*,* $\mathbf{n}_o \in H^1(\Omega, \mathbb{S}^2)$*,* $\mathbf{u}_o \in H^1(\Omega, \mathbb{R}^3)$*,* $\phi_o \in H^1(\Omega)$*. Let* $\mathcal{E}(\mathbf{n}, \mathbf{u}, \phi)$ *as in* (1.4.3)*. Then* $(\overline{\mathbf{n}}, \overline{\mathbf{u}}, \overline{\phi})$ *is a min-max critical point of* $\mathcal{E}$*, i.e.:*

$$\mathcal{E}(\overline{\mathbf{n}}, \overline{\mathbf{u}}, \overline{\phi}) = \min_{\mathcal{D}_n^{\Gamma_n} \times \{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}} \max_{H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}(\mathbf{n}, \mathbf{u}, \phi), \tag{1.4.7}$$

if and only if $(\overline{\mathbf{n}}, \overline{\mathbf{u}})$ *is a solution to this problem:*

$$\min_{\mathcal{D}_n^{\Gamma_n} \times \{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o\}} \mathcal{E}(\mathbf{n}, \mathbf{u}, \phi), \quad \text{sub Gauss law}, \tag{1.4.8}$$

with $\overline{\phi} = \Psi[\overline{\mathbf{n}}]$*.*

Here $\Psi[\mathbf{n}]$ is the solution to Gauss equation in dependence of a given $\mathbf{n}$ in $H^1(\Omega, \mathbb{S}^2)$. The proof of this theorem is analogous to that given for Theorem 6 in the frame of the biaxial theory. We can simply follow the lines of the proof in 'Outline of the proof of Theorem 6' with obvious adjustments. Again, existence and uniqueness of $\Psi[\mathbf{n}]$ follows from the fact that it solves the minimization problem for $\mathcal{F}_{ele}(\mathbf{n}, \phi)$. The proof of this can be derived easily from the results contained in Paragraph 1.2.2. Then, we plug $\Psi[\mathbf{n}]$ in $\mathcal{F}_{ele}(\mathbf{n}, \cdot)$ and $\mathcal{E}(\mathbf{n}, \mathbf{u}, \cdot)$ yielding $\mathcal{F}^*_{ele}(\mathbf{n})$ and $\mathcal{E}^*(\mathbf{n}, \mathbf{u})$. We minimize $\mathcal{E}^*(\mathbf{n}, \mathbf{u})$ in the set $\mathcal{D}_n^{\Gamma_n} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{u}_o\}$ by finding a bound for a minimizing sequence $\{\mathbf{n}_k, \mathbf{u}_k\}$ and proving the s.l.s.c. of the functional. As in (1.2.17), we get the boundedness of $\{\mathbf{u}_k\}$ in $H^1(\Omega, \mathbb{R}^3)$. Then, $\mathcal{F}_{nem}(\mathbf{n})$ controls the H^1 norm of $\{\mathbf{n}_k\}$. Notice that, since $\mathbf{n}(x) \in \mathbb{S}^2$ a.e. in Ω, we do not need to invoke Poincaré inequality. We can thus extract a subsequence which converges weakly to some $\mathbf{n}$ in $\mathcal{D}_n^{\Gamma_n}$ (since this set is weakly sequentially closed). Next step concerns the s.l.s.c. of $\mathcal{E}^*(\mathbf{n}, \mathbf{u})$ with respect to the weak topology of $H^1(\Omega, \mathbb{S}^2) \times H^1(\Omega, \mathbb{R}^3)$. In particular, notice that the strong convergence in $L^2(\Omega, \mathbb{M}^{3\times3})$ of sequences of maps in the form of (1.4.2) and of (1.4.4) follows trivially and yields the continuity of $\mathcal{F}^*_{ele}(\mathbf{n})$ by virtue of the argument of Proposition 4 which still holds provided we set $\mathbf{B}(x) := \mathbf{A}(\mathbf{n})(x)$ in (1.2.13). We conclude by observing that $\mathcal{F}_{nem}(\mathbf{n})$ and $\mathcal{F}_{mec}(\mathbf{n}, \mathbf{u})$ are s.l.s.c. in the weak topology of $H^1(\Omega, \mathbb{S}^2) \times H^1(\Omega, \mathbb{R}^3)$ by standard arguments.

Remark 10 Again, trivial adjustments allow to extend our proof to a min-max problem with slightly different boundary conditions and when a magnetic field is applied on the system. We refer to Remark 9 for an idea of the proof required.

Remark 11 R. Hardt, D. Kinderlehrer and F.H. Lin have studied in [38] an analogous optimization problem for nematic liquid crystals in the presence of an electric field. The functional they consider is comparable to our $\mathcal{F}_{nem}(\mathbf{n}) - \mathcal{F}_{ele}(\mathbf{n}, \phi)$, since their problem does not involve the mechanical displacement $\mathbf{u}$. Loosely speaking, their proof is based on the analysis of the Euler-Lagrange equations associated with problem (1.4.7) and problem (1.4.8), keeping in mind that $\mathcal{F}_{mec}(\mathbf{n}, \mathbf{u})$ is absent.

The case of the incompressible elastomers. It is straightforward to modify all the previous results in order to treat optimization problems for energies of incompressible elastomers which are modelled by constraining the divergence of $\mathbf{u}$ to be zero (notice that this is equivalent to set $\lambda \equiv +\infty$ in (1.1.6)). For the readers' convenience, we present a theorem which extends the results for systems of compressible elastomers in the presence of an applied electric field to the case of incompressible rubbers. This result will be applied in Chapter 3.

In the following theorem, X stands either for Fr, U or B.

Theorem 12 *Let $\Omega \subset \mathbb{R}^3$ be a simply connected and Lipschitz domain, let $\Gamma_u, \Gamma_\phi \subseteq \partial\Omega$ be open subsets with positive surface measure, let $\mathbf{u}_o \in H^1(\Omega, \mathbb{R}^3)$ with $\operatorname{div} \mathbf{u}_o = 0$, $\phi_o \in H^1(\Omega)$. Let $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$ as in (1.1.1), where $f_{nem}, f_{mec}, f_{ele}$ are given as in (1.1.3), (1.1.6), (1.1.8). Then, $(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \overline{\phi})$ is a min-max critical point of $\mathcal{E}$, i.e.:*

$$\mathcal{E}(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \overline{\phi}) = \min_{\substack{H^1(\Omega,\mathcal{Q}_X)\times \\ \{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o, \operatorname{div}\mathbf{u}=0\}}} \max_{H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi), \tag{1.4.9}$$

if and only if $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ is a solution to this problem:

$$\min_{\substack{H^1(\Omega,\mathcal{Q}_X)\times \\ \{H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{u}_o, \operatorname{div}\mathbf{u}=0\}}} \mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi), \quad \text{sub Gauss law,} \tag{1.4.10}$$

with $\overline{\phi} = \Psi[\overline{\mathbf{Q}}]$.

Proof. It follows as in the proof of Theorem 6 with some obvious changes. It is enough to take all sequence $\{\mathbf{u}_k\}$ with $\operatorname{div} \mathbf{u}_k = 0$. The constraint on the divergence is linear and, consequently, if we take $\{\mathbf{u}_k\} \subset H^1(\Omega, \mathbb{R}^3)$ such that

$$\mathbf{u}_k \rightharpoonup \mathbf{u} \ w\text{-}H^1(\Omega, \mathbb{R}^3), \text{ with } \operatorname{div} \mathbf{u}_k = 0,$$

then $\operatorname{div} \mathbf{u} = 0$. □

1.5 Phase diagrams

Let us assume $\Omega = (-X_1, X_1) \times (-X_2, X_2) \times (-X_3, X_3)$, for some $X_1, X_2, X_3 > 0$. Consider, for a moment, the biaxial theory and $\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi)$ as in Theorem 7. Labelling

O the origin in $\mathbb{R}^3$, let $\mathbf{u}_o = \mathbf{E}(x - O)$, for every x in $\partial\Omega$, for a given symmetric matrix $\mathbf{E}$, and $\phi_o = 0$ on $\Gamma_\phi \equiv \partial\Omega$. We find particular solutions which minimize the functional

$$\int_\Omega \Big(f_{nem}(\mathbf{Q}, \nabla\mathbf{Q}) + f_{mec}(\mathbf{Q}, \nabla\mathbf{u}) - f_{ele}(\mathbf{Q}, \nabla\phi) \Big) dx \tag{1.5.1}$$

with constant $\mathbf{Q}(x)$, with $\phi(x) \equiv 0$ and $\mathbf{u}(x) = \mathbf{E}(x - O)$ for every x in the closure of Ω. Plugging $\phi \equiv 0$ and neglecting the gradient of $\mathbf{Q}$, the integral in (1.5.1) reduces to

$$\int_\Omega \Big(\Psi_{LdG}(\mathbf{Q}) + \mu \big|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}\big|^2 + \frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2 \Big) dx. \tag{1.5.2}$$

Furthermore, let us neglect the LdG energy density. We can thus find solutions $(\mathbf{Q}, \mathbf{u})$ *algebraically*, by minimizing the integrand of (1.5.2). This hypothesis allows us to find exact asymptotic expressions for the minimizers of f_{mec}, parameterized by the boundary data, i.e., by $\mathbf{E}$. The pictorial representation of the essential features of these solutions as a function of $\mathbf{E}$ is a phase diagram.

In the next paragraphs we show how to construct the phase diagrams for the uniaxial and biaxial model discussing several of their properties, and for the Frank model. We refer to [27] for more comments on the director theory.

1.5.1 The uniaxial theory

We parameterize $\mathbf{Q}$ following Ericksen's theory. This is not restrictive for our purpose, since we do not impose boundary conditions on $\mathbf{Q}$. Furthermore, we find it convenient to express $\mathbf{E}$ as

$$\mathbf{E} = \frac{1}{3}(\operatorname{tr}\mathbf{E})\mathbf{I} + \Delta\mathbf{E}, \quad \Delta\mathbf{E} := \Big(\mathbf{E} - \frac{1}{3}(\operatorname{tr}\mathbf{E})\mathbf{I}\Big), \tag{1.5.3}$$

where we define $(1/3)(\operatorname{tr}\mathbf{E})\mathbf{I}$ the *spherical* component and $\Delta\mathbf{E}$ the *deviatoric* component of $\mathbf{E}$. According to this decomposition, $f_{mec}(s, \mathbf{n}, \mathbf{F})$ can be written as

$$f_{mec}(s, \mathbf{n}, \mathbf{F}) = \mu\Big(|\Delta\mathbf{E}|^2 - 2\gamma\Delta\mathbf{E} : s\mathbf{n}\otimes\mathbf{n} + \frac{2}{3}\gamma^2 s^2 \Big) + \Big(\frac{\lambda}{2} + \frac{\mu}{3}\Big)(\operatorname{tr}\mathbf{F})^2. \tag{1.5.4}$$

The energy density in (1.5.4) describes the mechanics of a material with microstructure, whose descriptors are precisely $(s, \mathbf{n})$. By minimizing over these internal degrees of freedom, we obtain a macroscopic model:

$$f_U(\mathbf{F}) := \min_{s\in[-0.5,1], \mathbf{n}\in\mathbb{S}^2} f_{mec}(s, \mathbf{n}, \mathbf{F}). \tag{1.5.5}$$

We describe $\mathbf{E}$ in terms of its ordered eigenvalues

$$e_1 \le e_2 \le e_3, \tag{1.5.6}$$

and the corresponding eigenvectors $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$. For convenience, we define the eigenvalues of $\Delta\mathbf{E}$ as $\Delta e_i := e_i - (\operatorname{tr}\mathbf{E})/3, i = 1, 2, 3$. Incompressibility condition (if introduced) reads: $\mathrm{tr}\,(\mathbf{F}) = \mathrm{tr}\,(\mathbf{E}) = 0$, yielding $\Delta e_i = e_i$. We label $(s^*, \mathbf{n}^*)$ the absolute minimizers of (1.5.4). To determine them, we have to separate the cases when s is positive or negative. We define $(s^{*+}, \mathbf{n}^{*+})$ the minimizer of (1.5.4) in the case of positive s. Analogously we define $(s^{*-}, \mathbf{n}^{*-})$ the minimizer in the case of negative s. First of all, it is easy to verify that the minimizer in $\mathbf{n}$ is always $\mathbf{n}^{*+} = \mathbf{n}_3$ in the case of positive s, and $\mathbf{n}^{*-} = \mathbf{n}_1$ in the case of negative s. Let us plug $\mathbf{n} = \mathbf{n}^{*+}$ in (1.5.4), yielding

$$f_{mec}(s, \mathbf{n}^{*+}, \mathbf{F}) = \mu\Big(|\Delta\mathbf{E}|^2 - 2\gamma s \Delta e_3 + \frac{2}{3}\gamma^2 s^2\Big) + \Big(\frac{\lambda}{2} + \frac{\mu}{3}\Big)(\mathrm{tr}\,\mathbf{F})^2. \tag{1.5.7}$$

Now we minimize (1.5.7) in $s \in [0,1]$. We equate to zero the first derivative in s of (1.5.7) when looking for minimum points in the open segment $(0,1)$, or we evaluate (1.5.7) for $s = \{0,1\}$. We see that s^{*+} and $\mathbf{n}^{*+}$ depend only on the components of the deviatoric part of $\mathbf{F}$. We define $f_U^+(\mathbf{F}) := f_{mec}(s^{*+}, \mathbf{n}^{*+}, \mathbf{F})$. Proceeding exactly as above, we find s^{*-} and introduce $f_U^-(\mathbf{F}) := f_{mec}(s^{*-}, \mathbf{n}^{*-}, \mathbf{F})$. We conclude obtaining (1.5.5) by

$$f_U(\mathbf{F}) = \min\big\{f_U^+(\mathbf{F}), f_U^-(\mathbf{F})\big\}. \tag{1.5.8}$$

Since stable phases are characterized by the lowest value of the energy, we define

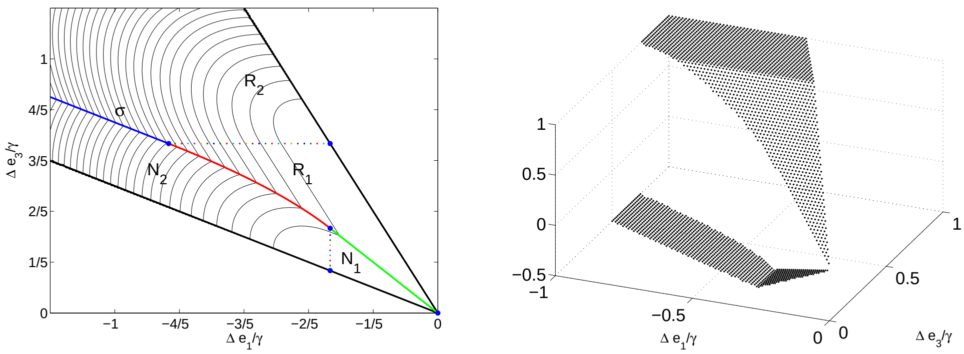

Figure 1.2: LEFT: Phase diagram and level curves. For convenience, we adopt a non-dimensional form here, expressing s^* as a function of $\Delta e_1/\gamma$ and $\Delta e_3/\gamma$. RIGHT: s^* represented as a function of $(\Delta e_1/\gamma, \Delta e_3/\gamma)$.

$$\big(s^*, \mathbf{n}^*\big) := \arg\Big(\min\big\{f_{mec}(s^{*+}, \mathbf{n}^{*+}, \mathbf{F}), f_{mec}(s^{*-}, \mathbf{n}^{*-}, \mathbf{F})\big\}\Big), \tag{1.5.9}$$

where $(s^*, \mathbf{n}^*)$ can be expressed as functions of $\Delta e_1, \Delta e_3$. In view of (1.5.6), not all the couples $(\Delta e_1, \Delta e_3)$ are admissible. From the constraints $e_1 \le e_2, e_2 \le e_3$ (equivalently, $\Delta e_1 \le \Delta e_2, \Delta e_2 \le \Delta e_3$) one easily gets that $-\Delta e_1/2 \le \Delta e_3 \le -2\Delta e_1$, for $\Delta e_1 \le 0$.

$$\big(s^*, \mathbf{n}^*\big) = \begin{cases} (\frac{3\Delta e_3}{2\gamma}, \mathbf{n}_3) & \text{on} \quad P_1 := \{(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}) : \sigma(\frac{\Delta e_3}{\gamma}) < \frac{\Delta e_1}{\gamma} \le -\frac{\Delta e_3}{2\gamma}, \frac{\Delta e_3}{\gamma} < \frac{2}{3}\} \\ (\frac{3\Delta e_1}{2\gamma}, \mathbf{n}_1) & \text{on} \quad N_1 := \{(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}) : -\frac{2\Delta e_3}{\gamma} \le \frac{\Delta e_1}{\gamma} < \sigma(\frac{\Delta e_3}{\gamma}), \frac{\Delta e_1}{\gamma} > -\frac{1}{3}\} \\ (1, \mathbf{n}_3) & \text{on} \quad P_2 := \{(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}) : \sigma(\frac{\Delta e_3}{\gamma}) < \frac{\Delta e_1}{\gamma} \le -\frac{\Delta e_3}{2\gamma}, \frac{\Delta e_3}{\gamma} \ge \frac{2}{3}\} \\ (-\frac{1}{2}, \mathbf{n}_1) & \text{on} \quad N_2 := \{(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}) : -\frac{2\Delta e_3}{\gamma} \le \frac{\Delta e_1}{\gamma} < \sigma(\frac{\Delta e_3}{\gamma}), \frac{\Delta e_1}{\gamma} \le -\frac{1}{3}\}. \end{cases}$$

Positive and negative phases of s^* are separated by the curve σ of equation

$$\sigma(t) := \begin{cases} -t & \text{for} \quad t \in [0, 1/3) \\ -1.5t^2 - 1/6 & \text{for} \quad t \in [1/3, 2/3) \\ -2t + 1/2 & \text{for} \quad t \geq 2/3. \end{cases}$$

A direct calculation allows to verify that the curve σ is C^1. On σ, s^* and $\mathbf{n}^*$ are not defined (see Fig. 1.2 RIGHT), while f_U is a continuous function of $\mathbf{E}$ and can be defined also on σ. Here is the expression for $f_U(\mathbf{F})$:

$$\frac{1}{\mu}\Big(f_U(\mathbf{F}) - \Big(\frac{\lambda}{2} + \frac{\mu}{3}\Big)(\operatorname{tr}\mathbf{F})^2\Big) = \begin{cases} (|\Delta\mathbf{E}|^2 - \frac{3}{2}\Delta e_3^2) & \text{on} \quad R_1 \\ (|\Delta\mathbf{E}|^2 - \frac{3}{2}\Delta e_1^2) & \text{on} \quad N_1 \\ (|\Delta\mathbf{E}|^2 - 2\gamma\Delta e_3 + \frac{2}{3}\gamma^2) & \text{on} \quad R_2 \\ (|\Delta\mathbf{E}|^2 + \gamma\Delta e_1 + \frac{\gamma^2}{6}) & \text{on} \quad N_2 \end{cases}$$

$$= \begin{cases} \frac{1}{2}(\Delta e_3 + 2\Delta e_1)^2 & \text{on} \quad R_1 \\ \frac{1}{2}(\Delta e_1 + 2\Delta e_3)^2 & \text{on} \quad N_1 \\ \frac{3}{2}(\Delta e_1 + \frac{\gamma}{3})^2 + & \\ \frac{1}{2}(\Delta e_1 + 2\Delta e_3 - \gamma)^2 & \text{on} \quad R_2, \\ \frac{3}{2}(\Delta e_3 - \frac{\gamma}{6})^2 + & \\ \frac{1}{2}(\Delta e_3 + 2\Delta e_1 + \frac{\gamma}{2})^2 & \text{on} \quad N_2, \end{cases}$$

where $R_1 := \{(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}) : \sigma(\frac{\Delta e_3}{\gamma}) \leq \frac{\Delta e_1}{\gamma} \leq -\frac{\Delta e_3}{2\gamma}, \frac{\Delta e_3}{\gamma} < \frac{2}{3}\}$, $R_2 := \{(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}) : \sigma(\frac{\Delta e_3}{\gamma}) \leq \frac{\Delta e_1}{\gamma} \leq -\frac{\Delta e_3}{2\gamma}, \frac{\Delta e_3}{\gamma} \geq \frac{2}{3}\}$.

Minimization of the magnetic energy

By minimizing the magnetic energy density $-f_{mag}(s, \mathbf{n}, \mathbf{h})$ in $(s, \mathbf{n})$ we understand the influence of the magnetic field on the nematic order.

Case $\chi_a > 0$. Again, it is convenient to consider separately the cases for positive and negative s. In brief, we comment the result

$$\min_{s\in[-0.5,1],\mathbf{n}\in\mathbb{S}^2}\big(-f_{mag}(s, \mathbf{n}, \mathbf{h})\big) = -\frac{\chi_o}{2}\Big(\chi_a\frac{2}{3}|\mathbf{h}|^2 + \overline{\chi}|\mathbf{h}|^2\Big). \tag{1.5.10}$$

The effect of a magnetic field is to orient $\mathbf{n}$ parallel to $\mathbf{h}$ and to push s to the value 1. We are enforcing the order of the system tightening the distribution of the molecules along the direction of the magnetic field.

Case $\chi_a < 0$. The minimization yields:

$$\min_{s\in[-0.5,1],\mathbf{n}\in\mathbb{S}^2}\big(-f_{mag}(s, \mathbf{n}, \mathbf{h})\big) = -\frac{\chi_o}{2}\Big(-\chi_a\frac{1}{3}|\mathbf{h}|^2 + \overline{\chi}|\mathbf{h}|^2\Big). \tag{1.5.11}$$

This result can be reached when $s = 1$ for any $\mathbf{n}$ perpendicular to $\mathbf{h}$ and equivalently when $s = -0.5$ for $\mathbf{n}$ parallel to $\mathbf{h}$.

1.5.2 The director theory

Setting $s \equiv 1$ in the previous construction we obtain the phase diagram for the macroscopic energy (see Figure 1.3-left)

$$f_{Fr}(\mathbf{F}) := \min_{\mathbf{n} \in \mathbb{S}^2} f_{mec}(\mathbf{n}, \mathbf{F})$$

whose expression (in components of the deviator of $\mathbf{F}$) is

$$\frac{1}{\mu}\Big(f_{Fr}(\mathbf{F}) - \Big(\frac{\lambda}{2} + \frac{\mu}{3}\Big)(\operatorname{tr}\mathbf{F})^2\Big) = \frac{3}{2}\Big(\Delta e_1 + \frac{\gamma}{3}\Big)^2 + \frac{1}{2}\Big(\Delta e_1 + 2\Delta e_3 - \gamma\Big)^2$$

$$\text{on } -\frac{1}{2}\Delta e_1 \leq \Delta e_3 \leq -2\Delta e_1,$$

1.5.3 The biaxial theory

Again, we minimize the mechanical energy density obtaining a new macroscopic model:

$$f_B(\mathbf{F}) := \min_{\mathbf{Q} \in \mathcal{Q}_B} f_{mec}(\mathbf{Q}, \mathbf{F}). \tag{1.5.12}$$

To compute (1.5.12) we choose a convenient parameterization for $\mathbf{Q} \in \mathcal{Q}_B$. Let

$$\mathbf{Q} = \sum_{i=1,2,3} (\lambda_i \mathbf{m}_i \otimes \mathbf{m}_i), \quad \sum_{i=1,2,3} \lambda_i = 0, \quad -1/3 \leq \lambda_i \leq 2/3, \tag{1.5.13}$$

with $\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3$ an orthonormal tern. By setting $\lambda_3 = \lambda_{max}(\mathbf{Q})$, $\lambda_1 = \lambda_{min}(\mathbf{Q})$, and $\lambda_2 = -\lambda_1 - \lambda_3$ we obtain a global parameterization for $-1 \leq 3\lambda_1 \leq 0 \leq 3\lambda_3 \leq 2$. Now, the minimization proceeds exactly as in Paragraph 1.5.1. We label $(\lambda_1^*, \lambda_2^*, \lambda_3^*)$ and $(\mathbf{m}_1^*, \mathbf{m}_2^*, \mathbf{m}_3^*)$ the functions which solve (1.5.12) (trivially, $\lambda_2^* = -\lambda_1^* - \lambda_3^*$). We define three regions in the plane $(\Delta e_1/\gamma, \Delta e_3/\gamma)$

$$\text{Liq} := \Big\{\Big(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}\Big) : -\frac{2\Delta e_3}{\gamma} \leq \frac{\Delta e_1}{\gamma} \leq -\frac{\Delta e_3}{2\gamma}, \frac{\Delta e_1}{\gamma} > -\frac{1}{3}\Big\}$$

$$\text{Sm} := \Big\{\Big(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}\Big) : -\frac{2\Delta e_3}{\gamma} \leq \frac{\Delta e_1}{\gamma} < -\frac{2\Delta e_3}{\gamma} + 1, \frac{\Delta e_1}{\gamma} \leq -\frac{1}{3}\Big\}$$

$$\text{Sol} := \Big\{\Big(\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}\Big) : -\frac{2\Delta e_3}{\gamma} + 1 \leq \frac{\Delta e_1}{\gamma} \leq -\frac{\Delta e_3}{2\gamma}, \frac{\Delta e_1}{\gamma} \leq -\frac{1}{3}\Big\}.$$

We skip all the details of the computation, and report only the results.

$$(\lambda_1^*, \lambda_3^*) = \begin{cases} (\frac{\Delta e_1}{\gamma}, \frac{\Delta e_3}{\gamma}) & \text{on Liq} \\ (-\frac{1}{3}, \frac{6\Delta e_3 + 3\Delta e_1 + \gamma}{6\gamma}) & \text{on Sm} \\ (-\frac{1}{3}, \frac{2}{3}) & \text{on Sol} \end{cases}$$

$$(\mathbf{m}_1^*, \mathbf{m}_2^*, \mathbf{m}_3^*) = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) \quad \text{on} \quad \text{Liq} \cup \text{Sm} \cup \text{Sol}$$

$$\frac{1}{\mu}\Big(f_B(\mathbf{F}) - \Big(\frac{\lambda}{2} + \frac{\mu}{3}\Big)(\operatorname{tr}\mathbf{F})^2\Big) = \begin{cases} 0 & \text{on Liq} \\ \frac{3}{2}(\Delta e_1 + \frac{\gamma}{3})^2 & \text{on Sm} \\ \frac{3}{2}(\Delta e_1 + \frac{\gamma}{3})^2 + & \\ \frac{1}{2}(\Delta e_1 + 2\Delta e_3 - \gamma)^2 & \text{on Sol.} \end{cases}$$

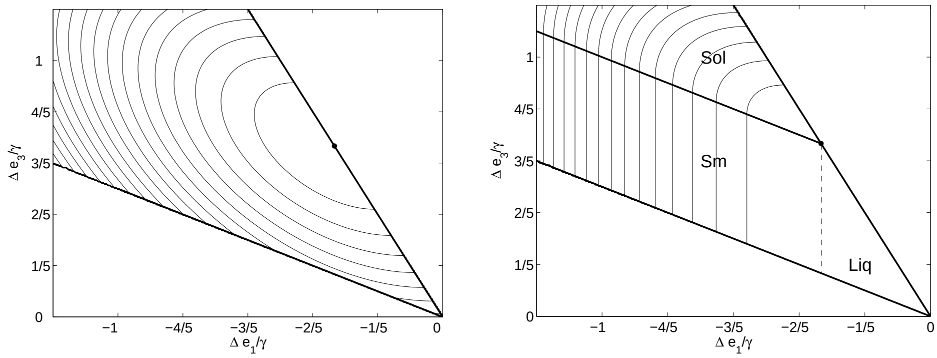

Figure 1.3: Phase diagram and level curves. LEFT: Frank model. RIGHT: Biaxial model.

1.6 Appendix to Chapter 1

1.6.1 Continuity properties of $\Phi[\mathbf{Q}]$

We describe the dependence of the solution to some elliptic equation on the matrix coefficients.

Proposition 6 *Let* $\phi_o \in H^1(\Omega)$, $\{\mathbf{B}_k\} \subset L^2(\Omega, \mathbb{M}^{3\times3}), \mathbf{B} \in L^2(\Omega, \mathbb{M}^{3\times3})$ *as in* (1.2.13) *and* $\mathbf{B}_k \to \mathbf{B}$ s-$L^2(\Omega, \mathbb{M}^{3\times3})$. *Consider the problems*

$$\begin{cases} \textit{Find } \phi \in H^1(\Omega) \textit{ s.t.} \\ \displaystyle\int_\Omega \big\langle \mathbf{B}(x)\nabla\phi, \nabla(\psi - \phi_o)\big\rangle dx = 0 \\ \phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \psi \in H^1(\Omega) \textit{ s.t. } \tau(\psi - \phi_o) = 0 \textit{ on } \Gamma_\phi \end{cases}$$

whose solution we denote Φ, *and*

$$\begin{cases} \textit{Find } \phi \in H^1(\Omega) \textit{ s.t.} \\ \displaystyle\int_\Omega \big\langle \mathbf{B}_k(x)\nabla\phi, \nabla(\psi - \phi_o)\big\rangle dx = 0 \\ \phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \psi \in H^1(\Omega) \textit{ s.t. } \tau(\psi - \phi_o) = 0 \textit{ on } \Gamma_\phi \end{cases}$$

whose solution is labelled Φ_k. *Then* $\Phi_k \to \Phi$ s-$H^1(\Omega)$.

Proof. From the strong convergence it follows that $\mathbf{B}_k(x) \to \mathbf{B}(x)$ a.e. in Ω (up to a subsequence not relabelled). The main point in the proof is to show that

$$\nabla\Phi_k \to \nabla\Phi \quad s\text{-}L^2(\Omega, \mathbb{R}^3). \tag{1.6.1}$$

We first prove that $\nabla\Phi_k \rightharpoonup \nabla\Phi$ w-$L^2(\Omega, \mathbb{R}^3)$. Setting $\psi = \Phi_k$ in the following identity

$$\begin{cases} \displaystyle\int_\Omega \big\langle \mathbf{B}_k(x)\nabla\Phi_k, \nabla(\psi-\phi_o)\big\rangle dx = 0 \\ \Phi_k - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \psi \in H^1(\Omega) \text{ s.t. } \tau(\psi-\phi_o) = 0 \text{ on } \Gamma_\phi, \end{cases}$$

we obtain

$$\int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\Phi_k\big\rangle dx = \int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\phi_o\big\rangle dx. \tag{1.6.2}$$

By using the uniform bounds (1.1.13), we can write

$$m\|\nabla\Phi_k\|^2_{L^2(\Omega,\mathbb{R}^3)} \le \int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\Phi_k\big\rangle dx \le M\int_\Omega \nabla\Phi_k\cdot\nabla\phi_o dx. \tag{1.6.3}$$

By Hölder's and Poincaré inequalities we can find some positive constant K_Ω such that

$$\|\Phi_k\|_{H^1(\Omega)} \le K_\Omega\|\nabla\phi_o\|_{L^2(\Omega,\mathbb{R}^3)}. \tag{1.6.4}$$

We have that Φ_k converges weakly in $H^1(\Omega)$ to some $\widetilde{\phi}$ at least up to a subsequence here not relabelled. In order to identify $\widetilde{\phi}$ suppose that

$$\int_\Omega \big\langle (\mathbf{B}_k\nabla\Phi_k - \mathbf{B}\nabla\widetilde{\phi}), \nabla(\psi-\phi_o)\big\rangle dx \to 0,\ \forall\,\psi\in H^1(\Omega)\,\text{s.t.}\,\tau(\psi-\phi_o)=0\,\text{on}\,\Gamma_\phi. \tag{1.6.5}$$

Thus, (1.6.5) shows that $\widetilde{\phi}$ is solution to the elliptic system

$$\begin{cases} \displaystyle\int_\Omega \big\langle \mathbf{B}(x)\nabla\widetilde{\phi}, \nabla(\psi-\phi_o)\big\rangle dx = 0 \\ \widetilde{\phi} - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \psi \in H^1(\Omega) \text{ s.t. } \tau(\psi-\phi_o) = 0 \text{ on } \Gamma_\phi, \end{cases}$$

and hence $\Phi = \widetilde{\phi}$ by the uniqueness of the solution to this problem. This proves the claim $\nabla\Phi_k \rightharpoonup \nabla\Phi$ w-$L^2(\Omega,\mathbb{R}^3)$. We prove that (1.6.5) is true. We verify the hypotheses of Lebesgue Dominated Convergence Theorem:

- $|\mathbf{B}_k\nabla(\psi-\phi_o)| \le M|\nabla(\psi-\phi_o)|$, where $\psi,\phi_o\in H^1(\Omega)$,
- $\mathbf{B}_k\nabla(\psi-\phi_o) \longrightarrow \mathbf{B}\nabla(\psi-\phi_o)$ pt. a.e. in Ω,

yielding: $\mathbf{B}_k\nabla(\psi-\phi_o)\to\mathbf{B}\nabla(\psi-\phi_o)$ s-$L^2(\Omega,\mathbb{R}^3)$. Since $\nabla\Phi_k \rightharpoonup \nabla\widetilde{\phi}$ w-$L^2(\Omega,\mathbb{R}^3)$, we have (1.6.5). Now it remains to pass from the weak to the strong convergence of $\nabla\Phi_k$ to $\nabla\Phi$. We can pass to the limit on the right hand side of (1.6.2) since we know that $\nabla\Phi_k \rightharpoonup \nabla\Phi$ w-$L^2(\Omega,\mathbb{R}^3)$ and $\mathbf{B}_k\nabla\phi_o \to \mathbf{B}\nabla\phi_o$ s-$L^2(\Omega,\mathbb{R}^3)$:

$$\int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\Phi_k\big\rangle dx = \int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\phi_o\big\rangle dx \overset{k\to\infty}{\longrightarrow} \int_\Omega \big\langle \mathbf{B}\nabla\Phi, \nabla\phi_o\big\rangle dx. \tag{1.6.6}$$

Plugging $\psi = \Phi$ in the identity

$$\begin{cases} \displaystyle\int_\Omega \big\langle \mathbf{B}(x)\nabla\Phi, \nabla(\psi - \phi_o)\big\rangle dx = 0 \\ \Phi - \phi_o \in H^1_{\Gamma_\phi}(\Omega) \\ \forall\, \psi \in H^1(\Omega) \text{ s.t. } \tau(\psi - \phi_o) = 0 \text{ on } \Gamma_\phi, \end{cases}$$

we have that $\int_\Omega \big\langle \mathbf{B}\nabla\Phi, \nabla\phi_o\big\rangle dx = \int_\Omega \big\langle \mathbf{B}\nabla\Phi, \nabla\Phi\big\rangle dx$, yielding, thanks to (1.6.6):

$$\int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\Phi_k\big\rangle dx \stackrel{k\to\infty}{\longrightarrow} \int_\Omega \big\langle \mathbf{B}\nabla\Phi, \nabla\Phi\big\rangle dx. \tag{1.6.7}$$

This fact turns out to be a key ingredient in the proof of (1.6.1). Let us now examine the expression below:

$$\int_\Omega \big\langle \mathbf{B}_k(\nabla\Phi_k - \nabla\Phi), \nabla\Phi_k - \nabla\Phi\big\rangle dx = \tag{1.6.8}$$

$$\int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\Phi_k\big\rangle dx - \int_\Omega \big\langle \mathbf{B}_k\nabla\Phi_k, \nabla\Phi\big\rangle dx - \int_\Omega \big\langle \mathbf{B}_k\nabla\Phi, \nabla\Phi_k\big\rangle dx + \int_\Omega \big\langle \mathbf{B}_k\nabla\Phi, \nabla\Phi\big\rangle dx.$$

By (1.6.7), we are allowed to take the limit in the first integral on the right hand side. The second and third integral converge since $\mathbf{B}_k\nabla\Phi \to \mathbf{B}\nabla\Phi$ s-$L^2(\Omega, \mathbb{R}^3)$ and $\nabla\Phi_k \rightharpoonup \nabla\Phi$ w-$L^2(\Omega, \mathbb{R}^3)$. Also the fourth piece converges trivially by Lebesgue Dominated Convergence Theorem. Hence, we deduce that

$$0 \le m \int_\Omega |\nabla\Phi_k - \nabla\Phi|^2 dx \le \int_\Omega \langle \mathbf{B}_k(\nabla\Phi_k - \nabla\Phi), \nabla\Phi_k - \nabla\Phi\rangle dx \to 0 \tag{1.6.9}$$

as $k \to +\infty$, proving (1.6.1). □

Part II

Ill-posed problems

Chapter 2

Relaxation of multi-well energies in linearized elasticity and applications to nematic elastomers

2.1 Introduction

We obtain the explicit expression of the relaxation of a free-energy functional which describes the order-strain interaction in nematic elastomers. We work in the regime of small strains (linearized kinematics). Adopting the uniaxial order tensor theory or Frank model to describe the liquid crystal order, we prove that the minima of the relaxed functional exhibit an effective biaxial microstructure, as in de Gennes tensor model. In particular, this implies that the response of the material is soft even if the order of the system is assumed to be fixed. The relaxed energy density satisfies a solenoidal quasiconvexification formula.

2.1.1 The mechanical model

We recall the mechanical model introduced in Chapter 1 for describing the coupling between strain and order in nematic elastomers

$$f_{mec}(\mathbf{Q},\mathbf{F}) := \frac{1}{2}\mathbb{C}\big(\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}\big) : (\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}) = \mu\big|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}\big|^2 + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2 \tag{2.1.1}$$

where μ, λ, γ are positive constants and $\mathbf{F} \in \mathbb{M}^{3\times 3}$, $\mathbf{Q} \in \mathcal{Q}_X$ where X stands either for Fr, U or B.

As anticipated in the Introduction to the thesis, the further development which we propose consists in minimizing (2.1.1) with respect to $\mathbf{Q}$ (see also Section 1.5 of Chapter 1). This new model can be defined as *macroscopic*, in the sense that the influence of the internal (*microscopic*) variable $\mathbf{Q}$ is perceived only through a direct coupling to the strain. Depending on the choice of the set where $\mathbf{Q}$ is allowed to vary, different results are obtained:

$$f_X(\mathbf{F}) := \inf_{\mathcal{Q}_X} f_{mec}(\mathbf{Q}, \mathbf{F}), \qquad \text{where } X \text{ stands for } Fr, U \text{ or } B. \tag{2.1.2}$$

It is clear that the macroscopic models thus obtained are the measure of the distance from the set $\gamma\mathcal{Q}_X$:

$$\begin{aligned} \inf_{\mathbf{Q}\in\mathcal{Q}_X} \Big\{\mu\big|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}\big|^2 + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2\Big\} &= \mu\Big(\inf_{\mathbf{Q}\in\mathcal{Q}_X} |\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}|\Big)^2 + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2 \qquad (2.1.3) \\ &= \mu\, dist^2\big(\mathbb{E}(\mathbf{F}), \gamma\mathcal{Q}_X\big) + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2. \end{aligned}$$

There exists a unique element $\overline{\mathbf{Q}}$ which minimizes in $\mathcal{Q}_B$ the function $\mathbf{Q} \mapsto |\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}|^2$. This is elementary, since the term proportional to the square of the trace is not subject to minimization and we are left with minimizing the square of the euclidian norm over the compact and convex set $\mathcal{Q}_B$. The matrix $\overline{\mathbf{Q}}$ is also called the *projection* of $\mathbb{E}(\mathbf{F})/\gamma$ onto $\mathcal{Q}_B$ and referred as $\pi^{\mathcal{Q}_B}(\mathbb{E}(\mathbf{F})/\gamma)$. This is the element of minimal distance from the set $\gamma\mathcal{Q}_B$. The projection of $\mathbb{E}(\mathbf{F})$ onto $\gamma\mathcal{Q}_B$ is $\pi^{\gamma\mathcal{Q}_B}(\mathbb{E}(\mathbf{F})) = \gamma\pi^{\mathcal{Q}_B}(\mathbb{E}(\mathbf{F})/\gamma)$. Since $\mathcal{Q}_{Fr} \subset \mathcal{Q}_U \subset \mathcal{Q}_B$, it follows that $f_B(\mathbf{F}) \leq f_U(\mathbf{F}) \leq f_{Fr}(\mathbf{F})$ and $f_B(\cdot)$ is a convex function. Notice that $\mathbf{F} \mapsto \pi^{\gamma\mathcal{Q}_B}(\mathbb{E}(\mathbf{Q}))$ is a Lipschitz continuous map in the space of matrices. The explicit expressions of f_{Fr}, f_U, f_B are reported in Section 1.5 (Chapter 1).

In the following, we discuss the problem of relaxing the integral energies obtained from f_{Fr} and f_U considering the constraint of incompressibility. In the case where we consider the energy density f_{Fr} and f_U, we are assuming that a Frank-like and a uniaxial description of the orientation and order of the molecules are allowed in the model. It can happen, however, that biaxial states which may seem unattainable according to (2.1.2) are allowed, in a suitable sense, by formation of a new microstructure. It turns out that f_{Fr} and f_U are non-convex energy densities, while f_B is. Even in the cases $X = Fr$ or U, the effective response of the material exhibits a richer microstructure if more favorable energetic paths are attainable. In fact, we show that microstructures are possible, and a biaxial tensor field is obtained *effectively*, via relaxation. More precisely, according to the Direct Method in the Calculus of Variations, the minimization of a non-lower semicontinuous energy may be an ill-posed problem. From the physical point of view, the material responds to outer solicitations by developing a microstructure accompanied by high oscillations of the strain. We overcome this degeneracy by reformulating the minimization problem in terms of its relaxation, namely the supremum in the class of all the lower semicontinuous functionals not exceeding the original one.

2.2 Relaxation theorems

As observed, the mechanical models f_{Fr}, f_U introduced in (2.1.2) are non-convex and, consequently, the associated integral functionals are not lower semicontinuous. We characterize the infima of the non-convex energies as the minima of the relaxed functionals.

According to well known relaxation theorems (see Acerbi-Fusco Theorem [1] and [8, Theorem 2.3]), the relaxation coincides with the integral of the quasiconvex envelope of the original non-convex density. Hence, our goal is to obtain the quasiconvexification explicitly. This can be computed in a practical way by proving that the rank-1 convex envelopes of f_{Fr} and f_U coincide with their convex envelopes. In the case of real-valued functions, this yields that the quasiconvex envelope coincides with the convex and rank-1 convex envelope, which are easier to compute.

On the other hand, experimental observations show that many nematic elastomers are nearly incompressible ($\lambda/\mu > 10^2$). The classical way to model such materials in linearized elasticity is to consider the limit ratio $\lambda/\mu = +\infty$, which is equivalent to restrict the admissible deformation gradients to the class of traceless matrices, and hence to define an energy functional in the presence of a linear constraint on the gradient of the displacement. We remark that the general way to treat such problems is with the tools of $\mathcal{A}$-quasiconvexification[10], the theory which studies the relaxation of non-convex functionals in the presence of linear constraints. In our particular case, in order to compute explicitly the relaxation of the energies, we use an argument due to Braides[8]. It is possible to prove that the relaxation of the incompressible models coincides with the limit of a sequence of relaxed models describing compressible materials with increasing bulk modulus, yielding an interesting physical interpretation which is discussed in Section 2.3.

We split the proof in several auxiliary propositions. In particular, we show that the projection of a constant strain onto $\gamma\mathcal{Q}_B$ can be obtained as a convex combination of elements which are compatible in the sense of (H_K) (see Definition 2 in Paragraph 0.1.2) and whose deviators belong to $\gamma\mathcal{Q}_{Fr}$ or $\gamma\mathcal{Q}_U$. We define the sets of matrices

$$\mathcal{K}_X := \Big\{ \mathbf{M} \in \mathbb{M}_0^{3\times 3} : \mathbb{E}(\mathbf{M}) \in \mathcal{Q}_X \Big\} \tag{2.2.1}$$

where X stands either for Fr, U or B. The sets $\mathcal{K}_X$ inherit from $\mathcal{Q}_X$ some of their properties. In particular $\mathcal{K}_B$ is convex and $\mathcal{K}_{Fr} \subset \mathcal{K}_U \subset \mathcal{K}_B$. We start by showing that $\mathcal{K}_U^{lc} = \mathcal{K}_B$. In the corollary to the following proposition we show that $\mathcal{K}_B$ coincides with the set of first order laminates of $\mathcal{K}_U$ (see (0.1.61)).

Proposition 7 *Denote with* $e_1(\mathbf{A}) \leq e_2(\mathbf{A}) \leq e_3(\mathbf{A})$ *the ordered eigenvalues of the symmetric* 3×3 *matrix* $\mathbf{A}$. *Let (here* $t \leq 0$*)*

$$\mathcal{M}_U^t := \Big\{ \mathbf{M} \in \mathbb{M}_0^{3\times 3} : e_1\big(\mathbb{E}(\mathbf{M})\big) = t, e_2\big(\mathbb{E}(\mathbf{M})\big), e_3\big(\mathbb{E}(\mathbf{M})\big) \in [t, -2t] \Big\}. \tag{2.2.2}$$

Then, the set $\mathcal{M}_U$ *defined by*

$$\mathcal{M}_U := \bigcup_{t \in [-1/3, 0]} \mathcal{M}_U^t \tag{2.2.3}$$

is contained in $\mathcal{K}_U^{(1)}$*, the set of first order laminates of* $\mathcal{K}_U$.

Proof. Let $\mathbf{M} \in \mathcal{M}_U$. By the spectral theorem and up to re-labelling the axes, we may assume that the symmetric part of $\mathbf{M}$ is diagonal in the form $\overline{\mathbf{X}} = \text{diag}\,(t, \mu_2, \mu_3)$. There is nothing to prove if μ_2 or μ_3 are equal to t, because in that case the remaining eigenvalue is equal to $-2t$. We show that, for $\mu_2, \mu_3 \in (t, -2t)$, there exists a positive $\delta = \delta(\mu_2, \mu_3)$ and

$$\mathcal{K}_U \ni \overline{\mathbf{V}}^{\pm} = \text{diag}\,(t, \widehat{\mathbf{V}}^{\pm}) \quad \text{where} \quad \widehat{\mathbf{V}}^{\pm} = \begin{pmatrix} \mu_2 & \pm 2\delta \\ 0 & \mu_3 \end{pmatrix},$$

such that $\overline{\mathbf{V}}^{+} - \overline{\mathbf{V}}^{-} = 4\delta \mathbf{i}_2 \otimes \mathbf{i}_3$ and $\overline{\mathbf{X}} = \frac{1}{2}(\overline{\mathbf{V}}^{+} + \overline{\mathbf{V}}^{-}) \in \mathcal{K}_U^{(1)}$. We define

$$\widehat{\mathbf{X}}^{\pm} := \mathbb{E}(\widehat{\mathbf{V}}^{\pm}) = \begin{pmatrix} \mu_2 & \pm\delta \\ \pm\delta & \mu_3 \end{pmatrix},$$

$$\overline{\mathbf{X}}^{\pm} := \mathbb{E}(\overline{\mathbf{V}}^{\pm}). \tag{2.2.4}$$

The eigenvalues $\theta_{\alpha,\beta}$ of $\widehat{\mathbf{X}}^{\pm}$ are the solutions of $\det(\widehat{\mathbf{X}}^{\pm} - \theta\mathbf{I}) = 0$, namely

$$\theta_{\alpha,\beta} = \Big(\frac{\mu_2 + \mu_3}{2}\Big) \pm \sqrt{\frac{(\mu_3 - \mu_2)^2}{4} + \delta^2}. \tag{2.2.5}$$

By imposing θ_α to be equal to $-2t$ and recalling that $t + \mu_2 + \mu_3 = 0$, we obtain

$$\delta^2 = (2t + \mu_3)(2t + \mu_2) > 0 \quad \text{since} \quad -2t > \mu_2, \mu_3 > t. \tag{2.2.6}$$

By observing that $\theta_\alpha + \theta_\beta = \mu_2 + \mu_3$, this choice of δ yields $\theta_\beta = t$ and $\overline{\mathbf{V}}^{\pm} \in \mathcal{K}_U$. Now, define $\mathbf{M}^{sk} := (\mathbf{M} - \mathbf{M}^T)/2$. Hence, $\mathbf{M} = \frac{1}{2}((\overline{\mathbf{V}}^{+} + \mathbf{M}^{sk}) + (\overline{\mathbf{V}}^{-} + \mathbf{M}^{sk}))$, $rank((\overline{\mathbf{V}}^{+} + \mathbf{M}^{sk}) - (\overline{\mathbf{V}}^{-} + \mathbf{M}^{sk})) \leq 1$ and $\mathbf{M}$ is in $\mathcal{K}_U^{(1)}$. □

Corollary 1

$$\mathcal{M}_U = \mathcal{K}_U^{(1)} = \mathcal{K}_U^{lc} = \mathcal{K}_U^{c} \equiv \mathcal{K}_B. \tag{2.2.7}$$

Proof. Since $\mathcal{K}_B$ is convex and $\mathcal{K}_U \subset \mathcal{K}_B$, then $\mathcal{K}_U^c \subseteq \mathcal{K}_B$. Then, it is straightforward to verify that $\mathcal{K}_B \subseteq \mathcal{M}_U$. □

Remark 12 As a by-product of Proposition 7, we deduce that $\mathcal{Q}_U^c = \mathcal{Q}_B$. Trivially, $\mathcal{Q}_U \subseteq \mathcal{Q}_B$ and $\mathcal{Q}_U^c \subseteq \mathcal{Q}_B$. To prove the opposite inclusion, notice that $\overline{\mathbf{X}}$ belongs to $\mathcal{Q}_B$ and it can be expressed as $\overline{\mathbf{X}} = \frac{1}{2}(\overline{\mathbf{X}}^{+} + \overline{\mathbf{X}}^{-})$, with $\overline{\mathbf{X}}^{\pm}$ in $\mathcal{Q}_U$.

With a similar argument we prove now that $\mathcal{K}_B$ coincides with the lamination-convex envelope of $\mathcal{K}_{Fr}$. In practice (see Corollary 2), it is enough to show that $\mathcal{K}_B$ coincides with the set of second order laminates of $\mathcal{K}_{Fr}$.

Proposition 8 *Denote with $e_1(\mathbf{A}) \leq e_2(\mathbf{A}) \leq e_3(\mathbf{A})$ the ordered eigenvalues of the symmetric 3×3 matrix $\mathbf{A}$. The set $\mathcal{M}_{Fr}$ defined by*

$$\mathcal{M}_{Fr} := \Big\{\mathbf{M} \in \mathbb{M}_0^{3\times 3} : e_1\big(\mathbb{E}(\mathbf{M})\big) = -\frac{1}{3}, e_2\big(\mathbb{E}(\mathbf{M})\big), e_3\big(\mathbb{E}(\mathbf{M})\big) \in \Big[-\frac{1}{3}, \frac{2}{3}\Big]\Big\} \quad (2.2.8)$$

is contained in $\mathcal{K}_{Fr}^{(1)}$, the se of first order laminates of $\mathcal{K}_{Fr}$.

Proof. The proof follows by taking t identically equal to $-1/3$ in the proof of Proposition 7. □

Corollary 2

$$\mathcal{M}_{Fr}^{(1)} = \mathcal{K}_{Fr}^{(2)} = \mathcal{K}_{Fr}^{lc} = \mathcal{K}_{Fr}^{c} \equiv \mathcal{K}_B. \quad (2.2.9)$$

Proof. As above, $\mathcal{K}_{Fr}^c \subseteq \mathcal{K}_B$. Then, it is enough to prove that $\mathcal{K}_B \subseteq \mathcal{M}_{Fr}^{(1)}$. Take $\mathbf{G} \in \mathcal{K}_B$. Again, it is not restrictive to assume that $\overline{\mathbf{X}} := \mathbb{E}(\mathbf{G})$ is diagonal in the form $\overline{\mathbf{X}} = \text{diag}\,(\mu_2, \mu_1, \mu_3)$ and $\mu_1 \leq \mu_2 \leq \mu_3$. If $\mu_1 = -1/3$ there is nothing to prove because this implies that $\mathbf{G} \in \mathcal{M}_{Fr}$. Similarly, we can assume $\mu_3 \neq 2/3$, otherwise the other two eigenvalues must be equal to $-1/3$. We show that, for $\mu_1, \mu_3 \in (-1/3, 2/3)$, there exists a positive $\delta = \delta(\mu_1, \mu_3)$ and

$$\mathcal{M}_{Fr} \ni \mathbf{G}^{\pm} = \text{diag}\,(\mu_2, \widehat{\mathbf{G}}^{\pm}) \quad \text{where} \quad \widehat{\mathbf{G}}^{\pm} = \begin{pmatrix} \mu_1 & \pm 2\delta \\ 0 & \mu_3 \end{pmatrix},$$

such that $\mathbf{G}^+ - \mathbf{G}^- = 4\delta \mathbf{i}_2 \otimes \mathbf{i}_3$ and $\overline{\mathbf{X}} = \frac{1}{2}(\mathbf{G}^+ + \mathbf{G}^-) \in \mathcal{M}_{Fr}^{(1)}$. We define

$$\widehat{\mathbf{H}}^{\pm} := \mathbb{E}(\widehat{\mathbf{G}}^{\pm}) = \begin{pmatrix} \mu_1 & \pm\delta \\ \pm\delta & \mu_3 \end{pmatrix},$$

$$\mathbf{H}^{\pm} := \mathbb{E}(\mathbf{G}^{\pm}). \quad (2.2.10)$$

The eigenvalues $\theta_{\alpha,\beta}$ of $\widehat{\mathbf{H}}^{\pm}$ are the solutions of $\det(\widehat{\mathbf{H}}^{\pm} - \theta\mathbf{I}) = 0$, namely

$$\theta_{\alpha,\beta} = \Big(\frac{\mu_1 + \mu_3}{2}\Big) \pm \sqrt{\frac{(\mu_3 - \mu_1)^2}{4} + \delta^2}. \quad (2.2.11)$$

By imposing θ_α to be equal to $-1/3$ and recalling that $\mu_1 + \mu_2 + \mu_3 = 0$ we obtain

$$\delta^2 = \Big(\frac{1}{3} + \mu_1\Big)\Big(\frac{1}{3} + \mu_3\Big) > 0 \quad \text{since} \quad -\frac{1}{3} < \mu_1 \leq \mu_3. \quad (2.2.12)$$

By observing that $\theta_\alpha + \theta_\beta = \mu_1 + \mu_3$, this choice of δ yields $\theta_\beta = -\mu_2 + \frac{1}{3}$, and $\mathbf{G}^{\pm} \in \mathcal{M}_{Fr}$. Now, define $\mathbf{G}^{sk} := (\mathbf{G} - \mathbf{G}^T)/2$. Hence, $\mathbf{G} = \frac{1}{2}((\mathbf{G}^+ + \mathbf{G}^{sk}) + (\mathbf{G}^- + \mathbf{G}^{sk}))$, $rank((\mathbf{G}^+ + \mathbf{G}^{sk}) - (\mathbf{G}^- + \mathbf{G}^{sk})) \leq 1$ and $\mathbf{G}$ is in $\mathcal{M}_{Fr}^{(1)}$. □

Remark 13 We deduce from Corollary 2 that $\mathcal{Q}^c_{Fr} = \mathcal{Q}_B$. Trivially, $\mathcal{Q}^c_{Fr} \subseteq \mathcal{Q}_B$. To prove the converse implication, notice that $\overline{\mathbf{X}}$ by definition belongs to $\mathcal{Q}_B$ and is expressed as a convex combination of two symmetric matrices $\mathbf{H}^{\pm}$ in $\mathcal{M}_{Fr} \subseteq \mathcal{K}^{(1)}_{Fr}$ with coefficients equal to 1/2. Hence there exist $\mathbf{H}^{\pm}_{1,2} \in \mathcal{K}_{Fr}$ such that $\mathbf{H}^{\pm} = \frac{1}{2}(\mathbf{H}^{\pm}_1 + \mathbf{H}^{\pm}_2)$. Now, $\overline{\mathbf{X}}$ can be expressed as a convex combination of the symmetric matrices $\mathbb{E}(\mathbf{H}^{\pm}_{1,2})$ in $\mathcal{Q}_{Fr}$ with coefficients equal to 1/4.

The explicit constructions in Corollaries 1 and 2 are used to compute the quasiconvex envelope of the square of the distance from the sets $\gamma\mathcal{Q}_U, \gamma\mathcal{Q}_{Fr}$ (there is nothing to prove for the case $X = B$ because the energy density f_B is already convex). This is done in the next Lemma through a *lamination* construction. Here and in the following, we repeatedly adopt the notation $\big(f(\xi)\big)^{qc} \equiv f^{qc}(\xi)$, and similarly for the other envelopes.

Lemma 2 *Let*

$$f_X(\xi) = \mu\, dist^2\big(\mathbb{E}(\xi), \gamma\mathcal{Q}_X\big) + \frac{\lambda}{2}(\mathrm{tr}\,\xi)^2, \tag{2.2.13}$$

where X stands either for Fr or U. Then,

$$\Big(f_X(\xi)\Big)^{qc} = f_B(\xi) = \mu\, dist^2\big(\mathbb{E}(\xi), \gamma\mathcal{Q}_B\big) + \frac{\lambda}{2}(\mathrm{tr}\,\xi)^2. \tag{2.2.14}$$

Proof. This is a consequence of (0.1.58) and of the chain of inequalities:

$$\big(f_X(\xi)\big)^{rc} \leq f_B(\xi) \leq \big(f_X(\xi)\big)^{c} \leq \big(f_X(\xi)\big)^{rc}, \tag{2.2.15}$$

where X stands either for Fr or U. The last inequality in (2.2.15) follows by definition. The second inequality is trivial if we consider that $f_B(\xi) \leq f_X(\xi)$ and if we take the convex envelope on both sides. We are left to prove the first inequality. To this end, we apply (0.1.57) characterizing the rank-1 convex envelope of a function by exhibiting a family of matrices and positive coefficients along which the infimum is attained. Fix $\varepsilon \in \mathbb{R}$ different from zero. For every $\xi \in \mathbb{M}^{3\times 3}$, $\mathbf{X} \in \mathcal{Q}_B$, $\mathbf{V} \in \mathcal{Q}_X$, a combination of the triangular and Young's inequalities yields

$$|\mathbb{E}(\xi) - \gamma\mathbf{V}|^2 \leq (1+\varepsilon^2)|\mathbb{E}(\xi) - \gamma\mathbf{X}|^2 + \Big(1 + \frac{1}{\varepsilon^2}\Big)|\gamma\mathbf{X} - \gamma\mathbf{V}|^2. \tag{2.2.16}$$

Write $\overline{\mathbf{X}} = \pi^{\mathcal{Q}_B}(\mathbb{E}(\xi)/\gamma)$ instead of $\mathbf{X}$ in (2.2.16). Now, (2.2.16) reads

$$|\mathbb{E}(\xi) - \gamma\mathbf{V}|^2 \leq (1+\varepsilon^2) dist^2\big(\mathbb{E}(\xi), \gamma\mathcal{Q}_B\big) + \Big(1 + \frac{1}{\varepsilon^2}\Big)|\gamma\overline{\mathbf{X}} - \gamma\mathbf{V}|^2. \tag{2.2.17}$$

We have to distinguish two cases. Suppose $\overline{\mathbf{X}} \in \mathcal{Q}_X$. Taking $\inf_{\mathbf{V}\in\mathcal{Q}_X}$ on both sides of (2.2.17), we obtain

$$dist^2\big(\mathbb{E}(\xi), \gamma\mathcal{Q}_X\big) \leq (1+\varepsilon^2) dist^2\big(\mathbb{E}(\xi), \gamma\mathcal{Q}_B\big) + 0, \tag{2.2.18}$$

taking the limit $\varepsilon \to 0$ we have

$$\mu\, dist^2\big(\mathbb{E}(\xi), \gamma\mathcal{Q}_X\big) + \frac{\lambda}{2}(\operatorname{tr}\xi)^2 \leq \mu\, dist^2\big(\mathbb{E}(\xi), \gamma\mathcal{Q}_B\big) + \frac{\lambda}{2}(\operatorname{tr}\xi)^2, \tag{2.2.19}$$

and then the claim follows by taking the rank-1 convex envelope.

Assume now $\overline{\mathbf{X}} \in \mathcal{Q}_B\backslash\mathcal{Q}_X$ and notice that $\overline{\mathbf{X}} \in \mathcal{K}_B\backslash\mathcal{K}_X$ as well. Corollaries 1 and 2 show that $\mathcal{K}_B$ can be laminated in the sense that $\mathcal{K}_B = \mathcal{K}_U^{(1)} = \mathcal{K}_{Fr}^{(2)}$. Precisely, there exist families of coefficients and matrices $\{\lambda_i\}_{i=1}^K \times \{\overline{\mathbf{V}}_i\}_{i=1}^K \in [0,1] \times \mathcal{K}_X$, with $\{\lambda_i, \overline{\mathbf{V}}_i\}_{1=1}^K$ satisfying (H_K) with K finite[1] such that $\overline{\mathbf{X}} = \sum_i \lambda_i \overline{\mathbf{V}}_i$. Define $\overline{\mathbf{X}}_i := \mathbb{E}(\overline{\mathbf{V}}_i) \in \mathcal{Q}_X$, $\xi^\perp := \xi - \gamma\overline{\mathbf{X}}$ and $\xi_i := \gamma\overline{\mathbf{V}}_i + \xi^\perp$ for any $i = 1, \ldots, K$. Trivially, $\{\lambda_i, \xi_i\}_{1=1}^K$ still satisfy (H_K) and $\xi = \sum_i \lambda_i \xi_i$. We can repeat the construction in (2.2.16) writing ξ_i and $\overline{\mathbf{X}}_i$ instead of $\xi, \mathbf{X}$ and take $\inf_{\mathbf{V}\in\mathcal{Q}_X}$ on both sides, yielding for every $i = 1, \ldots, K$

$$dist^2\big(\mathbb{E}(\xi_i), \gamma\mathcal{Q}_X\big) \leq (1+\varepsilon^2)|\mathbb{E}(\xi^\perp)|^2. \tag{2.2.20}$$

Here we use the fact that $\mathbb{E}(\xi_i) = \gamma\overline{\mathbf{X}}_i + \mathbb{E}(\xi^\perp)$. Then

$$\mu\, dist^2\big(\mathbb{E}(\xi_i), \gamma\mathcal{Q}_X\big) + \frac{\lambda}{2}(\operatorname{tr}\xi_i)^2 \leq \mu\,(1+\varepsilon^2)|\mathbb{E}(\xi^\perp)|^2 + (1+\varepsilon^2)\frac{\lambda}{2}(\operatorname{tr}\xi)^2, \tag{2.2.21}$$

because, by construction, $\operatorname{tr}\xi = \operatorname{tr}\xi_i\ \forall\, i = 1, \ldots, K$. Let us multiply both sides of formula (2.2.21) by λ_i and sum up in i yielding

$$\sum_i^K \lambda_i f_X(\xi_i) \leq \mu(1+\varepsilon^2)\sum_i^K \lambda_i|\mathbb{E}(\xi^\perp)|^2 + (1+\varepsilon^2)\frac{\lambda}{2}(\operatorname{tr}\xi)^2. \tag{2.2.22}$$

In view of (0.1.57) we finally obtain

$$\big(f_X(\xi)\big)^{rc} \leq (1+\varepsilon^2) f_B(\xi). \tag{2.2.23}$$

The claim is proved taking the limit $\varepsilon \to 0$. □

Remark 14 *We summarize some of the properties of the energy density f_X, where X stands either for Fr, U or B.*

$$f_X(\cdot) \text{ is continuous}, \tag{2.2.24}$$

$$0 \leq f_X(\mathbf{Z}), \tag{2.2.25}$$

$$-C_1 + C_2|\mathbb{E}(\mathbf{Z})|^2 \leq f_X(\mathbf{Z}), \tag{2.2.26}$$

$$f_X(\mathbf{Z}) \leq c_3|\mathbb{E}(\mathbf{Z})|^2 + C_4, \tag{2.2.27}$$

$$|f_X(\mathbf{Z}_1) - f_X(\mathbf{Z}_2)| \leq C_5\big(C_6 + |\mathbb{E}(\mathbf{Z}_1)| + |\mathbb{E}(\mathbf{Z}_2)|\big)\,\big|\mathbb{E}(\mathbf{Z}_1) - \mathbb{E}(\mathbf{Z}_2)\big|, \tag{2.2.28}$$

for every $\mathbf{Z}, \mathbf{Z}_1, \mathbf{Z}_2 \in \mathbb{M}^{3\times3}$ and were c_i with $i = 1, \ldots, 6$ are suitable positive constants. To prove (2.2.24) *and* (2.2.28) *we recall that the distance is a Lipschitz function. Then,* (2.2.25 − 2.2.27) *are trivial.*

[1] $K \leq 2$ for $X = U$ and $K \leq 4$ for $X = Fr$.

Proposition 9 ([1], [8]-Thm. 2.3) *Let Ω be any open, bounded subset of $\mathbb{R}^3$. Let $f : \mathbb{M}^{3\times 3} \mapsto [0, \infty[$ verify (2.2.24), (2.2.26) and (2.2.27). Let $\mathbf{u}_o(x) \in H^1(\Omega, \mathbb{R}^3)$. Define*

$$\mathcal{F}(\mathbf{u}) := \int_\Omega f(\nabla \mathbf{u})dx, \qquad \mathcal{F}^o(\mathbf{u}) := \begin{cases} \mathcal{F}(\mathbf{u}) & \text{on } \mathbf{u} \in H^1_o(\Omega, \mathbb{R}^3) + \mathbf{u}_o(x), \\ +\infty & \text{otherwise in } H^1(\Omega, \mathbb{R}^3). \end{cases}$$

Then, the relaxation of $\mathcal{F}$ and $\mathcal{F}^o$ is

$$\overline{\mathcal{F}}(\mathbf{u}) = \int_\Omega f^{qc}(\nabla \mathbf{u})dx, \qquad \overline{\mathcal{F}}^o(\mathbf{u}) = \begin{cases} \overline{\mathcal{F}}(\mathbf{u}) & \text{on } \mathbf{u} \in H^1_o(\Omega, \mathbb{R}^3) + \mathbf{u}_o(x), \\ +\infty & \text{otherwise in } H^1(\Omega, \mathbb{R}^3), \end{cases}$$

respectively. Then

$$\inf_{H^1(\Omega,\mathbb{R}^3)} \overline{\mathcal{F}}^o(\mathbf{u}) = \min_{H^1(\Omega,\mathbb{R}^3)} \overline{\mathcal{F}}^o(\mathbf{u}) \tag{2.2.29}$$

Here f^{qc} is the quasiconvex envelope of f, that is the greatest quasiconvex function less or equal f.

After these preparations, we are in a position to discuss our relaxation theorems.

2.2.1 The case of the compressible elastomers

A by-product of Lemma 2 and Proposition 9 is the relaxation of the non-convex mechanical energy for compressible materials, letting λ in (2.1.3) be finite.

Theorem 13 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain and denote with Γ_u an open subset of $\partial\Omega$ with positive surface measure. Take $f_X(\cdot)$ as defined in (2.1.2), where X stands either for Fr, U or B and take some function $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$. Let us define on $H^1(\Omega, \mathbb{R}^3)$*

$$\mathrm{J}_X(\mathbf{u}) = \int_\Omega f_X(\nabla \mathbf{u})dx. \tag{2.2.30}$$

Then, the relaxation of J_X is

$$\mathrm{J}_B(\mathbf{u}) = \int_\Omega f_B(\nabla \mathbf{u})dx. \tag{2.2.31}$$

Moreover, if we define $\mathrm{J}_X^{\Gamma_u,g}$ by setting $\mathrm{J}_X^{\Gamma_u,g} = \mathrm{J}_X$ on $\mathbf{g} + H^1_{\Gamma_u}(\Omega, \mathbb{R}^3)$ and $+\infty$ outside, the relaxation of $\mathrm{J}_X^{\Gamma_u,g}$ is equal to J_B on $\mathbf{g} + H^1_{\Gamma_u}(\Omega, \mathbb{R}^3)$ and $+\infty$ outside.

Proof. For $X = B$ these results are trivial. Define (here X stands either for Fr, U or B)

$$\mathrm{J}_X^o(\mathbf{u}) = \begin{cases} \mathrm{J}_X(\mathbf{u}) & \text{if } \mathbf{u} \in H^1_o(\Omega, \mathbb{R}^3), \\ +\infty & \text{otherwise in } H^1(\Omega, \mathbb{R}^3). \end{cases}$$

In the cases $X = Fr, U$, the quasiconvex envelope of f_X is f_B (Lemma 2) and hence the relaxation of J_X, J_X^o are J_B, J_B^o respectively (see [1] or [8]). In particular, the quasiconvexification formula can be expressed as ([36, Remark 5.3, pages 157-158], [9, Paragr. 6.2, pages 55-59])

$$\big(f_X\big)^{qc}(\mathbf{Z}) = \inf\Big\{|\omega|^{-1}\int_\omega f_X\big(\mathbf{Z}+\nabla\mathbf{w}(y)\big)dy : \mathbf{w}\in H_o^1(\omega,\mathbb{R}^3)\Big\}, \tag{2.2.32}$$

where ω is any open, bounded subset of $\mathbb{R}^3$ with $|\partial\omega| = 0$. The infimum in (2.2.32) can be taken in $C_c^\infty(\omega,\mathbb{R}^3)$. This is due to the density of C_c^∞ and the continuity of J_X in the strong convergence of H^1. Also, since $C_c^\infty(\omega,\mathbb{R}^3) \subset H_o^{1,\infty}(\omega,\mathbb{R}^3) \subset H_o^1(\omega,\mathbb{R}^3)$, we can simply consider test functions in $H_o^{1,\infty}(\omega,\mathbb{R}^3)$.

Now, we can extend the proof to more general boundary conditions. The relaxation result is true also if we choose some function $\mathbf{g}(x) \in H^1(\Omega,\mathbb{R}^3)$ and we define a new functional $\mathrm{J}_X^{o,\mathbf{g}}$ equal to $\int_\Omega f_X(\nabla\mathbf{u})dx$ only on the set $\{\mathbf{u}\in\mathbf{g}+H_o^1(\Omega,\mathbb{R}^3)\}$ and $+\infty$ outside. In fact, introduce $\mathbf{v} := \mathbf{u}-\mathbf{g}$ and $g_X(\nabla\mathbf{v}) := f_X(\nabla\mathbf{v}+\nabla\mathbf{g})$. Defining now (here X stands either for Fr, U or B)

$$\mathrm{G}_X^o(\mathbf{v}) = \begin{cases} \displaystyle\int_\Omega g_X(\nabla\mathbf{v})dx & \text{if } \mathbf{v}\in H_o^1(\Omega,\mathbb{R}^3), \\ +\infty & \text{otherwise in } H^1(\Omega,\mathbb{R}^3), \end{cases}$$

we obtain that the relaxation of G_X^o is G_B^o. Then, we can define $\mathrm{J}_X^{\Gamma_u,g}$ equal to $\int_\Omega f_X(\nabla\mathbf{u})dx$ only on the set $\{\mathbf{u}\in\mathbf{g}+H_{\Gamma_u}^1(\Omega,\mathbb{R}^3)\}$ and $+\infty$ otherwise in $H^1(\Omega,\mathbb{R}^3)$. It is immediate to see that the relaxation of $\mathrm{J}_X^{\Gamma_u,g}$ is $+\infty$ outside $\{\mathbf{u}\in\mathbf{g}+H_{\Gamma_u}^1(\Omega,\mathbb{R}^3)\}$ because this set is weakly closed. Fix $\mathbf{u}$ in $\mathbf{g}+H_{\Gamma_u}^1(\Omega,\mathbb{R}^3)$. Recalling that $\overline{\mathrm{J}_X^{\Gamma_u,\mathbf{g}}} = \Gamma\text{-}\lim \mathrm{J}_X^{\Gamma_u,g}$, we can write

$$\begin{aligned} \int_\Omega f_B(\nabla\mathbf{u})dx &= \Gamma\text{-}\liminf \mathrm{J}_X(\mathbf{u}) \le \Gamma\text{-}\liminf \mathrm{J}_X^{\Gamma_u,g}(\mathbf{u}) = \\ \Gamma\text{-}\liminf \mathrm{J}_X^{\Gamma_u,\widehat{g}}(\mathbf{u}) &\le \Gamma\text{-}\liminf \mathrm{J}_X^{o,\widehat{g}}(\mathbf{u}) = \int_\Omega f_B(\nabla\mathbf{u})dx, \end{aligned} \tag{2.2.33}$$

where $\widehat{\mathbf{g}} := \mathbf{u}$. The same inequality holds for the $\Gamma\text{-}\limsup$, proving the claim. □

2.2.2 The case of the incompressible elastomers

Theorem 14 *Let $\Omega\subset\mathbb{R}^3$ be a Lipschitz domain and denote with Γ_u an open subset of $\partial\Omega$ with positive surface measure. Take $f_X(\cdot)$ as in (2.1.2) (where X stands either for Fr, U or B) and define on $H^1(\Omega,\mathbb{R}^3)$*

$$\mathcal{J}_X(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_X(\nabla\mathbf{u})dx & \textit{if } \operatorname{div}\mathbf{u} = 0, \\ +\infty & \textit{otherwise.} \end{cases}$$

Then, the relaxation of $\mathcal{J}_X$ is

$$\mathcal{J}_B(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_B(\nabla\mathbf{u})dx & \textit{if } \operatorname{div}\mathbf{u} = 0, \\ +\infty & \textit{otherwise.} \end{cases}$$

Moreover, take $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$ *with* $\operatorname{div} \mathbf{g} = 0$ *a.e. in* Ω *and define* $\mathcal{J}_X^{\Gamma_u, g}$ *by setting* $\mathcal{J}_X^{\Gamma_u, g} = \mathcal{J}_X$ *on* $\mathbf{g} + H^1_{\Gamma_u}(\Omega, \mathbb{R}^3)$ *and* $+\infty$ *outside. Then the relaxation of* $\mathcal{J}_X^{\Gamma_u, g}$ *is equal to* $\mathcal{J}_B$ *on* $\mathbf{g} + H^1_{\Gamma_u}(\Omega, \mathbb{R}^3)$ *and* $+\infty$ *outside. Finally,* f_B *satisfies a solenoidal quasiconvexification formula, namely*

$$|\omega| f_B(\mathbf{Z}) = \inf\Big\{ \int_\omega f_X\big(\mathbf{Z} + \nabla \mathbf{w}(y)\big) dy : \mathbf{w} \in H^1_o(\omega, \mathbb{R}^3), \operatorname{div} \mathbf{w} = 0 \Big\} \ \forall \mathbf{Z} \in \mathbb{M}_0^{3\times 3}, \quad (2.2.34)$$

where ω *is any Lipschitz domain in* $\mathbb{R}^3$*.*

Remark 15 *Formula* (2.2.34) *holds under the hypotheses of Theorem* 14 *even if we replace* $\mathbf{w} \in H^1_o(\omega, \mathbb{R}^3)$ *with* $\mathbf{w} \in C_c^\infty(\omega, \mathbb{R}^3)$*, since the closure of* $\{\mathbf{w} \in C_c^\infty(\omega, \mathbb{R}^3), \operatorname{div} \mathbf{w} = 0\}$ *in* H^1 *is precisely* $\{\mathbf{w} \in H^1_o(\omega, \mathbb{R}^3), \operatorname{div} \mathbf{w} = 0\}$ *(see [48, Thm 1.6], [35, Sect. III.4] and [8]) and* $\mathcal{J}_X$ *is continuous in the strong topology of* H^1 *on the set* $\{\mathbf{u} \in H^1_o(\omega, \mathbb{R}^3), \operatorname{div} \mathbf{u} = 0\}$*.*

Proof. First of all, for $X = B$ there is nothing to prove because the energy density $f_B(\cdot)$ is convex. In the remaining cases, the relaxation result follows essentially from an idea of Braides[8]. For the readers' convenience, we recall the main lines of the proof when the functional is defined on $H^1(\Omega, \mathbb{R}^3)$. Let us introduce for any $h \in \mathbb{N}$

$$\mathrm{J}_X^h(\mathbf{u}) = \int_\Omega \big(f_X(\nabla \mathbf{u}) + h(\operatorname{div} \mathbf{u})^2\big) dx, \quad X = Fr, U, B. \quad (2.2.35)$$

The energy density appearing in (2.2.35) is still in the form of the square of the distance from the set $\gamma \mathcal{Q}_X$:

$$f_X^h(\mathbf{F}) := f_X(\mathbf{F}) + h(\operatorname{tr} \mathbf{F})^2 = \mu\, dist^2\big(\mathbb{E}(\mathbf{F}), \gamma \mathcal{Q}_X\big) + \Big(\frac{\lambda}{2} + h\Big)(\operatorname{tr} \mathbf{F})^2. \quad (2.2.36)$$

The main point of the proof is to show that

$$\overline{\mathcal{J}_X} = \Gamma\text{-}\lim_{h \to +\infty} \mathrm{J}_X^h = \Gamma\text{-}\lim_{h \to +\infty} \overline{\mathrm{J}_X^h} = \sup_h \overline{\mathrm{J}_X^h}. \quad (2.2.37)$$

Here, the second and the third equalities are a standard fact (see Proposition 2). We are left to prove the first equality. To this end, it is convenient to identify $\sup_h \overline{\mathrm{J}_X^h}(\mathbf{u})$. Notice that Theorem 13 applies to J_X^h for any $h \in \mathbb{N}$. Hence, the relaxation of J_X^h on $H^1(\Omega, \mathbb{R}^3)$ is the integral of the quasiconvex envelope of the energy density. The result of Lemma 2 applies to $f_X(\mathbf{F})$ if we replace λ with $\lambda' := \lambda + 2h$ in formula (2.2.13) yielding

$$\Big(f_X^h(\mathbf{F})\Big)^{qc} = \mu\, dist^2\big(\mathbb{E}(\mathbf{F}), \gamma \mathcal{Q}_B\big) + \Big(\frac{\lambda}{2} + h\Big)(\operatorname{tr} \mathbf{F})^2, \quad \text{where} \quad X = Fr, U,$$

and $\overline{\mathrm{J}_X^h} = \mathrm{J}_B^h$. Now, we take the limit of J_B^h as $h \to +\infty$. By Beppo-Levi's Theorem on monotone convergence, the supremum of a family of increasing integrals coincides with the integral of the pointwise limit of the energy densities

$$\lim_{h \to +\infty} \Big[\big(f_X^h(\mathbf{F})\big)^{qc}\Big] = \sup_h \Big[\inf_{\mathcal{Q}_B} \mu |\mathbb{E}(\mathbf{F}) - \gamma \mathbf{Q}|^2 + \Big(\frac{\lambda}{2} + h\Big)(\operatorname{tr} \mathbf{F})^2\Big] = \begin{cases} f_B(\mathbf{F}) & \text{if } \operatorname{tr} \mathbf{F} = 0, \\ +\infty & \text{otherwise,} \end{cases}$$

and hence $\sup_h \overline{\mathrm{J}_X^h} = \mathcal{J}_B$.

We are in a position to prove that $\overline{\mathcal{J}_X} = \mathcal{J}_B$. Since $\mathcal{J}_B$ is lower semicontinuous, then $\overline{\mathcal{J}_X}(\mathbf{u}) \geq \mathcal{J}_B(\mathbf{u})$. We are left to prove the converse inequality, that is

$$\overline{\mathcal{J}_X}(\mathbf{u}) \leq \mathcal{J}_B(\mathbf{u}). \tag{2.2.38}$$

This inequality is trivial if $\operatorname{div} \mathbf{u} \neq 0$ and in the rest of the proof we suppose $\operatorname{div} \mathbf{u} = 0$. Thanks to the coercivity condition (2.2.26) it is sufficient to prove that, for any sequence $\mathbf{u}_h \rightharpoonup \mathbf{u}$ w-$H^1(\Omega, \mathbb{R}^3)$, there exists a sequence $\{\mathbf{z}_h\}$ with $\operatorname{div} \mathbf{z}_h = 0$ and $\mathbf{z}_h \rightharpoonup \mathbf{u}$ w-$H^1(\Omega, \mathbb{R}^3)$ such that

$$\liminf_{h \to +\infty} \mathcal{J}_X(\mathbf{z}_h) \leq \liminf_{h \to +\infty} \mathrm{J}_X^h(\mathbf{u}_h). \tag{2.2.39}$$

Taking the infimum over all the sequences $\{\mathbf{u}_h\}$ weakly converging to $\mathbf{u}$, we obtain $\mathcal{J}_B$ on the right hand side of (2.2.39). Thanks to Theorem 13, we may restrict ourselves to sequences $\{\mathbf{u}_h\}$ such that $\mathbf{u}_h - \mathbf{u} \in H_o^1(\Omega, \mathbb{R}^3)$. We apply Proposition 1 in Paragraph 0.1.2 with $p = 2, n = 3$. For every $h \in \mathbb{N}$, let $\mathbf{w}_h \in H_o^1(\Omega, \mathbb{R}^3)$ such that

$$\begin{cases} \operatorname{div} \mathbf{w}_h = \operatorname{div} (\mathbf{u}_h - \mathbf{u}) = \operatorname{div} \mathbf{u}_h, \\ \|\mathbf{w}_h\|_{H^1(\Omega, \mathbb{R}^3)} \leq C_b \|\operatorname{div} \mathbf{u}_h\|_{L^2(\Omega)}. \end{cases} \tag{2.2.40}$$

Since $\mathcal{J}_B(\mathbf{u}) < +\infty$, we can suppose that $\mathrm{J}_X^h(\mathbf{u}_h) \leq Const$ for every h so that

$$\|\operatorname{div} \mathbf{u}_h\|^2_{L^2(\Omega)} \leq Const/h \tag{2.2.41}$$

and, by Proposition 1, we have that $\mathbf{w}_h \to 0$ strongly in $H^1(\Omega, \mathbb{R}^3)$ as $h \to +\infty$. If we define

$$\mathbf{z}_h := \mathbf{u}_h - \mathbf{w}_h, \tag{2.2.42}$$

we have that $\mathbf{z}_h \rightharpoonup \mathbf{u}$ w-$H^1(\Omega, \mathbb{R}^3)$, $\mathbf{z}_h - \mathbf{u}_h \in H_o^1(\Omega, \mathbb{R}^3)$ and $\operatorname{div} \mathbf{z}_h = 0$. Now, by (2.2.28) and Hölder's inequality, we have

$$\Big| \int_\Omega f_X(\nabla \mathbf{u}_h) dx - \int_\Omega f_X(\nabla \mathbf{z}_h) dx \Big| \leq Const \|\mathbb{E}(\nabla \mathbf{w}_h)\|_{L^2(\Omega, \mathbb{M}^{3\times3})} \tag{2.2.43}$$

and, in conclusion,

$$\begin{aligned} \overline{\mathcal{J}_X}(\mathbf{u}) \leq \liminf_{h \to +\infty} \mathcal{J}_X(\mathbf{z}_h) \leq \liminf_{h \to +\infty} \int_\Omega f_X(\mathbf{u}_h) dx + \lim_{h \to +\infty} \Big| \int_\Omega f_X(\mathbf{u}_h) dx - \mathcal{J}_X(\mathbf{z}_h) \Big| \quad (2.2.44) \\ \leq \liminf_{h \to +\infty} \mathrm{J}_X^h(\mathbf{u}_h) + 0. \end{aligned}$$

Theorem 14 holds also if we define a functional $\mathcal{J}_X^o(\mathbf{u})$ equal to $\mathcal{J}_X(\mathbf{u})$ on $H_o^1(\Omega, \mathbb{R}^3)$ and equal to $+\infty$ otherwise in $H^1(\Omega, \mathbb{R}^3)$. By proceeding as above, but taking all functions in $H_o^1(\Omega, \mathbb{R}^3)$ we obtain that $\overline{\mathcal{J}_X^o} = \mathcal{J}_B^o$. Now, we can extend the proof to more general boundary conditions. The relaxation result is true also if we choose some function $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$ with $\operatorname{div} \mathbf{g} = 0$ and we define a new functional $\mathcal{J}_X^{o,g}$ equal to $\int_\Omega f_X(\nabla \mathbf{u})dx$ only on the set $\{\mathbf{u} \in \mathbf{g} + H_o^1(\Omega, \mathbb{R}^3), \operatorname{div} \mathbf{u} = 0\}$ and $+\infty$ otherwise in $H^1(\Omega, \mathbb{R}^3)$. In fact, we can introduce $\mathbf{v} := \mathbf{u} - \mathbf{g}$ and $g_X(\nabla \mathbf{v}) := f_X(\nabla \mathbf{v} + \nabla \mathbf{g})$. Defining now

$$\mathcal{G}_X^o(\mathbf{v}) = \begin{cases} \displaystyle\int_\Omega g_X(\nabla \mathbf{v})dx & \text{if } \mathbf{v} \in H_o^1(\Omega, \mathbb{R}^3), \operatorname{div} \mathbf{v} = 0, \\ +\infty & \text{otherwise in } H^1(\Omega, \mathbb{R}^3). \end{cases}$$

we obtain that the relaxation of $\mathcal{G}_X^o$ is $\mathcal{G}_B^o$ (it is straightforward to prove that g_X verifies hypotheses $(2.2.26 - 2.2.28)$ possibly with different constants). Finally, we can define $\mathcal{J}_X^{\Gamma_u,g}$ equal to $\int_\Omega f_X(\nabla \mathbf{u})dx$ only on the set $\{\mathbf{u} \in \mathbf{g} + H_{\Gamma_u}^1(\Omega, \mathbb{R}^3), \operatorname{div} \mathbf{u} = 0\}$ and $+\infty$ otherwise in $H^1(\Omega, \mathbb{R}^3)$. It is immediate to see that the relaxation of $\mathcal{J}_X^{\Gamma_u,g}$ is $+\infty$ outside $\{\mathbf{u} \in \mathbf{g} + H_{\Gamma_u}^1(\Omega, \mathbb{R}^3), \operatorname{div} \mathbf{u} = 0\}$ because this set is weakly closed and then the claim follows as in the proof of Theorem 13.

Finally, formula (2.2.34) follows as in [8, Proposition 3.4]. □

2.3 Discussion

In this section we apply our relaxation result to some realistic examples. We show some physical implications of our analysis.

2.3.1 Physical implications

In the case when we consider the energy density f_{Fr}, we imply a direct coupling between strain and local orientation of the liquid crystal molecules. Experimental results show that a uniaxial stress typically aligns the molecules along the axis of the stress. Whether a macroscopic deformation may alter the local order of the molecules and not only the local direction is a debated problem. In particular, in the case when we consider the energy density f_U, we admit the possibility to enforce the melting of the order of the system ($\mathbf{Q} = 0$). More optimistically, with f_B we allow the whole class of biaxial states. We recall the main consequences of our relaxation result. In the following corollary, X stands either for Fr, U or B.

Corollary 3 *Under the hypotheses of Theorem* 13

$$\inf_{H^1(\Omega,\mathbb{R}^3)} \mathrm{J}_X^{\Gamma_u,g}(\mathbf{u}) = \min_{H^1(\Omega,\mathbb{R}^3)} \mathrm{J}_B^{\Gamma_u,g}(\mathbf{u}). \tag{2.3.1}$$

Moreover, under the hypotheses of Theorem 14

$$\inf_{H^1(\Omega,\mathbb{R}^3)} \mathcal{J}_X^{\Gamma_u,g}(\mathbf{u}) = \min_{H^1(\Omega,\mathbb{R}^3)} \mathcal{J}_B^{\Gamma_u,g}(\mathbf{u}). \tag{2.3.2}$$

Proof. This is a property of the relaxation (see [1], [21]). The right hand side in (4.2.36) and (2.3.2) is a minimum thanks to Korn's inequality (0.1.54) and Poincaré inequality. □

Notice that $\mathcal{J}_B$ is not strictly convex, since it is identically equal to zero for all the mechanical displacements whose symmetrized gradient lies in $\gamma\mathcal{Q}_B$.

Corollary 3 finds an application in traction problems. Let us assume $\Omega = (-X_1, X_1) \times (-X_2, X_2) \times (-X_3, X_3)$, $\Gamma_u = \{-X_1\} \times (-X_2, X_2) \times (-X_3, X_3) \cup \{X_1\} \times (-X_2, X_2) \times (-X_3, X_3)$ for some $X_1, X_2, X_3 > 0$, $\mathbf{g}(x) = \mathbf{F}\,(x - O)$ where $\mathbf{F}$ is a constant matrix with $\mathrm{tr}\,\mathbf{F} = 0$ and O is the origin. Then, the equilibrium solution to problem (2.3.2)-left is characterized by a biaxial tensor field. This is true not only if the elastomer is modelled in the frame of de Gennes tensor, but also in the case of the uniaxial tensors by developing an *effective* biaxial microstructure.

Remark 16 Let ξ be any matrix in $\mathbb{M}^{3\times3}$. Following [28], if $\pi^{\mathcal{Q}_B}(\mathbb{E}(\xi)/\gamma)$ belongs to $\mathcal{Q}_{Fr}$, we say that ξ belongs to the *solid* regime of the material. If $\pi^{\mathcal{Q}_B}(\mathbb{E}(\xi)/\gamma)$ belongs to $\mathcal{Q}_B \backslash \mathcal{Q}_{Fr}$, we say that ξ belongs to the *smectic* regime of the material if only one order of laminations is required to relax the energy, or to the *liquid* regime if two order of laminations are required (see Figure 1.3-right).

Remark 17 Another by-product of Theorem 14 is implicitly given by (2.2.37). This formula holds trivially when $X = B$ since $\mathrm{J}_B^h \equiv \overline{\mathrm{J}_B^h}$. This proves that the functional $\mathcal{J}_B$ of an incompressible material can be approximated in the sense of Gamma-convergence by a sequence of energies with increasing bulk moduli.

Chapter 3

Gamma-limits for large bodies and small particles

3.1 Introduction

This chapter concerns the asymptotic analysis of minima and minimizers of the functional

$$(\mathbf{Q}, \mathbf{u}) \mapsto \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2 |\nabla \mathbf{Q}|^2 + f_{mec}(\mathbf{Q}, \nabla \mathbf{u})\Big) dx & \\ \qquad\qquad\qquad \text{on } H^1(\Omega, \mathcal{Q}_X) \times H^1_o(\Omega, \mathbb{R}^3), \operatorname{div} \mathbf{u} = 0, & \\ +\infty \qquad\qquad \text{otherwise in } L^2(\Omega, \mathbb{M}^{3\times 3}) \times H^1(\Omega, \mathbb{R}^3), & \end{cases} \tag{3.1.1}$$

where the label X stands either for Fr, U or B. As it will be explained in the following sections, ε is a parameter defined as the ratio between the curvature constant of the liquid crystal and the characteristic length of the specimen. We obtain the Gamma-limit of (3.1.1) in the asymptotic cases of large bodies (as $\varepsilon \to 0$) and small particles (as $\varepsilon \to \infty$) and also for models of compressible elastomers.

In the asymptotic case for large bodies, even if the model of perfect order (Frank theory) is assumed to describe the local orientation of the liquid crystal molecules, we obtain a fully biaxial microstructure (that of the de Gennes theory) as a by-product of the relaxation phenomenon connected to the Gamma-convergence. We anticipate that the analysis of this problem is far from trivial. Since the proof is quite long, we subdivide it into two main subsections, the first one concerning the relaxation of the mechanical energy, the second one containing the Gamma-convergence argument.

On the other hand, in the asymptotic case for small particles, we prove that the Gamma-limit must exhibit a constant order tensor, thus justifying the solutions presented in Section 1.5 (the phase diagrams).

The last part of the chapter regards the analysis of the asymptotic energies of systems of nematic elastomers in the presence of applied fields.

3.1.1 Preliminaries

In what follows, letting $\{\mathbf{u}_k\} \subset H^1(\Omega, \mathbb{R}^3)$ and $\mathbf{u} \in H^1(\Omega, \mathbb{R}^3)$, we adopt the compact notation

$$\mathbf{u}_k \rightharpoonup \mathbf{u} \ w\text{-}H^1_o(\Omega, \mathbb{R}^3) \text{ as } k \to +\infty$$

instead of

$$\mathbf{u}_k \rightharpoonup \mathbf{u} \ w\text{-}H^1(\Omega, \mathbb{R}^3) \text{ with } (\mathbf{u}_k - \mathbf{u}) \in H^1_o(\Omega, \mathbb{R}^3) \text{ as } k \to +\infty.$$

Properties of the projection operators. We denote with $L^2(\Omega, \mathcal{Q}_X)$ where X stands either for Fr, U or B, three subsets of $L^2(\Omega, \mathbb{M}^{3\times 3})$. As observed in Chapter 1, they are strongly closed. Furthermore, $L^2(\Omega, \mathcal{Q}_B)$ is closed also in the sense of the weak topology, by convexity (Hahn-Banach Thm., see [11]). It can be proved (see Remark 18 in Section 3.2) that $L^2(\Omega, \mathcal{Q}_B)$ coincides with the (closed) convex envelope of $L^2(\Omega, \mathcal{Q}_{Fr})$ and hence also of $L^2(\Omega, \mathcal{Q}_U)$.

Now, given any tensor field $\mathbf{F}(x) \in L^2(\Omega, \mathbb{M}^{3\times 3})$, we define with $\pi^{L^2(\Omega,\gamma\mathcal{Q}_B)}(\mathbb{E}(\mathbf{F}))$ the projection of its symmetric part onto the subset $L^2(\Omega, \gamma\mathcal{Q}_B)$. Again, it is defined uniquely because $L^2(\Omega, \gamma\mathcal{Q}_B)$ is a convex, closed, and bounded subset of $L^2(\Omega, \mathbb{M}^{3\times 3})$. It follows that $\mathbf{F} \mapsto \pi^{L^2(\Omega,\gamma\mathcal{Q}_B)}(\mathbb{E}(\mathbf{F}))$ is a Lipschitz continuous map in the sense of L^2. If we define $\overline{\mathbf{F}} := \pi^{L^2(\Omega,\gamma\mathcal{Q}_B)}(\mathbb{E}(\mathbf{F}))$, then $\overline{\mathbf{F}}$ is the unique matrix field which solves the following minimization problem and which is the element of minimal distance from the set $L^2(\Omega, \gamma\mathcal{Q}_B)$

$$\min_{\mathbf{Q}\in L^2(\Omega,\mathcal{Q}_B)} \big\|\mathbb{E}(\mathbf{F}(x)) - \gamma\mathbf{Q}(x)\big\|^2_{L^2(\Omega,\mathbb{M}^{3\times 3})} = dist^2_{L^2}\big(\mathbb{E}(\mathbf{F}(x)), L^2(\Omega, \gamma\mathcal{Q}_B)\big). \tag{3.1.2}$$

The relation between $\pi^{\gamma\mathcal{Q}_B}(\cdot)$ and $\pi^{L^2(\Omega,\gamma\mathcal{Q}_B)}(\cdot)$ is shown in the following Proposition which we do not prove.

Proposition 10 *Let $\Omega \subset \mathbb{R}^3$ be a domain. Given any $\mathbf{F}(x) \in L^2(\Omega, \mathbb{M}^{3\times 3})$, then*

$$\big(\pi^{L^2(\Omega,\gamma\mathcal{Q}_B)}(\mathbf{F})\big)(x) = \pi^{\gamma\mathcal{Q}_B}\big(\mathbf{F}(x)\big) \tag{3.1.3}$$

for a.e. $x \in \Omega$.

It the follows

$$dist^2_{L^2}\big(\mathbb{E}(\mathbf{F}(x)), L^2(\Omega, \gamma\mathcal{Q}_B)\big) = \int_\Omega dist^2\big(\mathbb{E}(\mathbf{F}(x)), \gamma\mathcal{Q}_B\big)dx. \tag{3.1.4}$$

3.1.2 Domain rescaling

We consider a Lipschitz domain $\mathcal{B} \subset \mathbb{R}^3$ which we assume of volume Λ^3 with $\Lambda \in (0, \infty)$. We define the functional

$$\mathcal{F}^\kappa(\mathbf{Q}, \mathbf{u}; \mathcal{B}) := \int_{\mathcal{B}} \Big(\frac{\kappa^2}{2}|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q}, \nabla\mathbf{u})\Big)dx, \tag{3.1.5}$$

We write the minimization problem

$$\text{Minimize} \quad \mathcal{F}^{\kappa}(\mathbf{Q},\mathbf{u};\mathcal{B}), \text{ with } \mathbf{Q} \in H^1(\mathcal{B},\mathcal{Q}_X) \text{ and } \mathbf{u} \in H^1(\mathcal{B},\mathbb{R}^3), \mathbf{u}|_{\partial\mathcal{B}} \text{ assigned,} \tag{3.1.6}$$

where X stands either for Fr, U or B. It is intuitive that a predominance of the curvature energy onto the mechanical energy represented by the integral of f_{mec} yields minimizers of (3.1.6) with small gradients of $\mathbf{Q}$, while, in the reverse situation, we find minimizers with high oscillations of the gradient of $\mathbf{Q}$. We want to formulate in a rigorous form this observation. To understand how the contributions in (3.1.5) are affected by a volume rescaling, let $\mathbf{Q}_\Lambda : \mathcal{B} \mapsto \mathcal{Q}_X$, $\mathbf{u}_\Lambda : \mathcal{B} \mapsto \mathbb{R}^3$. Set $\Omega := (1/\Lambda)\mathcal{B}$ and define $\mathbf{Q} : \Omega \mapsto \mathcal{Q}_X$, $\mathbf{u} : \Omega \mapsto \mathbb{R}^3$ by

$$\mathbf{Q}\Big(\frac{1}{\Lambda}z\Big) := \mathbf{Q}_\Lambda(z), \quad \Lambda\,\mathbf{u}\Big(\frac{1}{\Lambda}z\Big) := \mathbf{u}_\Lambda(z), \qquad z \in \mathcal{B}.$$

Hence,

$$\frac{1}{|\mathcal{B}|}\mathcal{F}^{\kappa}(\mathbf{Q}_\Lambda,\mathbf{u}_\Lambda;\mathcal{B}) = \mathcal{F}^{\kappa/\Lambda}(\mathbf{Q},\mathbf{u};\Omega) = \int_\Omega \Big(\frac{\kappa^2}{2\Lambda^2}|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx, \tag{3.1.7}$$

and, if we define $\varepsilon^2 := \kappa^2/2\Lambda^2$, we obtain the integral expression presented in the Introduction to the thesis. Our aim is to study the asymptotic behavior of minima and minimizers of $\mathcal{F}^{\kappa/\Lambda}(\mathbf{Q},\mathbf{u};\Omega)$ as $\Lambda \to 0^+, +\infty$. We present the two asymptotic problems (here X stands either for Fr, U or B). By setting Λ identically equal to 0, (3.1.6) can be formulated as

$$\mathcal{P}_0 : \qquad \text{Minimize} \quad (\mathbf{Q},\mathbf{u}) \mapsto \int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx, \tag{3.1.8}$$
$$\text{with } \mathbf{Q} \in H^1(\Omega,\mathcal{Q}_X), \text{ constant and } \mathbf{u} \in H^1(\Omega,\mathbb{R}^3), \mathbf{u}|_{\partial\Omega} \text{ assigned.}$$

The asymptotic problem $\mathcal{P}_0$ for large bodies is well-posed and can be solved exactly for a relevant class of boundary conditions (see Paragraph 3.3.2). By setting Λ identically equal to $+\infty$, then (3.1.6) can be written in this form

$$\mathcal{P}_\infty : \qquad \text{Minimize} \quad (\mathbf{Q},\mathbf{u}) \mapsto \int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx, \tag{3.1.9}$$
$$\text{with } \mathbf{Q} \in L^2(\Omega,\mathcal{Q}_X) \text{ and } \mathbf{u} \in H^1(\Omega,\mathbb{R}^3), \mathbf{u}|_{\partial\Omega} \text{ assigned.}$$

The limit problem for small particles $\mathcal{P}_\infty$, in the case $X = Fr, U$ is ill-posed because the sets $L^2(\Omega,\mathcal{Q}_{Fr})$ and $L^2(\Omega,\mathcal{Q}_U)$ are not weakly closed. It may happen that a minimizing sequence $\{\mathbf{Q}_k\} \subset L^2(\Omega,\mathcal{Q}_{Fr})$ yields increasing oscillations and, consequently, the minimum may not be attained in the original set of admissible functions. This simple observation suggests that, instead of finding minima and minimizers of $\mathcal{P}_\infty$, we should study a relaxed problem $\mathcal{P}^*_\infty$.

In the next sections we prove rigourously that $\mathcal{P}_0$ and $\mathcal{P}_\infty$ appear as variational limits of problem (3.1.6) in the sense of Gamma-convergence. We anticipate that our Gamma-convergence results hold also in the presence of an additional constraint on the divergence of the displacement, in order to model incompressible materials and with slightly different boundary conditions.

3.1.3 Gathering of technical propositions

In this section we show several technical tools which are applied in the rest of the chapter. In the following propositions, let $\Omega \subset \mathbb{R}^3$ be a (non-empty) open, bounded and connected subset with Lipschitz boundary.

Proposition 11 *Let $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_B)$. Then, there exists a sequence $\{\mathbf{Q}_k\}$ of biaxial Lipschitz-continuous tensors such that $\mathbf{Q}_k \to \mathbf{Q}$ s-$L^2(\Omega, \mathbb{M}^{3\times 3})$ as $k \to +\infty$.*

Proof. We can take a sequence $\{\mathbf{M}_k\} \subset C_c^\infty(\Omega, \mathbb{M}^{3\times 3})$ of smooth tensors such that $\mathbf{M}_k \to \mathbf{Q}$ s-$L^2(\Omega, \mathbb{M}^{3\times 3})$ as $k \to +\infty$ (it is enough to apply [32, Thm. 2.78] to the components of $\mathbf{Q}$). Then, the new sequence of Lipschitz-continuous tensors $\mathbf{Z}_k := \pi^{\mathcal{Q}_B}(\mathbb{E}(\mathbf{M}_k))$ converges strongly to $\mathbf{Q} \equiv \pi^{\mathcal{Q}_B}(\mathbf{Q})$ in $L^2(\Omega, \mathbb{M}^{3\times 3})$, because the projection $\pi^{\mathcal{Q}_B}$ is a Lipschitz-continuous map in the space of matrices. □

Proposition 12 *Let $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_B)$. Then, there exists a sequence $\{\mathbf{Q}_k\} \subset L^2(\Omega, \mathcal{Q}_B)$ of piecewise-constant functions such that $\mathbf{Q}_k \to \mathbf{Q}$ s-$L^2(\Omega, \mathbb{M}^{3\times 3})$ as $k \to +\infty$.*

Proof. First of all, any $\mathbf{Q}(x)$ in $L^2(\Omega, \mathcal{Q}_B)$ can be approximated by a sequence of biaxial and continuous tensors in the strong topology of L^2. It is enough to take the sequence $\{\mathbf{Z}_k\}$ defined in the proof of Proposition 11 such that $\mathbf{Z}_k \to \mathbf{Q}$ s-$L^2(\Omega, \mathbb{M}^{3\times 3})$. Now we show that any continuous matrix $\mathbf{Z}_k \in C^o(\Omega, \mathcal{Q}_B)$ can be approximated by a sequence of piecewise-constant tensors $\{\widetilde{\mathbf{Q}}_{k,n}\}$. This means that there exists a partition of Ω consisting of a finite number of open and pairwise disjoint sets such that Ω coincides with the union of them up to a rest of measure equal to zero, and $\widetilde{\mathbf{Q}}_{k,n}$ is constant on each element of this partition. Let $\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$ be a family of orthonormal vectors in $\mathbb{R}^3$. For every $n \in \mathbb{N}$ we define the cubic lattice

$$L_n := \Big\{x \in \mathbb{R}^3 : x = \frac{1}{2^n}\sum_{i=1}^{3} \nu^i \mathbf{i}_i, \quad \nu^1, \nu^2, \nu^3 \in \mathbb{Z}\Big\}, \tag{3.1.10}$$

whose elementary cell is the open cube

$$U_n := \Big\{x \in \mathbb{R}^3 : x = \frac{1}{2^n}\sum_{i=1}^{3} \alpha^i \mathbf{i}_i, \quad 0 < \alpha^i < 1, i = 1, 2, 3\Big\}. \tag{3.1.11}$$

Since Ω is bounded, there exist $m = m(n) \in \mathbb{N}$ and a finite collection of $m(n)$ non-empty disjoint subsets of Ω of the form $\Omega_n^j := \Omega \cap \{x_j + U_n\}$, with $x_j \in L_n$ and $j = 1, \ldots, m$, and $\Omega = N \cup \bigcup_{j=1}^{m(n)} \Omega_n^j$, where N is a set such that $|N| = 0$. Now, for every $n \in \mathbb{N}$, we define

$$\widetilde{\mathbf{Q}}_{k,n}(y) := \frac{1}{|\Omega_n^j|}\int_{\Omega_n^j} \mathbf{Z}_k(x)dx \quad y \in \Omega_n^j,\ j = 1, \ldots, m(n). \tag{3.1.12}$$

Since $\mathbf{Z}_k(x)$ is a continuous function, it is a standard fact that $\widetilde{\mathbf{Q}}_{k,n} \to \mathbf{Z}_k$ s-$L^2(\Omega, \mathbb{M}^{3\times 3})$ as $n \to +\infty$. Then, also $\widehat{\mathbf{Q}}_{k,n} := \pi^{\mathcal{Q}_B}(\widetilde{\mathbf{Q}}_{k,n})$ converges strongly in L^2 as $n \to +\infty$ with $\widehat{\mathbf{Q}}_{k,n} \in L^2(\Omega, \mathcal{Q}_B)$ and piecewise constant. Choosing for every k an index $n = n(k)$ such that $\|\widehat{\mathbf{Q}}_{k,n} - \mathbf{Z}_k\|_{L^2(\Omega, \mathbb{M}^{3\times 3})} < 1/k$ and letting $\mathbf{Q}_k := \widehat{\mathbf{Q}}_{k,n(k)}$ proves the claim. □

Lemma 3 *For any* $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_{Fr})$ *there exists* $\{\mathbf{Q}_k\} \subset H^1(\Omega, \mathcal{Q}_{Fr})$ *s.t.*

$$\mathbf{Q}_k \to \mathbf{Q} \ s\text{-}L^2(\Omega, \mathbb{M}^{3\times 3}) \text{ as } k \to +\infty.$$

Proof. It is easy to prove that any $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_{Fr})$ can be written in the form $\mathbf{Q} = \mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}$ with $\mathbf{n} \in L^2(\Omega, \mathbb{S}^2)$. In fact, by the spectral theorem it is possible to set $\mathbf{Q}$ in diagonal form

$$\mathbf{Q} = \frac{2}{3}\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{m} \otimes \mathbf{m} - \frac{1}{3}\mathbf{p} \otimes \mathbf{p} \tag{3.1.13}$$

where $\{\mathbf{n}, \mathbf{m}, \mathbf{p}\}$ is an orthonormal frame. Since two of the eigenvalues of $\mathbf{Q}$ coincide, (3.1.13) is equivalent to

$$\mathbf{Q} = \frac{2}{3}\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) = \Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big).$$

Now, for any given $\mathbf{n} \in L^2(\Omega, \mathbb{S}^2)$, there exists a sequence

$$\mathbf{n}_k \to \mathbf{n} \ s\text{-}L^2(\Omega, \mathbb{R}^3) \quad \text{as} \quad k \to +\infty$$

with $\{\mathbf{n}_k\} \subset H^1(\Omega, \mathbb{S}^2)$ (see [26, Assertion 1, Pages 109-110, with $m_s = 1$]). Let us define

$$\mathbf{Q}_k := \mathbf{n}_k \otimes \mathbf{n}_k - \frac{1}{3}\mathbf{I}.$$

Every tensor field $\mathbf{Q}_k$ belongs to $H^1(\Omega, \mathcal{Q}_{Fr})$ by an elementary property of the product of essentially bounded H^1-functions. Then, it is sufficient to verify that $\mathbf{n}_k \otimes \mathbf{n}_k \to \mathbf{n} \otimes \mathbf{n} \, s\text{-}L^2(\Omega, \mathbb{M}^{3\times 3})$:

$$\begin{aligned}\int_\Omega |\mathbf{n}_k \otimes \mathbf{n}_k - \mathbf{n} \otimes \mathbf{n}|^2 dx &= \int_\Omega |\mathbf{n}_k \otimes \mathbf{n}_k - \mathbf{n}_k \otimes \mathbf{n} + \mathbf{n}_k \otimes \mathbf{n} - \mathbf{n} \otimes \mathbf{n}|^2 dx \\ &\leq a_1 \int_\Omega |\mathbf{n}_k| \, |\mathbf{n}_k - \mathbf{n}|^2 dx + a_2 \int_\Omega |\mathbf{n}||\mathbf{n}_k - \mathbf{n}|^2 dx \overset{k\to\infty}{\longrightarrow} 0,\end{aligned}$$

where a_1, a_2 are suitable positive constants[1]. □

3.2 Large bodies: asymptotics

We discuss the behavior of minima and minimizers of the family of functionals (3.1.1) by computing its Gamma-limit as $\varepsilon \to 0$, in the topology

$$\sigma := w\text{-}L^2(\Omega, \mathbb{M}^{3\times 3}) \times w\text{-}H^1(\Omega, \mathbb{R}^3). \tag{3.2.1}$$

In what follows, letting $\{\mathbf{Q}_h, \mathbf{u}_h\} \subset L^2(\Omega, \mathcal{Q}_X) \times H^1(\Omega, \mathbb{R}^3)$, where X stands either for Fr, U or B, we write

$$\mathbf{Q}_h, \mathbf{u}_h \overset{\sigma}{\rightharpoonup} \mathbf{Q}, \mathbf{u} \quad \text{ as } h \to +\infty, \tag{3.2.2}$$

[1]The lemma above proves that any Frank tensor in $L^2(\Omega, \mathcal{Q}_{Fr})$ can be approximated in the strong topology by a sequence of *oriented* Frank tensors, in the sense of [4]

instead of

$$\mathbf{u}_h \rightharpoonup \mathbf{u}\ w\text{-}H^1(\Omega,\mathbb{R}^3),\ \text{ and } \mathbf{Q}_h \rightharpoonup \mathbf{Q}\ w\text{-}L^2(\Omega,\mathbb{M}^{3\times3}) \text{ as } h \to +\infty. \tag{3.2.3}$$

We recall that the Gamma-convergence in the weak topology of $H^1(\Omega,\mathbb{R}^3)$ is equivalent to the Gamma-convergence in the strong topology of $L^2(\Omega,\mathbb{R}^3)$ because the functional bounds the L^2-norm of the gradient of $\mathbf{u}$ by Korn's inequality (0.1.53). Analogously, since $L^2(\Omega,\mathcal{Q}_X)$ (where X stands either for Fr, U or B) is contained in some closed and bounded ball of $L^2(\Omega,\mathbb{M}^{3\times3})$, then the weak topology over $L^2(\Omega,\mathcal{Q}_X)$ is metrizable (see [22, Chapt. 8]).

The idea of the proof is to show that the family (3.1.1) Gamma-converges to the relaxation of the mechanical energy defined as

$$\mathcal{F}^{\partial\Omega}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } L^2(\Omega,\mathcal{Q}_X)\times H^1_o(\Omega,\mathbb{R}^3), \operatorname{div}\mathbf{u}=0, \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

To start, we find the relaxation of $\mathcal{F}^{\partial\Omega}_{mec,X}$ in the sense of σ and we show that it always coincides with $\mathcal{F}^{\partial\Omega}_{mec,B}$ (Section 3.2.2) also in the case $X = Fr$ or U. The main difficulty is to treat the penalty function $+\infty$ if $\operatorname{div}\mathbf{u} \neq 0$. This requires an intermediate ingredient, that is the relaxation of the mechanical model for a compressible material (Section 3.2.1), that is when we remove the constraint on the divergence of the displacement. Then, we show that the relaxation of $\mathcal{F}^{\partial\Omega}_{mec,X}$ can be obtained as the Gamma-limit of a sequence of energies with finite and increasing bulk modulus. The last part (Section 3.2.3) consists in proving the Gamma-convergence result, that is to prove the *liminf* and the *limsup* inequalities.

3.2.1 Relaxation of energies of compressible elastomers

Theorem 15 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain. Let f_{mec} as in* (2.1.1) *and define (here X stands either for Fr, U or B)*

$$\mathrm{F}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } L^2(\Omega,\mathcal{Q}_X)\times H^1(\Omega,\mathbb{R}^3), \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3). \end{cases} \tag{3.2.4}$$

Then, the relaxation of $\mathrm{F}_{mec,X}$ in the sense of σ (see 3.2.1) is $\mathrm{F}_{mec,B}$.

Proof. We make the complete construction only in the case $X = Fr$. When $X = B$ the functional is lower semicontinuous by convexity. In the case $X = U$ the result follows automatically by an abstract argument explained in Paragraph 3.2.4. Recalling that $L^2(\Omega,\mathcal{Q}_{Fr}) \subset L^2(\Omega,\mathcal{Q}_B)$, we have that $\mathrm{F}_{mec,Fr} \geq \mathrm{F}_{mec,B}$ and if we relax both sides we obtain $\overline{\mathrm{F}}_{mec,Fr} \geq \mathrm{F}_{mec,B}$. Then, we notice that $\overline{\mathrm{F}}_{mec,Fr} \leq \mathrm{F}_{mec,B}$ is trivial if $\mathbf{Q} \notin L^2(\Omega,\mathcal{Q}_B)$. Hence, in what follows we may assume $(\mathbf{Q},\mathbf{u}) \in L^2(\Omega,\mathcal{Q}_B)\times H^1(\Omega,\mathbb{R}^3)$. We split the proof in three steps. First (Step 1), we discuss the relaxation in the case when the tensor field $\mathbf{Q}$ is constant by exhibiting a recovery sequence $\{\mathbf{Q}_n,\mathbf{u}_n\}$ which is optimal for the energy. Then (Step 2), we extend the proof to the case of piecewise-constant biaxial tensor fields. The last point (Step 3), concerns the density of L^2-biaxial tensor fields.

Step 1, $\mathbf{Q}(x)$ constant

As anticipated, we assume $\mathbf{u} \in H^1(\Omega, \mathbb{R}^3)$ and $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_B)$ and constant, and we construct a sequence $\{\mathbf{Q}_n, \mathbf{u}_n\}$ such that

$$\limsup_{n\to+\infty} \int_U f_{mec}(\mathbf{Q}_n, \nabla\mathbf{u}_n)dx \le \int_U f_{mec}(\mathbf{Q}, \nabla\mathbf{u})dx + o(1), \tag{3.2.5}$$

as

$$\mathbf{Q}_n \rightharpoonup \mathbf{Q}\ w\text{-}L^2(U, \mathbb{M}^{3\times3}), \quad \mathbf{u}_n \rightharpoonup \mathbf{u}\ w\text{-}H^1(U, \mathbb{R}^3) \text{ as } n \to +\infty, \tag{3.2.6}$$

with support$(\mathbf{u}_n - \mathbf{u}) \subset\subset U$, for every open set $U \subset \Omega$. Denoting with $\chi_U(x)$ the function which is identically equal to 1 in U and 0 in its complementary, we can write $\mathbf{Q}(x) = \mathrm{Q}\,\chi_U(x)$ with $\mathrm{Q} \in \mathcal{Q}_B$. With some abuse of notation, in what follows, we do not make any distinction between $\mathbf{Q}$ and Q. By the spectral theorem we can find a rotation $\mathbf{R} \in \mathbb{SO}(3)$ so that $\mathbf{Q}$ can be written in diagonal form

$$\mathbf{Q}_D = \mathbf{R}^T\mathbf{Q}\mathbf{R} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}$$

and with $a \le b \le c$, $a + b + c = 0$. Suppose for a moment $a \ne -1/3$. We denote with $\mathcal{D}$ the open parallelepiped in $\mathbb{R}^3$ defined as $\mathcal{D} = (-T, T) \times (-1, 1) \times (-1, 1)$ where

$$T := \sqrt{\frac{c + 1/3}{a + 1/3}}. \tag{3.2.7}$$

Let (see also Figure 3.1-left)

$$F_1 := \Big\{(x_1, x_2, x_3) : -\frac{1}{T}x_1 \le x_3 < -\frac{1}{T}(x_1 - T), 0 \le x_3 < 1, -T < x_1 < T, -1 < x_2 < 1\Big\},$$
$$F_3 := \Big\{(x_1, x_2, x_3) : \frac{1}{T}(x_1 - T) < x_3 \le \frac{1}{T}x_1, -1 < x_3 < 0, -T < x_1 < T, -1 < x_2 < 1\Big\},$$
$$F_2' := \Big\{(x_1, x_2, x_3) : x_3 < -\frac{1}{T}x_1, 0 \le x_3 < 1, -T < x_1 \le 0, -1 < x_2 < 1\Big\},$$
$$F_2'' := \Big\{(x_1, x_2, x_3) : -\frac{1}{T}(x_1 - T) \le x_3, 0 \le x_3 < 1, 0 < x_1 < T, -1 < x_2 < 1\Big\},$$
$$F_4' := \Big\{(x_1, x_2, x_3) : x_3 > \frac{1}{T}x_1, -1 < x_3 < 0, -T < x_1 < 0, -1 < x_2 < 1\Big\},$$
$$F_4'' := \Big\{(x_1, x_2, x_3) : x_3 \le \frac{1}{T}(x_1 - T), -1 < x_3 < 0, 0 < x_1 < T, -1 < x_2 < 1\Big\},$$
$$F_2 := F_2' \cup F_2'', \quad F_4 := F_4' \cup F_4''.$$

Now (see also Figure 3.1), we define the tensor field $\mathbf{H} : \mathcal{D} \to \mathbb{M}^{3\times3}$

$$\mathbf{H}(x) := \begin{cases} \mathbf{R}\mathbf{G}_1\mathbf{R}^T & \text{on} \quad F_1 \\ \mathbf{R}\mathbf{G}_2\mathbf{R}^T & \text{on} \quad F_2 \\ \mathbf{R}\mathbf{G}_3\mathbf{R}^T & \text{on} \quad F_3 \\ \mathbf{R}\mathbf{G}_4\mathbf{R}^T & \text{on} \quad F_4, \end{cases}$$

where $\mathbf{G}_i$ with $i = 1, \dots, 4$ are the following constant matrices

$$\mathbf{G}_1 = \begin{pmatrix} a & 0 & 2G_{a,c} \\ -2G_{a,b} & b & -2G_{b,c} \\ 0 & 0 & c \end{pmatrix}, \mathbf{G}_2 = \begin{pmatrix} a & 0 & 2G_{a,c} \\ 2G_{a,b} & b & 2G_{b,c} \\ 0 & 0 & c \end{pmatrix},$$

$$\mathbf{G}_3 = \begin{pmatrix} a & 0 & -2G_{a,c} \\ -2G_{a,b} & b & 2G_{b,c} \\ 0 & 0 & c \end{pmatrix}, \mathbf{G}_4 = \begin{pmatrix} a & 0 & -2G_{a,c} \\ 2G_{a,b} & b & -2G_{b,c} \\ 0 & 0 & c \end{pmatrix},$$

and where the constants $G_{a,b}$, $G_{a,c}$, $G_{b,c}$ are defined as follows

$$G_{a,b} = \sqrt{a+\frac{1}{3}}\sqrt{b+\frac{1}{3}}, G_{a,c} = \sqrt{a+\frac{1}{3}}\sqrt{c+\frac{1}{3}}, G_{b,c} = \sqrt{b+\frac{1}{3}}\sqrt{c+\frac{1}{3}}.$$

Suppose now $a = -1/3$. In this case we denote with $\mathcal{D}$ the open cube in $\mathbb{R}^3$ defined as $\mathcal{D} = (-1,1) \times (-1,1) \times (-1,1)$ and

$$F_5 := \big\{(x_1, x_2, x_3) \in \mathcal{D} : 0 \le x_3 < 1\big\}, \quad F_6 := \big\{(x_1, x_2, x_3) \in \mathcal{D} : -1 < x_3 < 0\big\}. \tag{3.2.8}$$

Then (see also Figure 3.2-left), we define the tensor field $\mathbf{H} : \mathcal{D} \to \mathbb{M}^{3\times3}$

$$\mathbf{H}(x) = \begin{cases} \mathbf{R}\mathbf{G}_5\mathbf{R}^T & \text{on } F_5 \\ \mathbf{R}\mathbf{G}_6\mathbf{R}^T & \text{on } F_6. \end{cases}$$

where

$$\mathbf{G}_5 = \begin{pmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & b & -2G_{b,c} \\ 0 & 0 & c \end{pmatrix}, \quad \mathbf{G}_6 = \begin{pmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & b & 2G_{b,c} \\ 0 & 0 & c \end{pmatrix}. \tag{3.2.9}$$

A straightforward computation shows that

$$\text{spectrum}\big(\mathbb{E}(\mathbf{G}_i)\big) = \Big\{-\frac{1}{3}, -\frac{1}{3}, \frac{2}{3}\Big\}, \text{with } i = 1, \dots, 6. \tag{3.2.10}$$

For the remaining part of the construction we address the interested readers to [32, Par. 2.2.2] as an additional reference. Now, define $\widetilde{\mathbf{H}}(x)$ as the extension of $\mathbf{H}(x)$ in $\mathbb{R}^3$ by periodicity (notice that it is constant in the direction $\mathbf{i}_2$) and define $\forall\, n \in \mathbb{N}$

$$\mathbf{F}_n(x) := \widetilde{\mathbf{H}}(n\,x_1, n\,x_2, n\,x_3).$$

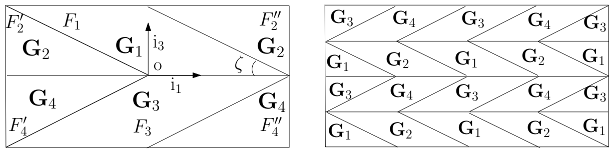

Figure 3.1: Geometry of the oscillating sequence $\mathbf{F}_n$ in the case $1 \leq T < +\infty$. The left panel is referred to the case $n = 1$ and the right panel to the case $n = 2$. Here ζ is an angle whose tangent has absolute value equal to $1/T$. Here $\mathbf{R} = \mathbf{I}$.

Figure 3.2: LEFT. Geometry of the oscillating sequence $\mathbf{F}_n$ in the case $a = -1/3$, $T = +\infty$. The left panel is referred to the case $n = 1$ and the right panel to the case $n = 2$. Here $\mathbf{R} = \mathbf{I}$. RIGHT. Sketch of the construction of the sequence $\{\mathbf{u}_n\}$, case $a = c = 0$.

Then, restricting the sequence $\{\mathbf{F}_n\}$ to U, we have

$$\mathbf{F}_n(x) \overset{*}{\rightharpoonup} \mathbf{Q} \quad w\text{-}L^\infty(U, \mathbb{M}^{3\times 3}) \text{ as } n \to +\infty,$$

and, in particular,

$$\mathbf{Q} = \frac{1}{|\mathcal{D}|} \int_{\mathcal{D}} \mathbf{H}(x)dx, \qquad Q_{ij} = \frac{1}{|\mathcal{D}|} \int_{\mathcal{D}} H_{ij}(x)dx, \qquad i, j \in \{1, 2, 3\}.$$

In fact, the coefficients of the matrix $\mathbf{Q}_D$ are obtained as a convex combination of the matrices $\mathbf{G}_i$ with $i = 1, \ldots, 4$ with coefficients equal to $1/4$ (case $a \neq -1/3$) or as a convex combination of the matrices $\mathbf{G}_i$ with $i = 5, 6$ (case $a = -1/3$) with coefficients equal to $1/2$ (see also Figures 3.1 and 3.2). This construction has a double purpose. The symmetric part of $\mathbf{H}$ yields an oscillating sequence which converges to $\mathbf{Q}$ if restricted to U:

$$\mathbf{Q}_n(x) := \mathbb{E}(\mathbf{F}_n) \overset{*}{\rightharpoonup} \mathbf{Q} \quad w\text{-}L^\infty(U, \mathbb{M}^{3\times 3}) \text{ as } n \to +\infty, \tag{3.2.11}$$

while the tensor field $\mathbf{F}_n(x)$ is itself the gradient of a sequence of functions which converges to $\mathbf{u}$ as the width of the oscillations tends to zero. For, we verify that the compatibility condition (see [45], [29]) holds for $\mathbf{G}(x)$:

$$\mathbf{G}_1 - \mathbf{G}_2 = \mathbf{a} \otimes \nu_1 \text{ and } \mathbf{G}_3 - \mathbf{G}_4 = \mathbf{a} \otimes \nu_2, \tag{3.2.12}$$

where

$$\mathbf{a} = -4\mathbf{i}_2\sqrt{b+\frac{1}{3}}\sqrt{\frac{2}{3}-b}, \nu_1 = \frac{\sqrt{a+1/3}}{\sqrt{2/3-b}}\mathbf{i}_1 + \frac{\sqrt{c+1/3}}{\sqrt{2/3-b}}\mathbf{i}_3, \nu_2 = \frac{\sqrt{a+1/3}}{\sqrt{2/3-b}}\mathbf{i}_1 - \frac{\sqrt{c+1/3}}{\sqrt{2/3-b}}\mathbf{i}_3$$

and ν_1 is perpendicular to the interface between $\mathbf{G}_1$ and $\mathbf{G}_2$ and ν_2 is perpendicular to the interface between $\mathbf{G}_3$ and $\mathbf{G}_4$;

$$\mathbf{G}_1 - \mathbf{G}_3 = \Big(4G_{a,c}\mathbf{i}_1 - 4G_{b,c}\mathbf{i}_2\Big)\otimes\mathbf{i}_3, \quad \mathbf{G}_2 - \mathbf{G}_4 = \Big(4G_{a,c}\mathbf{i}_1 + 4G_{b,c}\mathbf{i}_2\Big)\otimes\mathbf{i}_3, \tag{3.2.13}$$

$$\mathbf{G}_5 - \mathbf{G}_6 = \big(-4G_{b,c}\big)\mathbf{i}_2\otimes\mathbf{i}_3, \tag{3.2.14}$$

and $\mathbf{i}_3$ is perpendicular to the interface between $\mathbf{G}_1$ and $\mathbf{G}_3$, $\mathbf{G}_2$ and $\mathbf{G}_4$, $\mathbf{G}_5$ and $\mathbf{G}_6$.

Now we construct the sequence $\{\mathbf{u}_n\}$. Suppose for a moment $a \neq -1/3$. We define a vector field $\mathbf{g} : \mathcal{D} \mapsto \mathbb{R}^3$ as

$$\mathbf{g}(x) := \begin{cases} \mathbf{g}_i(x) & \text{on} \quad F_i, \quad i = 1,3 \\ \mathbf{g}'_i(x) & \text{on} \quad F'_i, \quad i = 2,4 \\ \mathbf{g}''_i(x) & \text{on} \quad F''_i, \quad i = 2,4, \end{cases} \tag{3.2.15}$$

where

$$\mathbf{g}_1(x) := \begin{cases} 2G_{a,c}\,x_3 \\ -2G_{a,b}\,x_1 - 2G_{b,c}\,x_3 \\ 0, \end{cases} \qquad \mathbf{g}_3(x) := \begin{cases} -2G_{a,c}\,x_3 \\ -2G_{a,b}\,x_1 + 2G_{b,c}\,x_3 \\ 0, \end{cases} \tag{3.2.16}$$

$$\mathbf{g}'_2(x) := \begin{cases} 2G_{a,c}\,x_3 \\ 2G_{a,b}\,x_1 + 2G_{b,c}\,x_3 \\ 0, \end{cases} \qquad \mathbf{g}'_4(x) := \begin{cases} -2G_{a,c}\,x_3 \\ 2G_{a,b}\,x_1 - 2G_{b,c}\,x_3 \\ 0, \end{cases} \tag{3.2.17}$$

$$\mathbf{g}''_2(x) := \begin{cases} 2G_{a,c}\,x_3 \\ 2G_{a,b}\,(x_1 - 2T) + 2G_{b,c}\,x_3 \\ 0, \end{cases} \quad \mathbf{g}''_4(x) := \begin{cases} -2G_{a,c}\,x_3 \\ 2G_{a,b}\,(x_1 - 2T) - 2G_{b,c}\,x_3 \\ 0. \end{cases} \tag{3.2.18}$$

Now, suppose $a = -1/3$. In this case we define a vector field $\mathbf{g} : \mathcal{D} \mapsto \mathbb{R}^3$ as

$$\mathbf{g}(x) := \begin{cases} \mathbf{g}_5(x) & \text{on} \quad F_5 \\ \mathbf{g}_6(x) & \text{on} \quad F_6, \end{cases} \tag{3.2.19}$$

where

$$\mathbf{g}_5(x) := \begin{cases} 0 \\ -2G_{b,c}\,x_3 \\ 0, \end{cases} \qquad \mathbf{g}_6(x) := \begin{cases} 0 \\ 2G_{b,c}\,x_3 \\ 0. \end{cases} \tag{3.2.20}$$

Now we define $\widetilde{\mathbf{g}}$ as the extension of $\mathbf{g}(x)$ on $\mathbb{R}^3$ by periodicity, $\mathbf{f}(x) := \mathbf{R}\widetilde{\mathbf{g}}(\mathbf{R}^T x) + \mathbf{Q}(x-O)$ and $\forall\, n \in \mathbb{N}$

$$\mathbf{f}_n(x) := \mathbf{f}(n\,x_1, n\,x_2, n\,x_3).$$

Notice that $\mathbf{f}(x)$ is a Lipschitz function, $\nabla \mathbf{f}_n(x) = \mathbf{F}_n$ and that $\mathbf{f}_n$ converges to $\mathbf{Q}(x-O)$ uniformly on compact sets as $n \to \infty$. In order to take into account the boundary conditions, we modify slightly the previous construction. We assign a positive real number ε_o which is defined in the next lines and let any ε such that $0 < \varepsilon \le \varepsilon_o$. Take a compact set K well contained in U defined as $K := \{x \in U : dist(x, U^c) \le \varepsilon\}$ and let $\theta(x) \in C_c^\infty(U)$ be a scalar test function whose support is $K' := \{x \in U : dist(x, U^c) \le \varepsilon/2\}$ and which is identically equal to 1 on K, $0 \le \theta \le 1$ (see also Figure 3.2-right for an idea of the construction). Now we can define ε_o as the largest number such that K, K' are not empty. Then, let

$$\mathbf{u}_n(x) := \mathbf{u}(x) + \gamma\theta(x)\big(\mathbf{f}_n(x) - \mathbf{Q}(x-O)\big). \tag{3.2.21}$$

By construction $\mathbf{u}_n \rightharpoonup \mathbf{u}$ w-$H^1(U, \mathbb{R}^3)$ and $\mathrm{supp}(\mathbf{u}_n - \mathbf{u}) \subset\subset U$.

We show that the sequence $\{\mathbf{Q}_n, \mathbf{u}_n\}$ defined by (3.2.11) and (3.2.21) yields (3.2.5). We observe that since $\mathbf{Q}_n$ ranges in $\mathcal{Q}_{Fr}$ for any $n \in \mathbb{N}$ (see (3.2.10)), then the energy functional $\mathrm{F}_{mec,Fr}$ takes finite values when evaluated at $\{\mathbf{Q}_n, \mathbf{u}_n\}$ and we can write

$$\int_U f_{mec}(\mathbf{Q}_n, \nabla\mathbf{u}_n)dx = \int_K f_{mec}(\mathbf{Q}_n, \nabla\mathbf{u}_n)dx + \int_{U\setminus K} f_{mec}(\mathbf{Q}_n, \nabla\mathbf{u}_n)dx. \tag{3.2.22}$$

Let us consider the first summand on the right hand side of (3.2.22). We have (since $\mathrm{tr}\,\mathbf{F}_n = \mathrm{tr}\,\mathbf{Q} = 0$)

$$\begin{aligned} &\int_K f_{mec}\big(\mathbf{Q}_n, \nabla\mathbf{u} + \gamma\mathbf{F}_n - \gamma\mathbf{Q}\big)dx = \\ &\int_K \Big\{\mu\big|\gamma\mathbf{Q}_n - \mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}_n + \gamma\mathbf{Q}\big|^2 + \frac{\lambda}{2}\Big(\mathrm{tr}\,\big(\nabla\mathbf{u} + \gamma\mathbf{F}_n - \gamma\mathbf{Q}\big)\Big)^2\Big\}dx = \\ &\int_K \Big(\mu\big|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}\big|^2 + \frac{\lambda}{2}(\mathrm{div}\,\mathbf{u})^2\Big)dx. \end{aligned} \tag{3.2.23}$$

We turn our attention to the second summand on the right hand side of (3.2.22) (here the constants may change from line to line while we maintain the same name). Recalling (2.2.27) (Remark 14) we can write

$$\begin{aligned} &\int_{U\setminus K} f_{mec}\Big(\mathbf{Q}_n, \nabla\mathbf{u} + \gamma\theta(\mathbf{F}_n - \mathbf{Q}) + \gamma\big(\nabla\theta \otimes (\mathbf{f}_n - \mathbf{Q}x)^T\big)\Big)dx \\ &\le \int_{U\setminus K} Const\Big\{1 + |\mathbb{E}(\nabla\mathbf{u})|^2 + \gamma^2|\mathbf{Q}_n - \mathbf{Q}|^2 + \gamma^2|\nabla\theta|^2|\mathbf{f}_n - \mathbf{Q}x|^2\Big\}dx. \end{aligned} \tag{3.2.24}$$

It is important to recall that $\nabla\theta$ is bounded since $\theta \in C_c^\infty(U)$ and that $\mathbf{f}_n(x)$ converges uniformly to $\mathbf{Q}(x-O)$ and, taking the limit in n, we have

$$\begin{aligned} \limsup_{n\to\infty} \int_U f_{mec}(\mathbf{Q}_n, \nabla\mathbf{u}_n)dx &\le \limsup_{n\to\infty} \int_K f_{mec}(\mathbf{Q}_n, \nabla\mathbf{u}_n)dx + Const\frac{\varepsilon}{m} = \\ &\int_K f_{mec}(\mathbf{Q}, \nabla\mathbf{u})dx + Const\frac{\varepsilon}{m}, \end{aligned} \tag{3.2.25}$$

where $m \in \mathbb{N}$ (the rôle of the natural number m will be clear in the next paragraph). Since f_{mec} is non-negative we can enlarge K to U

$$\limsup_{n\to\infty} \int_U f_{mec}(\mathbf{Q}_n, \nabla \mathbf{u}_n)dx \leq \int_U f_{mec}(\mathbf{Q}, \nabla \mathbf{u})dx + Const\frac{\varepsilon}{m}. \tag{3.2.26}$$

Since the constant is indeed independent of ε, in what follows we simply write $\frac{\varepsilon}{m}$ instead of $Const\frac{\varepsilon}{m}$.

Step 2, $\mathbf{Q}(x)$ piecewise-constant

Suppose now $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_B)$ and piecewise-constant, i.e. there exists a partition of Ω consisting of a finite number m of open and pairwise disjoint sets Ω^j s.t.

$$\Omega = \bigcup_{j=1}^{m} \Omega^j \cup N, \tag{3.2.27}$$

where $|N| = 0$ and $\mathbf{Q}^j := \mathbf{Q}|_{\Omega^j}$ is constant. By Step 1 we have that, for every Ω^j with $j = 1, \dots, m$, there exist

$$\mathbf{Q}^j_n \rightharpoonup \mathbf{Q}^j \ w\text{-}L^2(\Omega^j, \mathbb{M}^{3\times3}), \qquad \mathbf{u}^j_n \rightharpoonup \mathbf{u}^j \ w\text{-}H^1(\Omega^j, \mathbb{R}^3) \qquad \text{as } n \to +\infty, \tag{3.2.28}$$

with $\text{supp}(\mathbf{u}^j_n - \mathbf{u}) \subset\subset \Omega^j$ and where $\mathbf{u}^j$ is the restriction of $\mathbf{u}$ on Ω^j, and

$$\limsup_{n\to\infty} \int_{\Omega^j} f_{mec}\big(\mathbf{Q}^j_n, \nabla \mathbf{u}^j_n\big)dx \leq \int_{\Omega^j} f_{mec}(\mathbf{Q}^j, \nabla \mathbf{u}^j)dx + \frac{\varepsilon}{m}. \tag{3.2.29}$$

Now, let us define $\mathbf{u}_n := \mathbf{u}^j_n$ on Ω^j, $\mathbf{Q}_n := \mathbf{Q}^j_n$ on Ω^j, $j = 1, \dots, m$. Recalling that $\mathbf{u}^j_n - \mathbf{u}^j = 0$ on $\partial\Omega^j$, then $\mathbf{u}_n \in H^1(\Omega, \mathbb{R}^3)$ and $\mathbf{u}_n - \mathbf{u} \in H^1_o(\Omega, \mathbb{R}^3)$ and

$$\int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u})dx = \sum_{j=1}^{m} \int_\Omega f_{mec}(\mathbf{Q}^j, \nabla \mathbf{u}^j)dx. \tag{3.2.30}$$

By using (3.2.29) we have

$$\liminf_{n\to+\infty} \int_\Omega f_{mec}(\mathbf{Q}_n, \nabla \mathbf{u}_n)dx = \liminf_{n\to+\infty} \sum_{j=1}^{m} \int_{\Omega^j} f_{mec}\big(\mathbf{Q}^j_n, \nabla \mathbf{u}^j_n\big)dx \tag{3.2.31}$$

$$\leq \sum_{j=1}^{m} \limsup_{n\to+\infty} \int_{\Omega^j} f_{mec}\big(\mathbf{Q}^j_n, \nabla \mathbf{u}^j_n\big)dx \leq \sum_{j=1}^{m} \Big(\int_{\Omega^j} f_{mec}(\mathbf{Q}^j, \nabla \mathbf{u}^j)dx + \frac{\varepsilon}{m}\Big)$$

$$= \sum_{j=1}^{m} \int_{\Omega^j} f_{mec}(\mathbf{Q}^j, \nabla \mathbf{u}^j)dx + \varepsilon = \int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u})dx + \varepsilon.$$

Summarizing:

$$\overline{\mathrm{F}}_{mec,Fr}(\mathbf{Q}, \mathbf{u}) \leq \liminf_{n\to+\infty} \int_\Omega f_{mec}(\mathbf{Q}_n, \nabla \mathbf{u}_n)dx \leq \int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u})dx + \varepsilon. \tag{3.2.32}$$

Step 3, $\mathbf{Q}(x) \in L^2(\Omega, \mathcal{Q}_B)$

Let $(\mathbf{Q}, \mathbf{u}) \in L^2(\Omega, \mathcal{Q}_B) \times H^1(\Omega, \mathbb{R}^3)$. By Proposition 12 there exists a sequence $\{\mathbf{Q}_k\} \subset L^2(\Omega, \mathcal{Q}_B)$ of piecewise-constant and biaxial matrices such that

$$\mathbf{Q}_k \to \mathbf{Q} \quad s\text{-}L^2(\Omega, \mathbb{M}^{3\times 3}) \text{ as } k \to +\infty. \tag{3.2.33}$$

Hence, we can write

$$\overline{\mathrm{F}}_{mec,Fr}(\mathbf{Q}_k, \mathbf{u}) \leq \int_\Omega f_{mec}(\mathbf{Q}_k, \nabla \mathbf{u}) dx + \varepsilon, \tag{3.2.34}$$

and, in the limit as $k \to +\infty$, we have

$$\overline{\mathrm{F}}_{mec,Fr}(\mathbf{Q}, \mathbf{u}) \leq \liminf_{k\to+\infty} \overline{\mathrm{F}}_{mec,Fr}(\mathbf{Q}_k, \mathbf{u}) \leq \liminf_{k\to+\infty} \int_\Omega f_{mec}(\mathbf{Q}_k, \nabla \mathbf{u}) dx + \varepsilon. \tag{3.2.35}$$

Since the right hand side in (3.2.35) is continuous in the strong topology of $L^2(\Omega, \mathbb{M}^{3\times 3})$, we have

$$\overline{\mathrm{F}}_{mec,Fr}(\mathbf{Q}, \mathbf{u}) \leq \int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u}) dx + \varepsilon, \tag{3.2.36}$$

and, in the limit as $\varepsilon \to 0$,

$$\overline{\mathrm{F}}_{mec,Fr}(\mathbf{Q}, \mathbf{u}) \leq \mathrm{F}_{mec,B}(\mathbf{Q}, \mathbf{u}), \tag{3.2.37}$$

for any $(\mathbf{Q}, \mathbf{u}) \in L^2(\Omega, \mathcal{Q}_B) \times H^1(\Omega, \mathbb{R}^3)$. □

Remark 18 We Observe that $L^2(\Omega, \mathcal{Q}_B)$ coincides with $\overline{co}(L^2(\Omega, \mathcal{Q}_{Fr}))$, the closed convex hull of $L^2(\Omega, \mathcal{Q}_{Fr})$. The constructions contained in Step 1, Step 2 and Step 3 suggest that it is possible to approximate constant and piecewise-constant biaxial matrices in $L^2(\Omega, \mathcal{Q}_B)$ with weakly convergent sequences of tensor fields ranging in $\mathcal{Q}_{Fr}$ (see also [40, Thm.3 pag. 140]). Hence, we have

$$L^2(\Omega, \mathcal{Q}_B) \subseteq \overline{co}\big(L^2(\Omega, \mathcal{Q}_{Fr})\big).$$

The opposite inclusion is trivial because $L^2(\Omega, \mathcal{Q}_B)$ is closed, convex and contains $L^2(\Omega, \mathcal{Q}_{Fr})$ by definition. Then, since $L^2(\Omega, \mathcal{Q}_{Fr}) \subset L^2(\Omega, \mathcal{Q}_U) \subset L^2(\Omega, \mathcal{Q}_B)$, it also follows that $\overline{co}(L^2(\Omega, \mathcal{Q}_U)) = L^2(\Omega, \mathcal{Q}_B)$.

Remark 19 (Boundary conditions) From the previous construction it is clear that relaxation results can be obtained also with slightly different boundary conditions for the displacement $\mathbf{u}$, as shown in the following corollary.

Corollary 4 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, let $\Gamma_u \subseteq \partial\Omega$ be an open subset with positive surface measure, $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$ and f_{mec} as in (2.1.1). Define (here X stands either for Fr, U or B)*

$$\mathrm{F}^{\Gamma_u,g}_{mec,X}(\mathbf{Q}, \mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u}) dx & \text{on } L^2(\Omega, \mathcal{Q}_X) \times H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{g}, \\ +\infty & \text{otherwise in } L^2(\Omega, \mathbb{M}^{3\times 3}) \times H^1(\Omega, \mathbb{R}^3). \end{cases}$$

Then, the relaxation of $\mathrm{F}^{\Gamma_u,g}_{mec,X}$ in the sense of σ (see (3.2.1)) is $\mathrm{F}^{\Gamma_u,g}_{mec,B}$.

Proof. The same proof of Theorem 15 works also for this case, because the trace of the vector field $\mathbf{u}_n$ defined in Paragraph 3.2.1-Step 2 is equal to the trace of $\mathbf{u}$ for every $n \in \mathbb{N}$. $\square$

3.2.2 Relaxation of energies of incompressible elastomers

We show that the result of Theorem 15 can be extended to the case of incompressible materials, where we formally assign $\lambda = +\infty$, that is an infinite penalization if the displacement $\mathbf{u}$ is not divergence-free.

Theorem 16 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain. Let f_{mec} as in* (2.1.1) *and define (here X stands either for Fr, U or B)*

$$\mathcal{F}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } L^2(\Omega,\mathcal{Q}_X)\times H^1(\Omega,\mathbb{R}^3), \operatorname{div}\mathbf{u}=0,\\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3).\end{cases}$$

Then, the relaxation of $\mathcal{F}_{mec,X}$ in the sense of σ (see (3.2.1)) is $\mathcal{F}_{mec,B}$.

Proof. Again, if $X = B$ there is nothing to prove. We postpone the discussion of the case $X = U$ to Paragraph 3.2.4. In the case when $X = Fr$, the proof is essentially based on an argument due to Braides[8] and largely employed also in Chapter 2. We prove that $\overline{\mathcal{F}}_{mec,Fr} = \mathcal{F}_{mec,B}$ by showing two inequalities. The same argument that proves that $\mathrm{F}_{mec,B} \le \overline{\mathrm{F}}_{mec,Fr}$, yields also that $\mathcal{F}_{mec,B} \le \overline{\mathcal{F}}_{mec,Fr}$. We are left with the opposite inequality. For convenience, we label with $\mathrm{F}^\lambda_{mec,X}$ the functional introduced in (3.2.4) i.e.

$$\mathrm{F}^\lambda_{mec,X}(\mathbf{Q},\mathbf{u}) := \begin{cases} \displaystyle\int_\Omega \Big(\mu|\mathbb{E}(\nabla\mathbf{u})-\gamma\mathbf{Q}|^2 + \frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2\Big)dx & \text{on } L^2(\Omega,\mathcal{Q}_X)\times H^1(\Omega,\mathbb{R}^3),\\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3),\end{cases}$$

where X stands either for Fr, U or B. Therefore, the relaxation of $\mathrm{F}^\lambda_{mec,X}$ in the sense of σ is $\mathrm{F}^\lambda_{mec,B}$. We want to show that $\overline{\mathcal{F}}_{mec,Fr}$ is the Gamma-limit of the sequence of functionals $\mathrm{F}^\lambda_{mec,X}$ as $\lambda \to +\infty$. We extract a countable subsequence $\{\lambda_h\}$ such that $\lambda_h \to +\infty$. We claim that

$$\Gamma\text{-}\lim_{h\to+\infty} \mathrm{F}^{\lambda_h}_{mec,Fr}(\mathbf{Q},\mathbf{u}) = \sup_h \overline{\mathrm{F}}^{\lambda_h}_{mec,Fr}(\mathbf{Q},\mathbf{u}) = \sup_h \mathrm{F}^{\lambda_h}_{mec,B}(\mathbf{Q},\mathbf{u}) = \mathcal{F}_{mec,B}(\mathbf{Q},\mathbf{u}). \tag{3.2.38}$$

The first equality in (3.2.38) follows from Proposition 2, the second equality is due to Theorem 15 and the last equality is an application of Beppo-Levi theorem for monotone sequences of integrals:

$$\lim_{h\to+\infty}\Big(\mu|\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}|^2 + \frac{\lambda_h}{2}(\operatorname{tr}\mathbf{F})^2\Big) = \begin{cases} \mu|\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}|^2 & \text{if } \operatorname{tr}\mathbf{F}=0\\ +\infty & \text{otherwise.}\end{cases}$$

Now, if $\operatorname{div}\mathbf{u} \neq 0$ or $\mathbf{Q} \notin L^2(\Omega,\mathcal{Q}_B)$, the inequality $\overline{\mathcal{F}}_{mec,Fr} \le \mathcal{F}_{mec,B}$ is trivial. Thus, in what follows, we assume $\mathbf{u} \in H^1(\Omega,\mathbb{R}^3)$ with $\operatorname{div}\mathbf{u} = 0$ and $\mathbf{Q} \in L^2(\Omega,\mathcal{Q}_B)$. Since the Gamma-convergence is metrizable, we prove that for any sequence $\{\mathbf{Q}_h, \mathbf{u}_h\} \subset L^2(\Omega, \mathcal{Q}_{Fr}) \times H^1(\Omega, \mathbb{R}^3)$ such that (see (3.2.2) for an example of this notation)

$$\mathbf{Q}_h, \mathbf{u}_h \stackrel{\sigma}{\rightharpoonup} \mathbf{Q}, \mathbf{u} \quad \text{as } h \to +\infty, \tag{3.2.39}$$

there exists a sequence $\mathbf{z}_h \rightharpoonup \mathbf{u}$ w-$H^1(\Omega, \mathbb{R}^3)$ with $\operatorname{div} \mathbf{z}_h = 0$ such that

$$\overline{\mathcal{F}}_{mec,Fr}(\mathbf{Q}, \mathbf{u}) \le \liminf_{h\to+\infty} \mathcal{F}_{mec,Fr}(\mathbf{Q}_h, \mathbf{z}_h) \le \liminf_{h\to+\infty} \mathrm{F}^{\lambda_h}_{mec,Fr}(\mathbf{Q}_h, \mathbf{u}_h). \tag{3.2.40}$$

Thanks to (3.2.38) and Remark 19 (Corollary 4) we have

$$\mathcal{F}_{mec,B}(\mathbf{Q}, \mathbf{u}) = \inf\big\{\liminf_{h\to+\infty} \mathrm{F}^{\lambda_h}_{mec,Fr}(\mathbf{Q}_h, \mathbf{u}_h), \mathbf{Q}_h, \mathbf{u}_h \stackrel{\sigma}{\rightharpoonup} \mathbf{Q}, \mathbf{u}\big\} = \tag{3.2.41}$$

$$\inf\big\{\liminf_{h\to+\infty} \mathrm{F}^{\lambda_h}_{mec,Fr}(\mathbf{Q}_h, \mathbf{u}_h), \mathbf{Q}_h, \mathbf{u}_h \stackrel{\sigma}{\rightharpoonup} \mathbf{Q}, \mathbf{u}, \text{with } \mathbf{u}_h - \mathbf{u} \in H^1_o(\Omega, \mathbb{R}^3)\big\}.$$

Now, for any $h \in \mathbb{N}$, let $\mathbf{w}_h(x)$ be a solution to the following problem (see Proposition 1 with $p = 2, n = 3$)

$$\begin{cases} \mathbf{w}_h \in H^{1,p}_o(\Omega, \mathbb{R}^n), \\ \operatorname{div} \mathbf{w}_h = \operatorname{div} \mathbf{u}_h = \operatorname{div} (\mathbf{u}_h - \mathbf{u}), \\ \|\mathbf{w}_h\|_{H^{1,p}(\Omega,\mathbb{R}^n)} \le C_b(\Omega, n, p) \|\operatorname{div} \mathbf{u}_h\|_{L^p(\Omega)}. \end{cases}$$

Since $\mathcal{F}_{mec,B}(\mathbf{Q}, \mathbf{u}) < +\infty$ we may suppose to take sequences in (3.2.40) such that

$$\mathrm{F}^{\lambda_h}_{mec,Fr}(\mathbf{Q}_h, \mathbf{u}_h) \le Const \quad \forall\, h \in \mathbb{N},$$

so that $\|\operatorname{div} \mathbf{u}_h\|^2_{L^2} \le Const/\lambda_h$ and $\lim_{h\to\infty} \|\operatorname{div} \mathbf{u}_h\|_{L^2(\Omega)} = 0$, and hence

$$\mathbf{w}_h \to 0 \quad s\text{-}H^1(\Omega, \mathbb{R}^3) \text{ as } h \to \infty. \tag{3.2.42}$$

Thus, if we define $\mathbf{z}_h := \mathbf{u}_h - \mathbf{w}_h$ we have

$$\mathbf{z}_h \rightharpoonup \mathbf{u} \ w\text{-}H^1(\Omega, \mathbb{R}^3),\ \mathbf{z}_h - \mathbf{u}_h \in H^1_o(\Omega, \mathbb{R}^3), \quad \text{and } \operatorname{div} \mathbf{z}_h = 0. \tag{3.2.43}$$

We conclude by computing

$$\liminf_{h\to+\infty} \mathcal{F}_{mec,Fr}(\mathbf{Q}_h, \mathbf{z}_h) = \liminf_{h\to+\infty} \int_\Omega \mu |\mathbb{E}(\nabla \mathbf{z}_h) - \gamma \mathbf{Q}_h|^2 dx \le$$

$$\liminf_{h\to+\infty} \int_\Omega \mu |\mathbb{E}(\nabla \mathbf{u}_h) - \gamma \mathbf{Q}_h|^2 dx + \lim_{h\to+\infty} \Big| \int_\Omega \mu \Big(|\mathbb{E}(\nabla \mathbf{z}_h) - \gamma \mathbf{Q}_h|^2 - |\mathbb{E}(\nabla \mathbf{u}_h) - \gamma \mathbf{Q}_h|^2 \Big) dx \Big|$$

$$= \liminf_{h\to+\infty} \int_\Omega \mu |\mathbb{E}(\nabla \mathbf{u}_h) - \gamma \mathbf{Q}_h|^2 dx + 0 \le \liminf_{h\to+\infty} \mathrm{F}^{\lambda_h}_{mec,Fr}(\mathbf{Q}_h, \mathbf{u}_h). \tag{3.2.44}$$

We stress that (3.2.44) follows because

$$\Big| \int_\Omega \Big(|\mathbb{E}(\nabla \mathbf{u}_h) - \gamma \mathbf{Q}_h|^2 - |\mathbb{E}(\nabla \mathbf{z}_h) - \gamma \mathbf{Q}_h|^2 \Big) dx \Big| \tag{3.2.45}$$

$$\le \int_\Omega \Big| |\mathbb{E}(\nabla \mathbf{u}_h) - \gamma \mathbf{Q}_h|^2 - |\mathbb{E}(\nabla \mathbf{z}_h) - \gamma \mathbf{Q}_h|^2 \Big| dx \stackrel{h\to\infty}{\longrightarrow} 0,$$

since $\mathbf{w}_h = \mathbf{u}_h - \mathbf{z}_h$ and thanks to (3.2.42). □

Remark 20 The result above holds also with slightly different boundary conditions, as shown in the next corollary.

Corollary 5 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, $\Gamma_u \subseteq \partial\Omega$ an open subset with positive surface measure and $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$ with $\operatorname{div}\mathbf{g}(x) = 0$ a.e. in Ω. Let f_{mec} as in (2.1.1) and define for $X = Fr, U, B$*

$$\mathcal{F}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } L^2(\Omega,\mathcal{Q}_X) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \operatorname{div}\mathbf{u} = 0, \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times 3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Then, the relaxation of $\mathcal{F}^{\Gamma_u,g}_{mec,X}$ in the sense of σ (see (3.2.1)) is $\mathcal{F}^{\Gamma_u,g}_{mec,B}$.

Proof. To start, let $\Gamma_u \equiv \partial\Omega$ and $\mathbf{g} \equiv 0$. In this case the result is immediate by taking $\mathbf{u} \in H^1_o(\Omega,\mathbb{R}^3)$ in the proof of Theorem 16. Then, the general case follows from a standard argument, since we have

$$\mathcal{F}_{mec,Fr}(\mathbf{Q},\mathbf{u}) \leq \mathcal{F}^{\Gamma_u,g}_{mec,Fr}(\mathbf{Q},\mathbf{u}) \leq \mathcal{F}^{\partial\Omega,\widehat{g}}_{mec,Fr}(\mathbf{Q},\mathbf{u}), \tag{3.2.46}$$

where $\widehat{\mathbf{g}} \equiv \mathbf{u}$. If we relax all the functionals in (3.2.46), we obtain that the relaxation of $\mathcal{F}^{\Gamma_u,g}_{mec,Fr}$ is equal to $\mathcal{F}_{mec,B}$ if $(\mathbf{Q},\mathbf{u}) \in L^2(\Omega,\mathcal{Q}_B) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \operatorname{div}\mathbf{u} = 0$ and $+\infty$ otherwise in $L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3)$, because the set $L^2(\Omega,\mathcal{Q}_B) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \operatorname{div}\mathbf{u} = 0$ is closed in σ (this is a property of the relaxation). □

3.2.3 Gamma-convergence theorem

Theorem 17 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, let $\Gamma_u \subseteq \partial\Omega$ be an open subset with positive surface measure and $\mathbf{g}(x) \in H^1(\Omega,\mathbb{R}^3)$ with $\operatorname{div}\mathbf{g}(x) = 0$ a.e. in Ω. Let f_{mec} as in (2.1.1) and (here X stands either for Fr, U or B)*

$$\mathcal{F}_{\varepsilon,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx & \text{on } H^1(\Omega,\mathcal{Q}_X) \times H^1(\Omega,\mathbb{R}^3), \operatorname{div}\mathbf{u} = 0 \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3) \end{cases}$$

and

$$\mathcal{F}^{\Gamma_u,g}_{\varepsilon,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx \\ \qquad \text{on } H^1(\Omega,\mathcal{Q}_X) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \operatorname{div}\mathbf{u} = 0 \\ +\infty \qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Then

$$\Gamma(\sigma)\text{-}\lim_{\varepsilon\to 0} \mathcal{F}_{\varepsilon,X} = \mathcal{F}_{mec,B} \tag{3.2.47}$$

and

$$\Gamma(\sigma)\text{-}\lim_{\varepsilon\to 0} \mathcal{F}^{\Gamma_u,g}_{\varepsilon,X} = \mathcal{F}^{\Gamma_u,g}_{mec,B}, \tag{3.2.48}$$

where $\mathcal{F}_{mec,B}$ and $\mathcal{F}^{\Gamma_u,g}_{mec,B}$ are defined in Theorem 16 and Corollary 5 and σ is defined in (3.2.1).

Proof. We start by proving (3.2.48) in the case $X = Fr$. We use the characterization of the Gamma-limit of a sequence of functionals involving the *liminf* and *limsup* inequality (here in the version of Gamma-*limsup* inequality), see [22], [7]. Notice that if $\mathbf{Q} \notin L^2(\Omega, \mathcal{Q}_B)$, then there is nothing to prove. Let $\{\varepsilon_j\}$ be a countable sequence such that $\varepsilon_j \to 0$ as $j \to +\infty$.

Liminf inequality. We show that $\forall \{\mathbf{Q}_j, \mathbf{u}_j\} \subset L^2(\Omega, \mathcal{Q}_B) \times H^1(\Omega, \mathbb{R}^3)$, such that

$$\mathbf{Q}_j, \mathbf{u}_j \stackrel{\sigma}{\rightharpoonup} \mathbf{Q}, \mathbf{u} \quad \text{as } j \to +\infty, \tag{3.2.49}$$

(see (3.2.2) for an explanation of this notation) we have $\mathcal{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q}, \mathbf{u}) \leq \liminf_j \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q}_j, \mathbf{u}_j)$. To start, we can restrict our attention to sequences along which the functional is finite, and, passing to subsequences (not re-labelled), uniformly bounded by some positive constant C. We have

$$\liminf_{j\to+\infty} \int_\Omega \mu \left|\mathbb{E}(\nabla \mathbf{u}_j) - \gamma \mathbf{Q}_j\right|^2 dx \leq \liminf_{j\to+\infty} \int_\Omega \left(\varepsilon_j^2 |\nabla \mathbf{Q}_j|^2 + \mu \left|\mathbb{E}(\nabla \mathbf{u}_j) - \gamma \mathbf{Q}_j\right|^2\right) dx \leq C.$$

By weak convergence, Korn's theorem and the properties of the trace we easily see that the limit functional is finite over the set $L^2(\Omega, \mathcal{Q}_B) \times H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{g}(x), \operatorname{div} \mathbf{u} = 0$. By invoking the relaxation result of Corollary 5, the claim follows.

Limsup inequality. In this paragraph we find it convenient to introduce the Γ-limsup in the form

$$\Gamma\text{-}\limsup_{j\to+\infty} \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q}, \mathbf{u}) = \inf\left\{\limsup_{j\to+\infty} \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q}_j, \mathbf{u}_j),\ \mathbf{Q}_j, \mathbf{u}_j \stackrel{\sigma}{\rightharpoonup} \mathbf{Q}, \mathbf{u}\right\},$$

where $\{\mathbf{Q}_j, \mathbf{u}_j\} \subset L^2(\Omega, \mathcal{Q}_B) \times H^1(\Omega, \mathbb{R}^3)$. If $\mathbf{u} \notin \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{g}(x), \operatorname{div} \mathbf{u} = 0\}$, then the claim is obtained by taking the trivial recovery sequence $\widehat{\mathbf{Q}}_j \equiv \mathbf{Q}, \widehat{\mathbf{u}}_j \equiv \mathbf{u}$. Now, let us assume for a moment $(\mathbf{Q}, \mathbf{u}) \in H^1(\Omega, \mathcal{Q}_{Fr}) \times H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{g}(x)$, $\operatorname{div} \mathbf{u} = 0$ and take the trivial recovery sequence $\widehat{\mathbf{Q}}_j \equiv \mathbf{Q}, \widehat{\mathbf{u}}_j \equiv \mathbf{u}$. We have

$$\Gamma\text{-}\overline{\lim_{j\to\infty}} \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q}, \mathbf{u}) \leq \overline{\lim_{j\to\infty}} \int_\Omega \left(\varepsilon_j^2 |\nabla \widehat{\mathbf{Q}}_j|^2 + f_{mec}(\widehat{\mathbf{Q}}_j, \nabla \widehat{\mathbf{u}}_j)\right) dx = \int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u}) dx \tag{3.2.50}$$

By Lemma 3, for every $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_{Fr})$ there exists a sequence $\{\mathbf{Q}_k\} \subset H^1(\Omega, \mathcal{Q}_{Fr})$ such that

$$\mathbf{Q}_k \to \mathbf{Q} \ \ s\text{-}L^2(\Omega, \mathbb{M}^{3\times 3}) \quad \text{as } k \to \infty,$$

and plugging $\mathbf{Q}_k$ instead of $\mathbf{Q}$ in (3.2.50), we have

$$\Gamma\text{-}\limsup_{j\to+\infty} \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q}_k, \mathbf{u}) \leq \int_\Omega \mu \left|\mathbb{E}(\nabla \mathbf{u}) - \gamma \mathbf{Q}_k\right|^2 dx \tag{3.2.51}$$

for every $k \in \mathbb{N}$. Recalling that the Gamma-limsup is a lower semicontinuous functional[22] and that the integral on the right hand side of (3.2.51) is continuous in the strong $L^2(\Omega, \mathbb{M}^{3\times 3})$-topology, we have

$$\Gamma\text{-}\limsup_{j\to+\infty} \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q},\mathbf{u}) \le \liminf_{k\to+\infty}\Big(\Gamma\text{-}\limsup_{j\to+\infty} \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q}_k,\mathbf{u})\Big) \le \int_\Omega \mu|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}_k|^2 dx \overset{k\to\infty}{\longrightarrow} \int_\Omega \mu|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}|^2 dx. \tag{3.2.52}$$

Summarizing, for every $(\mathbf{Q},\mathbf{u}) \in L^2(\Omega, \mathbb{M}^{3\times 3}) \times H^1(\Omega, \mathbb{R}^3)$ we have

$$\Gamma\text{-}\limsup_{j\to+\infty} \mathcal{F}^{\Gamma_u,g}_{Fr,\varepsilon_j}(\mathbf{Q},\mathbf{u}) \le \mathcal{F}^{\Gamma_u,g}_{mec,Fr}(\mathbf{Q},\mathbf{u}), \tag{3.2.53}$$

and to conclude it is sufficient to relax both sides by applying Corollary 5.
The proof of (3.2.47) in the case $X = Fr$ follows as above.
Then, considering the case $X = B$, the proof of (3.2.48) (and of (3.2.47)) is even easier. The *liminf* inequality becomes trivial, and the *limsup* inequality can be modified as follows. We observe that the proof for the Frank model is based on the approximaton of $L^2(\Omega, \mathcal{Q}_{Fr})$-tensors with $H^1(\Omega, \mathcal{Q}_{Fr})$-tensors in the strong L^2-topology. In the biaxial case, the result follows by approximating $L^2(\Omega, \mathcal{Q}_B)$-tensors with biaxial Lipschitz continuous tensors in the strong L^2-topology by applying Proposition 11. The remaining case $X = U$ is discussed in Paragraph 3.2.4. □

The Gamma-convergence result holds also if we remove the constraint on the divergence of $\mathbf{u}$, as shown in the next corollary.

Corollary 6 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, let $\Gamma_u \subseteq \partial\Omega$ be an open subset with positive surface measure and $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$. Let f_{mec} as in* (2.1.1)*. Define (here X stands either for Fr, U or B)*

$$\mathrm{F}_{\varepsilon,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx & \text{on } H^1(\Omega,\mathcal{Q}_X) \times H^1(\Omega,\mathbb{R}^3), \\ +\infty & \text{other. in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3), \end{cases}$$

$$\mathrm{F}^{\Gamma_u,g}_{\varepsilon,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx & \text{on } H^1(\Omega,\mathcal{Q}_X) \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3) + \mathbf{g}(x), \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3}) \times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Then

$$\Gamma(\sigma)\text{-}\lim_{\varepsilon\to0} \mathrm{F}_{\varepsilon,X} = \mathrm{F}_{mec,B}, \tag{3.2.54}$$

and

$$\Gamma(\sigma)\text{-}\lim_{\varepsilon\to0} \mathrm{F}^{\Gamma_u,g}_{\varepsilon,X} = \mathrm{F}^{\Gamma_u,g}_{mec,B}, \tag{3.2.55}$$

where $\mathrm{F}_{mec,B}$ and $\mathrm{F}^{\Gamma_u,g}_{mec,B}$ are defined in Theorem 15 *and Corollary* 4*.*

Proof. This result follows as in the proof of Theorem 17. The only point is that we do not have to take sequences of displacements with divergence equal to zero. □

3.2.4 Uniaxial models

We show how to obtain the relaxations and Gamma-convergence results for the uniaxial model $X = U$. Recalling that $\mathcal{Q}_{Fr} \subset \mathcal{Q}_U \subset \mathcal{Q}_B$ (and also that $L^2(\Omega, \mathcal{Q}_{Fr}) \subset L^2(\Omega, \mathcal{Q}_U) \subset L^2(\Omega, \mathcal{Q}_B)$), it easily follows that

$$\mathrm{F}_{mec,B} \leq \mathrm{F}_{mec,U} \leq \mathrm{F}_{mec,Fr}, \quad \mathcal{F}_{mec,B} \leq \mathcal{F}_{mec,U} \leq \mathcal{F}_{mec,Fr}, \tag{3.2.56}$$

where all the functionals above are defined in Theorem 15 and 16 respectively. Now, taking the relaxation of all the functionals in (3.2.56) we have

$$\mathrm{F}_{mec,B} \quad = \overline{\mathrm{F}}_{mec,B} \leq \overline{\mathrm{F}}_{mec,U} \leq \overline{\mathrm{F}}_{mec,Fr} = \quad \overline{\mathrm{F}}_{mec,B}. \tag{3.2.57}$$

$$\mathcal{F}_{mec,B} \quad = \overline{\mathcal{F}}_{mec,B} \leq \overline{\mathcal{F}}_{mec,U} \leq \overline{\mathcal{F}}_{mec,Fr} = \quad \overline{\mathcal{F}}_{mec,B}, \tag{3.2.58}$$

This shows that the relaxation of $\mathrm{F}_{mec,U}$ and $\mathcal{F}_{mec,U}$ is $\mathrm{F}_{mec,B}$ and $\mathcal{F}_{mec,B}$ respectively. Analogously, we obtain $\overline{\mathrm{F}}^{\Gamma_u,g}_{mec,U} = \mathrm{F}^{\Gamma_u,g}_{mec,B}$ and $\overline{\mathcal{F}}^{\Gamma_u,g}_{mec,U} = \mathcal{F}^{\Gamma_u,g}_{mec,B}$ (these functionals are defined in Corollary 4 and 5 respectively) . The same chain of inequalities holds for the Gamma-limits (defined in Theorem 17)

$$\mathcal{F}_{mec,B} = \Gamma\text{-}\lim_{\varepsilon\to 0} \mathcal{F}_{B,\varepsilon} \leq \Gamma\text{-}\liminf_{\varepsilon\to 0} \mathcal{F}_{U,\varepsilon} \leq \Gamma\text{-}\limsup_{\varepsilon\to 0} \mathcal{F}_{U,\varepsilon} \leq \Gamma\text{-}\limsup_{\varepsilon\to 0} \mathcal{F}_{Fr,\varepsilon} = \mathcal{F}_{mec,B}$$

and we obtain that $\Gamma\text{-}\lim_{\varepsilon\to 0} \mathcal{F}_{U,\varepsilon} = \mathcal{F}_{mec,B}$. Analogously,

$$\Gamma\text{-}\lim_{\varepsilon\to 0} \mathcal{F}^{\Gamma_u,g}_{U,\varepsilon} = \mathcal{F}^{\Gamma_u,g}_{mec,B}, \quad \Gamma\text{-}\lim_{\varepsilon\to 0} \mathrm{F}_{U,\varepsilon} = \mathrm{F}_{mec,B}, \quad \Gamma\text{-}\lim_{\varepsilon\to 0} \mathrm{F}^{\Gamma_u,g}_{U,\varepsilon} = \mathrm{F}^{\Gamma_u,g}_{mec,B}. \tag{3.2.59}$$

3.2.5 Discussion

Physical interpretation. The results contained in Section 3.2 allow us to model engineering traction problems. Under the hypotheses of Theorem 15 and Corollary 4, we have

$$\inf_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathrm{F}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \min_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathrm{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q},\mathbf{u}), \tag{3.2.60}$$

and, under the hypotheses of Theorem 16 and Corollary 5,

$$\inf_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathcal{F}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \min_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathcal{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q},\mathbf{u}). \tag{3.2.61}$$

The infimum on the left hand side of (3.2.60) or (3.2.61) may not be attained in the case where $X = Fr$ or U, because $L^2(\Omega, \mathcal{Q}_{Fr})$ and $L^2(\Omega, \mathcal{Q}_U)$ are not weakly closed. We show that the right hand side is a minimum. Consider (3.2.60). The functional $\mathrm{F}^{\Gamma_u,g}_{mec,B}$ is weakly lower semicontinuous because the function $(\mathbf{Q},\mathbf{u}) \mapsto \mu|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}|^2 + \frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2$ is convex. Since $\mathcal{Q}_B$ is a compact subset of $\mathbb{M}^{3\times3}$, the L^2-norm of $\mathbf{Q}$ is bounded. Therefore, also the L^2-norm of the symmetric part of the gradient of $\mathbf{u}$ is bounded. Korn's second inequality and Poincaré inequality yield the control of the H^1-norm of $\mathbf{u}$.

Then, the minimum in (3.2.61) is attained essentially for the same reason. We have only to take sequences of displacements with divergence equal to zero, which is equivalent to study minimization problems for the functional with the penalty $+\infty$ if $\operatorname{div}\mathbf{u} \neq 0$. In that case we have to take $\mathbf{g}(x)$ with $\operatorname{div}\mathbf{g}(x) = 0$ a.e. in Ω. The divergence is a linear operator, and hence the constraint on the divergence is weakly closed.

Moreover, we remark that, letting $\mathbf{E} = \mathcal{E}(\mathbf{F})$, the function $(\mathbf{Q}, \mathbf{E}) \mapsto |\mathbf{E} - \gamma\mathbf{Q}|^2$ with $\mathbf{Q} \in \mathcal{Q}_B$ is convex, but not strictly convex. On the other hand, $\mathbf{Q} \mapsto |\mathbf{E} - \gamma\mathbf{Q}|^2$, with $\mathbf{E} \in \mathbb{M}^{3\times3}$ and $\mathbf{E} \mapsto |\mathbf{E} - \gamma\mathbf{Q}|^2$, with $\mathbf{Q} \in \mathcal{Q}_B$ are two strictly convex functions. These observations are applied in what follows.

The relaxation of the *macroscopic* models of Chapter 2. In this section we want to relate the Gamma-convergence results of Section 3.2 to the relaxation of the non-convex models f_X (where X stands, in particular, for Fr or U) describing the order-strain interaction in nematic elastomers and discussed in Chapter 2.

Properties of the Gamma-limit $\mathcal{F}^{\Gamma_u,g}_{mec,B}$ and of the macroscopic model $\mathcal{J}_B^{\Gamma_u,g}$. We show the relation between $\mathcal{F}^{\Gamma_u,g}_{mec,B}$ and $\mathcal{J}_B^{\Gamma_u,g}$. We start by manipulating (3.2.61):

$$\min_{\substack{L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q},\mathbf{u}) = \inf_{\mathbf{Q}\in L^2(\Omega,\mathcal{Q}_B)} \min_{\substack{\mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}(x),\\ \operatorname{div}\mathbf{u}=0}} \int_\Omega \mu|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}|^2 dx \tag{3.2.62}$$

$$= \inf_{\substack{\mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}(x),\\ \operatorname{div}\mathbf{u}=0}} \min_{\mathbf{Q}\in L^2(\Omega,\mathcal{Q}_B)} \int_\Omega \mu|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}|^2 dx = \tag{3.2.63}$$

$$\inf_{\substack{\mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}(x),\\ \operatorname{div}\mathbf{u}=0}} \mu\, dist^2_{L^2}\Big(\mathbb{E}(\nabla\mathbf{u}), \gamma L^2(\Omega,\mathcal{Q}_B)\Big).$$

The minimization problem

$$\min_{\mathbf{Q}\in L^2(\Omega,\mathcal{Q}_B)} \int_\Omega \mu|\mathbb{E}(\nabla\mathbf{u}) - \gamma\mathbf{Q}|^2 dx, \tag{3.2.64}$$

has a unique solution equal to $\pi^{L^2(\Omega,\mathcal{Q}_B)}\big(\mathbb{E}(\nabla\mathbf{u})/\gamma\big)$ for any $\mathbf{u} \in H^1(\Omega,\mathbb{R}^3)$. Thanks to Proposition 10 and Eq. (3.1.4) we have

$$\mu\, dist^2_{L^2}\Big(\mathbb{E}(\nabla\mathbf{u}), L^2(\Omega,\gamma\mathcal{Q}_B)\Big) = \mu\int_\Omega dist^2\big(\mathbb{E}(\nabla\mathbf{u}), \gamma\mathcal{Q}_B\big)dx. \tag{3.2.65}$$

Summarizing, we obtain

$$\min_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathcal{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q},\mathbf{u}) = \inf_{H^1(\Omega,\mathbb{R}^3)} \mathcal{J}_B^{\Gamma_u,g}(\mathbf{u}), \tag{3.2.66}$$

and the infimum in (3.2.66)-right is indeed a minimum, by convexity. Concretely, we bring the minimization over $L^2(\Omega, \mathcal{Q}_B)$ (3.2.63) *inside* the integral and we transform it into a pointwise minimization in the space of matrices. Furthermore, let us define $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ a minimizer of (3.2.66)-left and $\overline{\overline{\mathbf{u}}}$ a minimizer of (3.2.66)-right. Therefore, we can write

$$\mu\|\mathbb{E}(\nabla\overline{\mathbf{u}}) - \gamma\overline{\mathbf{Q}}\|^2_{L^2(\Omega,\mathbb{M}^{3\times 3})} = \mathcal{F}^{\Gamma_u,g}_{mec,B}(\overline{\mathbf{Q}}, \overline{\mathbf{u}}) = \mathcal{J}^{\Gamma_u,g}_B(\overline{\overline{\mathbf{u}}}) = \mu\int_\Omega \left|\mathbb{E}(\nabla\overline{\overline{\mathbf{u}}}) - \gamma\overline{\overline{\mathbf{Q}}}\right|^2 dx \quad (3.2.67)$$

where $\overline{\overline{\mathbf{Q}}} := \pi^{\mathcal{Q}_B}(\mathbb{E}(\nabla\overline{\overline{\mathbf{u}}})/\gamma)$. This yields an interesting interpretation for the minimizers of the problem (3.2.66). Notice that the minimizer $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ may be not unique since $\mathcal{F}^{\Gamma_u,g}_{mec,B}$ is not strictly convex in the pair $(\mathbf{Q}, \mathbf{u})$. Anyway, once $\overline{\mathbf{u}}$ is given, then $\overline{\mathbf{Q}}$ is uniquely determined as $\overline{\mathbf{Q}} = \pi^{\mathcal{Q}_B}(\mathbb{E}(\nabla\overline{\mathbf{u}})/\gamma)$. Analogously, since $\mathcal{J}^{\Gamma_u,g}_B$ is not strictly convex, the minimizer $\overline{\overline{\mathbf{u}}}$ may be not unique. As above, the optimal microstructure $\overline{\overline{\mathbf{Q}}}$ in (3.2.67)-right is uniquely determined since it is precisely equal to $\overline{\overline{\mathbf{Q}}} = \pi^{\mathcal{Q}_B}(\mathbb{E}(\nabla\overline{\overline{\mathbf{u}}})/\gamma)$. Hence, if $\overline{\mathbf{u}} = \overline{\overline{\mathbf{u}}}$ a.e. in Ω, then $\overline{\mathbf{Q}} = \overline{\overline{\mathbf{Q}}}$. It is obvious that, if $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ minimizes (3.2.66)-left and $(\overline{\overline{\mathbf{Q}}}, \overline{\overline{\mathbf{u}}})$ minimizes (3.2.66)-right, then it is also true that $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ minimizes (3.2.66)-right and $(\overline{\overline{\mathbf{Q}}}, \overline{\overline{\mathbf{u}}})$ minimizes (3.2.66)-left. This observation is useful in the remarkable case when $\Gamma_u = \partial\Omega$ and $\mathbf{g}(x) = \mathbf{F}(x - O)$ where O is the origin in $\mathbb{R}^3$ and $\mathbf{F} \in \mathbb{M}^{3\times 3}_0$. A solution to (3.2.66)-right is represented by the pair $\overline{\mathbf{u}}(x) = \mathbf{F}(x - O)$, $\overline{\mathbf{Q}}(x) = \pi^{\mathcal{Q}_B}(\mathbb{E}(\mathbf{F})/\gamma)$ in $\overline{\Omega}$. This holds because f_B satisfies a solenoidal quasiconvexification formula (see (2.2.34) in the trivial case $X = B$)

$$\int_\Omega f_B(\mathbf{F})dx \le \int_\Omega f_B(\mathbf{F} + \nabla\mathbf{w})dx \quad \forall\,\mathbf{w} \in H^1_o(\Omega, \mathbb{R}^3), \operatorname{div}\mathbf{w} = 0. \quad (3.2.68)$$

Hence, a possible minimizer of (3.2.66)-left is the pair

$$(\overline{\mathbf{Q}}, \overline{\mathbf{u}}) = \Big(\pi^{\mathcal{Q}_B}\big(\mathbb{E}(\mathbf{F})/\gamma\big), \mathbf{F}(x - O)\Big). \quad (3.2.69)$$

Analogous results hold also if we remove the constraint of incompressibility

$$\min_{L^2(\Omega,\mathbb{M}^{3\times 3})\times H^1(\Omega,\mathbb{R}^3)} \mathrm{F}^{\Gamma_u,g}_{mec,B}(\mathbf{Q}, \mathbf{u}) = \min_{H^1(\Omega,\mathbb{R}^3)} \mathrm{J}^{\Gamma_u,g}_{mec,B}(\mathbf{u}). \quad (3.2.70)$$

As above, we have the same characterization for the minimizers of (3.2.70). Then, taking $\mathbf{F} \in \mathbb{M}^{3\times 3}$ and $\mathbf{g}(x) = \mathbf{F}(x - O)$, a solution to (3.2.70)-right is represented by the pair $\mathbf{Q}(x) = \pi^{\mathcal{Q}_B}(\mathbb{E}(\mathbf{F})/\gamma)$, $\mathbf{u}(x) = \mathbf{F}(x - O)$ in $\overline{\Omega}$. In this case we can directly invoke convexity to show that the minimum of $\mathrm{F}^{\Gamma_u,g}_{mec,B}$ amongst functions in $H^1_o(\Omega, \mathbb{R}^3) + \mathbf{F}(x - O)$ is attained at $\mathbf{F}(x - O)$.

3.3 Small particles: asymptotics

We turn our attention to the asymptotic analysis for small particles. We show that any relaxation phenomenon is forbidden by the predominance of the curvature energy on the mechanical energy.

3.3.1 Gamma-convergence theorem

In this section the space $L^2(\Omega,\mathbb{M}^{3\times 3})\times H^1(\Omega,\mathbb{R}^3)$ is endowed with the strong-L^2 topology for the tensor field $\mathbf{Q}$ and the weak-H^1 topology for the variable $\mathbf{u}$ and we write

$$\sigma' := s\text{-}L^2(\Omega,\mathbb{M}^{3\times 3}) \times w\text{-}H^1(\Omega,\mathbb{R}^3). \tag{3.3.1}$$

Theorem 18 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, $\Gamma_u \subseteq \partial\Omega$ be an open subset with positive surface measure and $\mathbf{g}(x) \in H^1(\Omega,\mathbb{R}^3)$ with $\operatorname{div}\mathbf{g} = 0$. Let f_{mec} as in* (2.1.1)*, $\mathcal{F}_{\varepsilon,X}$, $\mathcal{F}^{\Gamma_u,g}_{\varepsilon,X}$ as in Theorem* 17 *where X stands either for Fr, U or B. Then*

$$\mathcal{G}_{mec,X} = \Gamma(\sigma')\text{-}\lim_{\varepsilon\to+\infty} \mathcal{F}_{\varepsilon,X} \tag{3.3.2}$$

and

$$\mathcal{G}^{\Gamma_u,g}_{mec,X} = \Gamma(\sigma')\text{-}\lim_{\varepsilon\to+\infty} \mathcal{F}^{\Gamma_u,g}_{\varepsilon,X}, \tag{3.3.3}$$

where

$$\mathcal{G}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } \{\mathbf{Q}\in\mathcal{Q}_X, const.\}\times H^1(\Omega,\mathbb{R}^3), \operatorname{div}\mathbf{u}=0,\\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times 3})\times H^1(\Omega,\mathbb{R}^3),\end{cases}$$

and

$$\mathcal{G}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \\ & \text{on } \{\mathbf{Q}\in\mathcal{Q}_X, const.\}\times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}(x), \operatorname{div}\mathbf{u}=0,\\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times 3})\times H^1(\Omega,\mathbb{R}^3).\end{cases}$$

Remark 21 We denote with

$$\{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X), \text{const.}\},\ \text{ where } X \text{ stands either for } Fr, U \text{ or } B, \tag{3.3.4}$$

a subset in the subspace of constant tensors endowed with the weak topology of H^1. It is closed in the weak topology of $H^1(\Omega,\mathbb{M}^{3\times 3})$ and in the strong topology of $L^2(\Omega,\mathbb{M}^{3\times 3})$.

Proof. We prove (3.3.3). As $\varepsilon\to+\infty$ we extract a countable subsequence $\{\varepsilon_j\}$ such that $\varepsilon_j\to+\infty$ as $j\to+\infty$. We characterize the Gamma-limit with the *liminf* and *limsup* inequality.

Liminf inequality. Given any $(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times 3})\times H^1(\Omega,\mathbb{R}^3)$, we have to show that

$$\mathcal{G}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) \le \liminf_{j\to+\infty} \mathcal{F}^{\Gamma_u,g}_{\varepsilon_j,X}(\mathbf{Q}_j,\mathbf{u}_j) \tag{3.3.5}$$

for every sequence

$$\mathbf{Q}_j\to\mathbf{Q}\ s\text{-}L^2(\Omega,\mathbb{M}^{3\times 3}),\quad \mathbf{u}_j\rightharpoonup\mathbf{u}\ w\text{-}H^1(\Omega,\mathbb{R}^3) \text{ as } j\to+\infty. \tag{3.3.6}$$

We suppose that the right-hand side of (3.3.5) is not identically infinite and, up to a subsequence, also uniformly bounded by some positive constant C, so that

$$\left\{ \quad \int_\Omega \varepsilon_j^2 |\nabla \mathbf{Q}_j|^2 dx, \quad \int_\Omega (C_2 |\mathbb{E}(\nabla \mathbf{u}_j)|^2 - C_1) dx \quad \right\} \qquad \leq \mathcal{F}^{\Gamma_u, g}_{\varepsilon_j, X}(\mathbf{Q}_j, \mathbf{u}_j) \leq C. \tag{3.3.7}$$

By Korn's and Poincaré inequalities, the properties of the trace, and noticing that $\int_\Omega |\nabla \mathbf{Q}_j|^2 dx \leq Const/\varepsilon_j^2 \to 0$ as $j \to +\infty$, it follows that

$$\mathbf{Q}_j \to \mathbf{Q} \ s\text{-}H^1(\Omega, \mathbb{M}^{3\times3}), \qquad \mathbf{u}_j \rightharpoonup \mathbf{u} \ w\text{-}H^1(\Omega, \mathbb{R}^3) \text{ as } j \to +\infty \tag{3.3.8}$$

to some constant tensor $\mathbf{Q}$. Hence, the set where the functional is finite is

$$\{\mathbf{Q} \in H^1(\Omega, \mathcal{Q}_X), \text{const.}\} \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{g}(x), \operatorname{div} \mathbf{u} = 0\}. \tag{3.3.9}$$

Then, we have

$$\liminf_{j\to+\infty} \int_\Omega |\mathbb{E}(\nabla \mathbf{u}_j) - \gamma \mathbf{Q}_j|^2 dx \leq \liminf_{j\to+\infty} \int_\Omega \Big(\varepsilon_j^2 |\nabla \mathbf{Q}_j|^2 + |\mathbb{E}(\nabla \mathbf{u}_j) - \gamma \mathbf{Q}_j|^2 \Big) dx \tag{3.3.10}$$

and the claim follows because the functional on the left-hand side is lower semicontinuous in the sense of σ'.

Limsup inequality. Given any $(\mathbf{Q}, \mathbf{u}) \in L^2(\Omega, \mathbb{M}^{3\times3}) \times H^1(\Omega, \mathbb{R}^3)$ we have to exhibit a sequence $\{\widehat{\mathbf{Q}}_j, \widehat{\mathbf{u}}_j\} \subset L^2(\Omega, \mathbb{M}^{3\times3}) \times H^1(\Omega, \mathbb{R}^3)$ such that

$$\widehat{\mathbf{Q}}_j \to \mathbf{Q} \ s\text{-}L^2(\Omega, \mathbb{M}^{3\times3}), \quad \widehat{\mathbf{u}}_j \rightharpoonup \mathbf{u} \ w\text{-}H^1(\Omega, \mathbb{R}^3) \text{ as } j \to +\infty, \tag{3.3.11}$$

and such that

$$\mathcal{G}^{\Gamma_u, g}_{mec, X}(\mathbf{Q}, \mathbf{u}) = \limsup_{j\to+\infty} \mathcal{F}^{\Gamma_u, g}_{\varepsilon_j, X}(\widehat{\mathbf{Q}}_j, \widehat{\mathbf{u}}_j). \tag{3.3.12}$$

To obtain the claim it is enough to take the trivial sequence $\{\widehat{\mathbf{Q}}_j, \widehat{\mathbf{u}}_j\} \equiv (\mathbf{Q}, \mathbf{u})$.
The proof of (3.3.2) is analogous. □

The previous Gamma-convergence result works also in the case of the compressible elastomers, as shown in the following corollary.

Corollary 7 *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain and $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$. Let $F_{\varepsilon,X}$ and $F^{\Gamma_u, g}_{\varepsilon,X}$ as in Corollary* 6*, f_{mec} as in* (2.1.1) *(here X stands either for Fr, U or B). Then*

$$\mathrm{G}_{mec,X} = \Gamma(\sigma')\text{-}\lim_{j\to+\infty} \mathrm{F}_{\varepsilon,X} \tag{3.3.13}$$

and

$$\mathrm{G}^{\Gamma_u, g}_{mec,X} = \Gamma(\sigma')\text{-}\lim_{j\to+\infty} \mathrm{F}^{\Gamma_u, g}_{\varepsilon,X} \tag{3.3.14}$$

where

$$\mathrm{G}_{mec,X}(\mathbf{Q}, \mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q}, \nabla \mathbf{u}) dx & \text{on } \{\mathbf{Q} \in H^1(\Omega, \mathcal{Q}_X), \text{const}\} \times H^1(\Omega, \mathbb{R}^3), \\ +\infty & \text{otherwise in } L^2(\Omega, \mathbb{M}^{3\times3}) \times H^1(\Omega, \mathbb{R}^3). \end{cases}$$

and

$$\mathrm{G}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx & \text{on } \{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),\text{const}\}\times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \\ +\infty & \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Proof. It is analogous to the proof of Theorem 18 for the case of incompressible rubbers. The only point is that it is not necessary to take sequences of divergence-free displacements. □

3.3.2 Discussion

We turn to the analysis of problem $\mathcal{P}_0$ (3.1.8) and of the phase diagrams of Section 1.5. We apply Theorem 18 obtaining

$$\min_{\substack{L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{G}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \inf_{\substack{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),\\ \text{const.}}} \min_{\substack{\mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)\\ +\mathbf{g},\operatorname{div}\mathbf{u}=0}} \int_\Omega \mu|\mathbb{E}(\nabla\mathbf{u})-\gamma\mathbf{Q}|^2dx. \tag{3.3.15}$$

We denote with $\overline{\mathbf{u}}$ the solution to the problem

$$\min_{\mathbf{u}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\operatorname{div}\mathbf{u}=0} \int_\Omega \mu|\mathbb{E}(\nabla\mathbf{u})-\gamma\mathbf{Q}|^2dx, \tag{3.3.16}$$

where $\mathbf{Q}$ is assigned in $H^1(\Omega,\mathcal{Q}_X)$ and constant. Notice that $\overline{\mathbf{u}}$ is unique by the strict convexity of the function $\mathbf{E}\mapsto|\mathbf{E}-\gamma\mathbf{Q}|^2$, where $\mathbf{E}=\mathbb{E}(\mathbf{F})$, $\mathbf{F}\in\mathbb{M}^{3\times3}_0$. Now, we introduce $\overline{\mathbf{E}}^{av}\in\mathbb{M}^{3\times3}_0$ the average in Ω of the tensor field $\mathbb{E}(\nabla\overline{\mathbf{u}})$, whose components $\overline{E}^{av}_{ij}$ are defined as [2]

$$\overline{E}^{av}_{ij} := \frac{1}{|\Omega|}\int_\Omega \big(\mathbb{E}(\nabla\overline{\mathbf{u}})\big)_{ij}\,dx \qquad \text{with } i,j\in\{1,2,3\} \tag{3.3.17}$$

and $\overline{\mathbf{E}}^{\sim}(x) := \mathbb{E}(\nabla\overline{\mathbf{u}})-\overline{\mathbf{E}}^{av}$. Notice that $\int_\Omega \overline{\mathbf{E}}^{\sim}(x)=0$ and that

$$\int_\Omega \big(\overline{\mathbf{E}}^{av}-\gamma\mathbf{Q}\big):\overline{\mathbf{E}}^{\sim}(x)dx=0, \tag{3.3.18}$$

since $\overline{\mathbf{E}}^{av}$ and $\mathbf{Q}$ are constant matrices. Hence, we can rewrite (3.3.16) as

$$\int_\Omega \mu|(\overline{\mathbf{E}}^{av}-\gamma\mathbf{Q})+\overline{\mathbf{E}}^{\sim}(x)|^2dx = \mu\int_\Omega\Big(|\overline{\mathbf{E}}^{av}-\gamma\mathbf{Q}|^2+|\overline{\mathbf{E}}^{\sim}(x)|^2\Big)dx. \tag{3.3.19}$$

Then, problem (3.3.15)-left can be formulated as follows:

$$\begin{aligned}\min_{\substack{L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{G}^{\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) &= \inf_{\substack{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),\\ \text{const.}}} \int_\Omega \mu|\overline{\mathbf{E}}^{av}-\gamma\mathbf{Q}|^2dx + \int_\Omega \mu|\overline{\mathbf{E}}^{\sim}(x)|^2dx \\ &= \mu\int_\Omega dist^2\big(\overline{\mathbf{E}}^{av},\gamma\mathcal{Q}_X\big)dx + \int_\Omega \mu|\overline{\mathbf{E}}^{\sim}(x)|^2dx. \end{aligned} \tag{3.3.20}$$

[2] again, we identify a constant matrix $\mathbf{E}(x)\in L^2(\Omega,\mathbb{M}^{3\times3}_{sym})$ with the matrix $\mathbf{E}\in\mathbb{M}^{3\times3}_{sym}$ itself

In order to obtain more precise results regarding engineering traction experiments, in the next paragraph we specify even further the boundary conditions.

Physical interpretation. Let $\Gamma_u = \partial\Omega$ and $\mathbf{g}(x) = \mathbf{F}(x - O)$ with $\mathbf{F} \in \mathbb{M}_0^{3\times3}$. Then, we can compute the unique minimizer of (3.3.16). Assume $\mathbf{Q} \in H^1(\Omega, \mathcal{Q}_X)$ and constant. Then

$$\int_\Omega \mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}|^2 dx \leq \int_\Omega \mu|\mathbb{E}(\mathbf{F} + \nabla\mathbf{w}) - \gamma\mathbf{Q}|^2 dx \ \forall\, \mathbf{w} \in H_o^1(\Omega, \mathbb{R}^3), \operatorname{div}\mathbf{w} = 0, \tag{3.3.21}$$

and $\overline{\mathbf{u}} = \mathbf{F}(x - O)$ for every x in $\overline{\Omega}$. Since $\overline{\mathbf{E}}^{\sim}(x) \equiv 0$, then (3.3.20) becomes ($\overline{\mathbf{E}} = \overline{\mathbf{E}}^{av}$)

$$\min_{L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)} \mathcal{G}_{mec,X}^{\partial\Omega,Fx}(\mathbf{Q}, \mathbf{u}) = \mu \int_\Omega dist^2\big(\overline{\mathbf{E}}, \gamma\mathcal{Q}_X\big) dx. \tag{3.3.22}$$

We can find solutions $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ of (3.3.22) *algebraically*, by minimizing $f_{mec}(\cdot, \cdot)$. We find the exact asymptotic expressions of the minimizers of f_{mec}, parameterized by the symmetric part of the boundary datum i.e. by $\mathbf{E} = \mathbb{E}(\mathbf{F})$. As a consequence, we obtain a rigorous justification of the particular solutions presented in the phase diagrams (Section 1.5).

Analogous results hold also for the case of the compressible elastomers. The proofs are even simpler because it is not necessary to impose the constraint on the the divergence of the displacement.

Comparison between the two different limit problems

We summarize the main properties of the minimizers of $\mathcal{F}_{mec,X}^{\Gamma_u,g}$ (large bodies) and $\mathcal{G}_{mec,X}^{\Gamma_u,g}$ (small particles).

- The minimization problem for $\mathcal{F}_{mec,X}^{\Gamma_u,g}$ may be ill-posed in the cases when X stands either for Fr or U, while the minimization problem for $\mathcal{G}_{mec,X}^{\Gamma_u,g}$ is always well-posed for $X = Fr, U$ or B.
- Let $\mathbf{g}(x) = \mathbf{F}(x - O)$, with $\mathbf{F} \in \mathbb{M}_0^{3\times3}$ and with $\Gamma_u = \partial\Omega$. The solution of the minimization problem for $\mathcal{F}_{mec,B}^{\partial\Omega,Fx}$ may be not unique. Anyway, letting $(\overline{\mathbf{Q}}, \overline{\mathbf{u}})$ be a possible minimizer of $\mathcal{F}_{mec,B}^{\partial\Omega,Fx}$, then the optimal order tensor is uniquely determined as $\overline{\mathbf{Q}} = \pi^{\mathcal{Q}_B}(\mathbb{E}(\nabla\overline{\mathbf{u}})/\gamma)$.
  The solution of the minimization problem for $\mathcal{G}_{mec,X}^{\partial\Omega,Fx}$ may also be not unique, but for a different reason. In the cases $X = Fr$ or U, letting $(\mathbf{Q}_1, \mathbf{u}_1)$ and $(\mathbf{Q}_2, \mathbf{u}_2)$ be two possible minimizers of $\mathcal{G}_{mec,X}^{\partial\Omega,Fx}$, then $\mathbf{u}_1 \equiv \mathbf{u}_2$, while it may be $\mathbf{Q}_1 \neq \mathbf{Q}_2$. In the case $X = B$ we must have $\mathbf{Q}_1 \equiv \mathbf{Q}_2$, since the minimizer is unique.
- A common minimizer of $\mathcal{F}_{mec,B}^{\partial\Omega,Fx}$ and $\mathcal{G}_{mec,B}^{\partial\Omega,Fx}$ is the pair $\big(\pi^{\mathcal{Q}_B}(\mathbb{E}(\mathbf{F})/\gamma), \mathbf{F}(x - O)\big)$.

3.4 Continuous perturbations

In the last part of the chapter, we extend the previous Gamma-convergence results to systems of particles under the presence of applied fields. We compute exactly the Gamma-limit for the case of an applied magnetic field both in the limit for small particles and large bodies, by showing that the magnetostatic energy is a continuous perturbation for all the energy functionals previously introduced. Then, we discuss the case of the electric field. We describe the behavior of minima and minimizers only in the asymptotic case of small-particles and we briefly present an open problem for the case of large bodies.

The following proposition is a well known result [22, Prop. 6.21] (here H is any topological space).

Proposition 13 *Let $\mathcal{F}_2 : H \mapsto \mathbb{R}$ be a continuous functional. If $\{\mathcal{F}_h\}$ Gamma-converges to $\mathcal{F}_1$ in H, then $\{\mathcal{F}_h + \mathcal{F}_2\}$ Gamma-converges to $\mathcal{F}_1 + \mathcal{F}_2$ in H.*

3.4.1 The magnetic field

We recall that the magnetostatic energy is defined in Paragraph 1.2.4 and is given by

$$\mathcal{F}_{mag}(\mathbf{Q}, \mathbf{h}) = \int_\Omega \frac{\chi_o}{2} \langle (\overline{\chi}\mathbf{I} + \chi_a \mathbf{Q})\mathbf{h}, \mathbf{h}\rangle dx. \tag{3.4.1}$$

We recall that, as a typical assumption for liquid crystals[49], $\mathbf{h}$ is imposed. We want to show that $\mathcal{F}_{mag}(\cdot, \mathbf{h})$ is a continuous perturbation both for the topology σ and σ', so that the full energy of the system Gamma-converges, both in the limit for small particles and large bodies, also in the presence of the magnetostatic correction. In this second case the result is immediate since

$$\langle \mathbf{Q}_h\mathbf{h}, \mathbf{h}\rangle \to \langle \mathbf{Q}\mathbf{h}, \mathbf{h}\rangle \ s\text{-}L^2(\Omega, \mathbb{M}^{3\times3}) \text{ as } \mathbf{Q}_h \to \mathbf{Q} \ s\text{-}L^2(\Omega, \mathbb{M}^{3\times3}), \text{ as } h \to +\infty \tag{3.4.2}$$

and hence

$$\int_\Omega \frac{\chi_o}{2} \langle (\overline{\chi}\mathbf{I} + \chi_a \mathbf{Q}_h)\mathbf{h}, \mathbf{h}\rangle dx \overset{h\to+\infty}{\longrightarrow} \int_\Omega \frac{\chi_o}{2} \langle (\overline{\chi}\mathbf{I} + \chi_a \mathbf{Q})\mathbf{h}, \mathbf{h}\rangle dx. \tag{3.4.3}$$

We show that $\mathcal{F}_{mag}(\cdot, \mathbf{h})$ is continuous also for the weak $L^2(\Omega, \mathbb{M}^{3\times3})$-convergence.

Lemma 4 *Let $\Omega \subset \mathbb{R}^3$ be an open, bounded set. Let $\{\mathbf{Q}_h\}$ be a sequence of matrices such that $\mathbf{Q}_h : \Omega \mapsto \mathcal{Q}_X$, for any $h \in \mathbb{N}$, where X stands either for Fr, U or B and let $\mathbf{Q} : \Omega \mapsto \mathcal{Q}_B$. Then,*

$$\mathbf{Q}_h \rightharpoonup \mathbf{Q} \ w\text{-}L^2(\Omega, \mathbb{M}^{3\times3}) \quad \textit{if and only if} \quad \mathbf{Q}_h \overset{*}{\rightharpoonup} \mathbf{Q} \ w\text{-}L^\infty(\Omega, \mathbb{M}^{3\times3}). \tag{3.4.4}$$

Proof. Suppose that $\mathbf{Q}_h \rightharpoonup \mathbf{Q}$ w-$L^2(\Omega, \mathbb{M}^{3\times3})$. Since $\{\mathbf{Q}_h\} \subset L^\infty(\Omega, \mathcal{Q}_X)$ by definition, then, up to a subsequence, we have

$$\mathbf{Q}_{h_j} \overset{*}{\rightharpoonup} \overline{\mathbf{Q}} \quad \text{i.e.} \int_\Omega \mathbf{Q}_{h_j} : \mathbf{T} dx \overset{j\to+\infty}{\longrightarrow} \int_\Omega \overline{\mathbf{Q}} : \mathbf{T} dx, \quad \forall\, \mathbf{T} \in L^1(\Omega, \mathbb{M}^{3\times3}) \tag{3.4.5}$$

to $\overline{\mathbf{Q}} \in L^\infty(\Omega, \mathcal{Q}_B)$. In particular, since $L^2(\Omega, \mathbb{M}^{3\times3}) \subset L^1(\Omega, \mathbb{M}^{3\times3})$, we can take some $\overline{\mathbf{T}} \in L^2(\Omega, \mathbb{M}^{3\times3})$ in (3.4.5) and hence

$$\int_\Omega \mathbf{Q}_{h_j} : \overline{\mathbf{T}} dx \to \int_\Omega \overline{\mathbf{Q}} : \overline{\mathbf{T}} dx \text{ as } j \to +\infty$$

and, by assumption, we have $\overline{\mathbf{Q}} = \mathbf{Q}$ for any subsequence and hence for the whole sequence.
The converse implication is trivial. □

Thanks to Lemma 4, we have that, if $\mathbf{Q}_h, \mathbf{u}_h \overset{\sigma}{\rightharpoonup} \mathbf{Q}, \mathbf{u}$, with $\{\mathbf{Q}_h\} \subset L^2(\Omega, \mathcal{Q}_X)$, $\{\mathbf{u}_h\} \subset H^1(\Omega, \mathbb{R}^3)$, then $\mathbf{Q}_h \overset{*}{\rightharpoonup} \mathbf{Q}$ w-$L^\infty(\Omega, \mathbb{M}^{3\times3})$ and hence (3.4.3) follows since $\mathbf{h}$ is an assigned vector field in $L^2(\Omega, \mathbb{R}^3)$.

3.4.2 The electric field

In the presence of an electric field, an energy contribution has to be added to all the energies introduced in Sections 3.2, 3.3. Denoting with $\phi : \Omega \mapsto \mathbb{R}$ the electric potential, we recall the expression of the electrostatic energy (see (1.1.8) and below). Neglecting the LdG free-energy density, we re-write the energy of the system in the form

$$\mathcal{E}(\mathbf{Q}, \mathbf{u}, \phi) = \int_\Omega \Big(\frac{\kappa^2}{2} |\nabla \mathbf{Q}|^2 + f_{mec}(\mathbf{Q}, \nabla \mathbf{u}) - \big\langle \mathbf{A}(\mathbf{Q}) \nabla \phi, \nabla \phi \big\rangle \Big) dx. \tag{3.4.6}$$

In what follows, we study the asymptotic behavior of minima and minimizers of (3.4.6) in the small-particle limit under the constraint of Gauss law. To this aim, we recall that Gauss law coincides with the first variation of $\phi \mapsto \mathcal{F}_{ele}(\mathbf{Q}, \phi)$ defined in (1.1.10), i.e.

$$\mathcal{F}_{ele}(\mathbf{Q}, \phi) = \int_\Omega \big\langle \mathbf{A}(\mathbf{Q}) \nabla \phi, \nabla \phi \big\rangle dx.$$

Then, letting $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_X)$, where X stands either for Fr, U or B, and letting Ω, Γ_ϕ, ϕ_o as in Theorem 12, we can define the non-local functional $\mathcal{F}^*_{ele}$

$$\min_{\phi \in H^1_{\Gamma_\phi}(\Omega) + \phi_o} \mathcal{F}_{ele}(\mathbf{Q}, \phi) = \mathcal{F}_{ele}(\mathbf{Q}, \Phi[\mathbf{Q}]) =: \mathcal{F}^*_{ele}(\mathbf{Q}). \tag{3.4.7}$$

Now, take $\{\mathbf{Q}_h\} \subset L^2(\Omega, \mathcal{Q}_X)$, $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_X)$ such that

$$\mathbf{Q}_h \to \mathbf{Q} \quad s\text{-}L^2(\Omega, \mathbb{M}^{3\times3}) \quad \textit{as } h \to +\infty, \tag{3.4.8}$$

and let us denote the (unique) solutions of Gauss equation (1.2.5) associated with $\mathbf{Q}_h \in L^2(\Omega, \mathcal{Q}_X)$, $\forall\, h \in \mathbb{N}$ and to $\mathbf{Q} \in L^2(\Omega, \mathcal{Q}_X)$ with

$$\Phi_h = \Phi[\mathbf{Q}_h] \quad \text{and} \quad \Phi = \Phi[\mathbf{Q}], \tag{3.4.9}$$

respectively. Then, thanks to the result of Paragraph 1.2.2 (Proposition 4) regarding the continuity properties of $\Phi[\mathbf{Q}]$, there follows that

$$\Phi[\mathbf{Q}_h] \to \Phi[\mathbf{Q}] \quad s\text{-}H^1(\Omega), \tag{3.4.10}$$

and (Remark 3)

$$\int_\Omega \big\langle \mathbf{A}(\mathbf{Q}_h)\nabla\Phi_h, \nabla\Phi_h\big\rangle dx \to \int_\Omega \big\langle \mathbf{A}(\mathbf{Q})\nabla\Phi, \nabla\Phi\big\rangle dx. \tag{3.4.11}$$

Adopting the notation of (3.4.7), then (3.4.11) can be written in the following way

$$\mathcal{F}^*_{ele}(\mathbf{Q}_h) \to \mathcal{F}^*_{ele}(\mathbf{Q}) \quad \text{as} \quad \mathbf{Q}_h \to \mathbf{Q}\ s\text{-}L^2(\Omega, \mathcal{Q}_X) \quad (h \to +\infty) \tag{3.4.12}$$

where X stands either for Fr, U or B, and hence $\mathcal{F}^*_{ele} : L^2(\Omega, \mathcal{Q}_X) \mapsto \mathbb{R}$ is continuous in the strong topology of $L^2(\Omega, \mathbb{M}^{3\times3})$.

Rescaling. We repeat the procedure of Paragraph 3.1.2 in order to discuss how the energy $\mathcal{E}^\kappa(\cdot,\cdot,\cdot;\mathcal{B})$ defined as

$$\mathcal{E}^\kappa(\mathbf{Q}, \mathbf{u}, \phi; \mathcal{B}) := \int_\mathcal{B} \Big(\frac{\kappa^2}{2}|\nabla\mathbf{Q}|^2 dx + f_{mec}(\mathbf{Q}, \nabla\mathbf{u}) - \big\langle \mathbf{A}(\mathbf{Q})\nabla\phi, \nabla\phi\big\rangle\Big) dx \tag{3.4.13}$$

rescales if we dilate the reference domain $\mathcal{B} \in \mathbb{R}^3$.
Let $\mathcal{B} \subset \mathbb{R}^3$ be a Lipschitz domain with volume Λ^3, where $\Lambda \in (0, \infty)$. Set $\Omega := (1/\Lambda)\mathcal{B}$. Let $\phi_\Lambda : \mathcal{B} \mapsto \mathbb{R}$ and define $\phi : \Omega \mapsto \mathbb{R}$ by

$$\Lambda\,\phi\Big(\frac{1}{\Lambda}z\Big) := \phi_\Lambda(z), \qquad z \in \mathcal{B}. \tag{3.4.14}$$

Hence,

$$\frac{1}{|\mathcal{B}|}\int_\mathcal{B} \big\langle \mathbf{A}(\mathbf{Q}_\Lambda)\nabla\phi_\Lambda, \nabla\phi_\Lambda\big\rangle dx_\Lambda = \int_\Omega \big\langle \mathbf{A}(\mathbf{Q})\nabla\phi, \nabla\phi\big\rangle dx. \tag{3.4.15}$$

Using the uniqueness of the solution to Gauss equation (1.2.5), we easily prove that

$$\Lambda\Phi\Big(\frac{1}{\Lambda}z\Big) = \Lambda\,\Phi[\mathbf{Q}] = \Phi_\Lambda[\mathbf{Q}_\Lambda] := \Phi_\Lambda(z)$$

and then

$$\frac{1}{|\mathcal{B}|}\mathcal{E}^\kappa(\mathbf{Q}_\Lambda, \mathbf{u}_\Lambda, \Phi_\Lambda; \mathcal{B}) = \mathcal{E}^{\kappa/\Lambda}(\mathbf{Q}, \mathbf{u}, \Phi; \Omega). \tag{3.4.16}$$

In view of this rescaling, it makes sense to investigate the behavior of critical values and critical points of $\mathcal{E}^{\kappa/\Lambda}(\cdot,\cdot,\cdot;\Omega)$ as Λ tends to zero (limit case of small particles) and to $+\infty$ (limit case of large bodies).

In what follows, we discuss the small-particle limit.

Theorem 19 *Let $\Omega \subset \mathbb{R}^3$ be a simply connected and Lipschitz domain, let $\mathbf{g}(x) \in H^1(\Omega, \mathbb{R}^3)$ with $\operatorname{div}\mathbf{g} = 0$. Let f_{mec} as in* (2.1.1)*, $\mathcal{F}^*_{ele}$ as in* (3.4.7) *and define (here $X = Fr, U, B$)*

$$\mathcal{E}^*_{\varepsilon,X}(\mathbf{Q}, \mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q}, \nabla\mathbf{u})\Big)dx - \mathcal{F}^*_{ele}(\mathbf{Q}) & \\ \qquad\qquad\qquad \textit{on } H^1(\Omega, \mathcal{Q}_X) \times H^1(\Omega, \mathbb{R}^3), \operatorname{div}\mathbf{u} = 0 \\ +\infty \qquad \textit{otherwise in } L^2(\Omega, \mathbb{M}^{3\times3}) \times H^1(\Omega, \mathbb{R}^3), \end{cases}$$

$$\mathcal{E}^{*\Gamma_u,g}_{\varepsilon,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u})\Big)dx - \mathcal{F}^*_{ele}(\mathbf{Q}) \\ \qquad\qquad \text{on } H^1(\Omega,\mathcal{Q}_X)\times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div}\mathbf{u}=0 \\ +\infty \qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Then

$$\Gamma(\sigma')\text{-}\lim_{\varepsilon\to+\infty}\mathcal{E}^*_{\varepsilon,X} = \mathcal{E}^*_{mec,X} \tag{3.4.17}$$

and

$$\Gamma(\sigma')\text{-}\lim_{\varepsilon\to+\infty}\mathcal{E}^{*\Gamma_u,g}_{\varepsilon,X} = \mathcal{E}^{*\Gamma_u,g}_{mec,X} \tag{3.4.18}$$

where

$$\mathcal{E}^*_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx - \mathcal{F}^*_{ele}(\mathbf{Q}) \\ \qquad\qquad \text{on } \{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),\text{const}\}\times H^1(\Omega,\mathbb{R}^3), \operatorname{div}\mathbf{u}=0 \\ +\infty \qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3), \end{cases}$$

$$\mathcal{E}^{*\Gamma_u,g}_{mec,X}(\mathbf{Q},\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega f_{mec}(\mathbf{Q},\nabla\mathbf{u})dx - \mathcal{F}^*_{ele}(\mathbf{Q}) \\ \qquad\qquad \text{on } \{\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X),\text{const}\}\times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div}\mathbf{u}=0 \\ +\infty \qquad \text{otherwise in } L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3). \end{cases}$$

Proof. It is enough to apply Theorem 18 together with Proposition 13. We recall that $\mathcal{F}^*_{ele}$ is continuous (see (3.4.12)) with respect to the convergence $\mathbf{Q}_j \to \mathbf{Q}$ s-$L^2(\Omega,\mathbb{M}^{3\times3})$ with $\{\mathbf{Q}_j\}\subset L^2(\Omega,\mathcal{Q}_X)$, where X stands either for Fr, U or B. □

To obtain the convergence of minima and minimizers of $\mathcal{E}^{*X}_{\Gamma_u,g}(\mathbf{Q},\mathbf{u})$, we have to verify the equicoercivity of the functional. This condition is trivial for all the functionals analyzed in the previous sections and also in the presence of the magnetostatic energy. Let $\mathbf{Q}\in H^1(\Omega,\mathcal{Q}_X)$. By minimality and (1.1.13) we have

$$M\int_\Omega |\nabla\phi_o|^2dx \geq \int_\Omega \big\langle \mathbf{A}(\mathbf{Q})\nabla\phi_o,\nabla\phi_o\big\rangle dx \geq \inf_{\phi\in H^1_{\Gamma_\phi}(\Omega)+\phi_o}\int_\Omega\big\langle\mathbf{A}(\mathbf{Q})\nabla\phi,\nabla\phi\big\rangle dx. \tag{3.4.19}$$

Now, recalling (2.2.26), we can write (here $\varepsilon^2>0$ is assigned)

$$\int_\Omega\Big\{\varepsilon^2|\nabla\mathbf{Q}|^2+\mu|\mathbb{E}(\nabla\mathbf{u})-\gamma\mathbf{Q}|^2+\frac{\lambda}{2}(\operatorname{div}\mathbf{u})^2\Big\}dx \tag{3.4.20}$$
$$-\inf_{\phi\in H^1_{\Gamma_\phi}(\Omega)+\phi_o}\int_\Omega\big\langle\mathbf{A}(\mathbf{Q})\nabla\phi,\nabla\phi\big\rangle dx \geq \varepsilon^2\int_\Omega|\nabla\mathbf{Q}|^2dx + C_2\int_\Omega|\mathbb{E}(\nabla\mathbf{u})|^2dx - Const,$$

for every $(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X)\times H^1(\Omega,\mathbb{R}^3)$, where X stands either for Fr, U or B, and hence equicoercivity is obtained in $H^1(\Omega,\mathcal{Q}_X)\times H^1(\Omega,\mathbb{R}^3)$ by applying Korn's and Poincaré inequality and the fact that $L^2(\Omega,\mathcal{Q}_X)$ is a bounded set. As a consequence, we obtain the following theorem.

Theorem 20 (Fundamental theorem of Gamma-convergence) *Under the hypotheses of Theorem 19, there follows (here X stands either for Fr, U or B)*

$$\min_{\substack{(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{E}^{*\Gamma_u,g}_{mec,X} = \lim_{j\to+\infty}\left(\min_{\substack{(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}\right) \text{ (convergence of minima).}$$

Then, let $\{\mathbf{Q}_j,\mathbf{u}_j\}\subset L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)$ be a minimizing sequence for $\{\mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}\}$ (i.e. $\lim_j \mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}(\mathbf{Q}_j,\mathbf{u}_j) = \lim_j \inf \mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}$). Then, up to a subsequence, $\mathbf{Q}_{j_k}\to\overline{\mathbf{Q}}$, $\mathbf{u}_{j_k}\rightharpoonup\overline{\mathbf{u}}$ in $L^2(\Omega,\mathbb{M}^{3\times3})\times H^1(\Omega,\mathbb{R}^3)$ and with $\overline{\mathbf{Q}}$ constant, where

$$\mathcal{E}^{*\Gamma_u,g}_{mec,X}(\overline{\mathbf{Q}},\overline{\mathbf{u}}) = \min_{\substack{(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{E}^{*\Gamma_u,g}_{mec,X} \quad \text{(convergence of minimum points).} \tag{3.4.21}$$

Proof. This is a standard result. We can take a minimizing sequence $(\widehat{\mathbf{Q}}_j,\widehat{\mathbf{u}}_j)$ directly in $H^1(\Omega,\mathcal{Q}_X)\times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}(x)$ with $\operatorname{div}\widehat{\mathbf{u}}_j=0$ such that

$$\liminf_{j\to+\infty} \mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}(\widehat{\mathbf{Q}}_j,\widehat{\mathbf{u}}_j) = \liminf_{j\to+\infty}\left(\min_{\substack{(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}\right). \tag{3.4.22}$$

Thanks to (3.4.20), up to a subsequence we have

$$\widehat{\mathbf{Q}}_{j_k}\rightharpoonup\overline{\mathbf{Q}}\ w\text{-}H^1(\Omega,\mathbb{M}^{3\times3}),\quad \widehat{\mathbf{u}}_{j_k}\rightharpoonup\overline{\mathbf{u}}\ w\text{-}H^1(\Omega,\mathbb{R}^3), \tag{3.4.23}$$

to some $\overline{\mathbf{Q}}\in H^1(\Omega,\mathcal{Q}_B)$ and $\overline{\mathbf{u}}\in H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}(x)$ with $\operatorname{div}\mathbf{u}=0$. In view of Theorem 18, $\overline{\mathbf{Q}}$ must be constant. Now we regard $\widehat{\mathbf{Q}}_{j_k},\widehat{\mathbf{u}}_{j_k}$ as a subsequence of a new sequence $\mathbf{Q}_j,\mathbf{u}_j$ defined as

$$\mathbf{Q}_j=\begin{cases}\widehat{\mathbf{Q}}_{j_k} & \text{if } j=j_k\\ \overline{\mathbf{Q}} & \text{otherwise,}\end{cases}\qquad \mathbf{u}_j=\begin{cases}\widehat{\mathbf{u}}_{j_k} & \text{if } j=j_k\\ \overline{\mathbf{u}} & \text{otherwise,}\end{cases} \tag{3.4.24}$$

so that $\mathbf{Q}_j\rightharpoonup\overline{\mathbf{Q}}$, $\mathbf{u}_j\rightharpoonup\overline{\mathbf{u}}$ and

$$\lim_{k\to+\infty}\mathcal{E}^{*\Gamma_u,g}_{\varepsilon_{j_k},X}(\widehat{\mathbf{Q}}_{j_k},\widehat{\mathbf{u}}_{j_k}) = \liminf_{j\to+\infty}\mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}(\widehat{\mathbf{Q}}_j,\widehat{\mathbf{u}}_j). \tag{3.4.25}$$

We then have

$$\limsup_{j\to+\infty}\left(\min_{\substack{(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}\right) \leq \min_{\substack{(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{E}^{*\Gamma_u,g}_{mec,X} \leq \tag{3.4.26}$$

$$\mathcal{E}^{*\Gamma_u,g}_{mec,X}(\overline{\mathbf{Q}},\overline{\mathbf{u}}) \leq \liminf_{j\to+\infty}\mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}(\mathbf{Q}_j,\mathbf{u}_j) \leq \liminf_{k\to+\infty}\mathcal{E}^{*\Gamma_u,g}_{\varepsilon_{j_k},X}(\widehat{\mathbf{Q}}_{j_k},\widehat{\mathbf{u}}_{j_k}) =$$

$$\liminf_{j\to+\infty}\mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}(\widehat{\mathbf{Q}}_j,\widehat{\mathbf{u}}_j) = \liminf_{j\to+\infty}\left(\min_{\substack{(\mathbf{Q},\mathbf{u})\in L^2(\Omega,\mathbb{M}^{3\times3})\\ \times H^1(\Omega,\mathbb{R}^3)}} \mathcal{E}^{*\Gamma_u,g}_{\varepsilon_j,X}\right).$$

The first inequality in (3.4.26) follows from the *limsup* inequality, the second inequality is a trivial fact and the third inequality follows from the *liminf* inequality. Then, the extraction of the subsequence as in (3.4.24) yields the fourth inequality, and the remaining equalities are a property of the minimizing sequence. □

Gamma-convergence results for a min-max problem

The previous theorem may be interpreted to obtain Gamma-convergence-like results for min-max problems. Since a literature on the asymptotics of min-max problems is missing to our knowledge, in what follows we simply extend the terminology of Gamma-convergence for minimum problems to the case of min-max problems. Setting $\varepsilon^2 = \kappa^2/\Lambda^2$ in (3.4.16) and dropping the dependence on the domain in (3.4.13), we label

$$\mathcal{E}^{\varepsilon}(\mathbf{Q},\mathbf{u},\phi) := \int_\Omega \Big(\varepsilon^2|\nabla\mathbf{Q}|^2 + f_{mec}(\mathbf{Q},\nabla\mathbf{u}) - \langle\mathbf{A}(\mathbf{Q})\nabla\phi,\nabla\phi\rangle\Big)dx, \tag{3.4.27}$$

$$\mathcal{E}_{mec}(\mathbf{Q},\mathbf{u},\phi) := \int_\Omega \Big(f_{mec}(\mathbf{Q},\nabla\mathbf{u}) - \langle\mathbf{A}(\mathbf{Q})\nabla\phi,\nabla\phi\rangle\Big)dx. \tag{3.4.28}$$

Corollary 8 (Fundamental theorem of Γ-convergence for min-max problems) *Let $\mathcal{E}^\varepsilon$, $\mathcal{E}_{mec}$ defined as in* (3.4.27) *and* (3.4.28)*. Under the hypotheses of Theorems* 12 *and* 20 *(here X stands either for Fr, U or B) we have:*

1. (Convergence of min-max values)

$$\min_{\substack{(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X),const\times\\ H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0}} \max_{\phi\in H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}_{mec} = \lim_{j\to\infty}\left(\inf_{\substack{(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X)\times\\ H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0}} \max_{\phi\in H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}^{\varepsilon_j}\right).$$

Then, denote with $\Phi = \Phi[\mathbf{Q}]$ the solution to Gauss equation (1.2.5)*. Let* $\{\mathbf{Q}_j, \mathbf{u}_j, \Phi_j\} \subset H^1(\Omega, \mathcal{Q}_X) \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{g}, \operatorname{div} \mathbf{u} = 0\} \times H^1_{\Gamma_\phi}(\Omega) + \phi_o(x)$ *be a min-maximizing sequence for* $\{\mathcal{E}^{\varepsilon_j}\}$*, i.e.*

$$\lim_{j \to +\infty} \mathcal{E}^{\varepsilon_j}\left(\mathbf{Q}_j, \mathbf{u}_j, \Phi_j\right) = \lim_{j \to +\infty} \inf_{\substack{(\mathbf{Q},\mathbf{u}) \in H^1(\Omega,\mathcal{Q}_X) \times \\ H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div} \mathbf{u}=0}} \max_{\phi \in H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}^{\varepsilon_j}(\mathbf{Q}, \mathbf{u}, \phi),$$

Then, up to a subsequence, $\mathbf{Q}_{j_k} \to \overline{\mathbf{Q}}$*,* $\mathbf{u}_{j_k} \rightharpoonup \overline{\mathbf{u}}$ *in* $L^2(\Omega, \mathbb{M}^{3\times3}) \times H^1(\Omega, \mathbb{R}^3)$ *with* $\overline{\mathbf{Q}}$ *constant and* $\Phi[\mathbf{Q}_{j_k}] \to \Phi[\overline{\mathbf{Q}}]$ s-$H^1(\Omega)$*, and:*

2. (Convergence of min-max points)

$$\mathcal{E}_{mec}(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \Phi[\overline{\mathbf{Q}}]) = \min_{\substack{(\mathbf{Q},\mathbf{u}) \in H^1(\Omega,\mathcal{Q}_X), const \\ \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div} \mathbf{u}=0}} \max_{\phi \in H^1_{\Gamma_\phi}(\Omega)+\phi_o} \mathcal{E}_{mec}(\mathbf{Q}, \mathbf{u}, \phi).$$

Proof. We only notice that, thanks to Proposition 1.2.2, $\Phi[\mathbf{Q}_{j_k}] \to \Phi[\overline{\mathbf{Q}}]$ s-$H^1(\Omega)$ as $\mathbf{Q}_{j_k} \to \overline{\mathbf{Q}}$. □

Remark 22 By virtue of Theorem 12, the result of Corollary 8 can be written in the following alternative way.

1. (Convergence of min-max values). It is equivalent to:

$$\begin{aligned} &\min_{\substack{(\mathbf{Q},\mathbf{u}) \in H^1(\Omega,\mathcal{Q}_X), const, \\ \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div} \mathbf{u}=0}} \Big\{\mathcal{E}_{mec}(\mathbf{Q}, \mathbf{u}, \phi) \text{ sub Gauss law (1.2.5)}\Big\} \\ &= \lim_{j \to +\infty} \left(\inf_{\substack{(\mathbf{Q},\mathbf{u}) \in H^1(\Omega,\mathcal{Q}_X) \times \\ H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div} \mathbf{u}=0}} \Big\{\mathcal{E}^{\varepsilon_j}(\mathbf{Q}, \mathbf{u}, \phi) \text{ sub Gauss law (1.2.5)}\Big\} \right). \end{aligned} \tag{3.4.29}$$

2. (Convergence of min-max points). It is equivalent to the following formulation.

Denote with $\Phi = \Phi[\mathbf{Q}]$ the solution to Gauss equation (1.2.5). Let $\{\mathbf{Q}_j, \mathbf{u}_j, \Phi_j\} \subset H^1(\Omega, \mathcal{Q}_X) \times \{H^1_{\Gamma_u}(\Omega, \mathbb{R}^3) + \mathbf{g}, \operatorname{div} \mathbf{u} = 0\} \times H^1_{\Gamma_\phi}(\Omega) + \phi_o(x)$ be a min-maximizing sequence for $\{\mathcal{E}^{\varepsilon_j}\}$, i.e.

$$\begin{aligned} &\lim_{j \to +\infty} \mathcal{E}^{\varepsilon_j}\left(\mathbf{Q}_j, \mathbf{u}_j, \Phi_j\right) = \\ &\lim_{j \to +\infty} \inf_{\substack{(\mathbf{Q},\mathbf{u}) \in H^1(\Omega,\mathcal{Q}_X) \times \\ H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g}, \operatorname{div} \mathbf{u}=0}} \Big\{\mathcal{E}^{\varepsilon_j}(\mathbf{Q}, \mathbf{u}, \phi) \text{ sub Gauss law (1.2.5)}\Big\}. \end{aligned} \tag{3.4.30}$$

Then, up to a subsequence, $\mathbf{Q}_{j_k} \to \overline{\mathbf{Q}}$, $\mathbf{u}_{j_k} \rightharpoonup \overline{\mathbf{u}}$ in $L^2(\Omega, \mathbb{M}^{3\times 3}) \times H^1(\Omega, \mathbb{R}^3)$ with $\overline{\mathbf{Q}}$ constant and $\Phi[\mathbf{Q}_{j_k}] \to \Phi[\overline{\mathbf{Q}}]$ s-$H^1(\Omega)$ and

$$\mathcal{E}_{mec}\big(\overline{\mathbf{Q}}, \overline{\mathbf{u}}, \Phi[\overline{\mathbf{Q}}]\big) = \min_{\substack{(\mathbf{Q},\mathbf{u})\in H^1(\Omega,\mathcal{Q}_X),const \\ \times H^1_{\Gamma_u}(\Omega,\mathbb{R}^3)+\mathbf{g},\mathrm{div}\,\mathbf{u}=0}} \Big\{\mathcal{E}_{mec}(\mathbf{Q}, \mathbf{u}, \phi) \text{ sub Gauss law (1.2.5)}\Big\}.$$

Remark 23 Theorem 20, Corollary 8 and Remark 22 still hold for models of compressible elastomers, that is in the absence of the constraint on the divergence of $\mathbf{u}$. The proofs are even simpler since it is not necessary to take sequences $\{\mathbf{u}_k\}$ with $\mathrm{div}\,\mathbf{u}_k = 0$. Moreover, it is not necessary to take the boundary datum $\mathbf{g}(x)$ with divergence equal to zero.

Open problem. The above results describe the asymptotic energies of small particles in the presence of an applied electric field. The main ingredient in all the proofs is the continuity of the electrostatic energy $\mathcal{F}^*_{ele}(\mathbf{Q})$ (that is, $\mathcal{F}_{ele}(\mathbf{Q}, \phi)$ under the constraint of Gauss law) in the strong L^2-convergence. This is a standard result for elliptic integrals.

On the other hand, the analysis of the large-body limit in the presence of an applied electric field is extremely difficult. In general, if we denote with $\Phi[\mathbf{Q}]$ the solution to Gauss equation (1.2.5), then it is not true that

$$\Phi[\mathbf{Q}_h] \to \Phi[\mathbf{Q}] \ s\text{-}H^1(\Omega) \quad \text{as} \quad \mathbf{Q}_h \rightharpoonup \mathbf{Q} \ w\text{-}L^2(\Omega, \mathbb{M}^{3\times 3}) \qquad (h \to +\infty)$$

and $\mathbf{Q} \mapsto \mathcal{F}^*_{ele}(\mathbf{Q})$ is not continuous in the weak topology of $L^2(\Omega, \mathbb{M}^{3\times 3})$. As a consequence, The characterization of the energy of the system in the presence of an electric field in the large-body asimptotics does not follow from the construction contained in the previous sections and is an open problem. In particular, we recall that the explicit characterization of

$$\inf\Big\{\int_\Omega \big\langle \mathbf{A}(\mathbf{Q}_h)\nabla\Phi[\mathbf{Q}_h], \nabla\Phi[\mathbf{Q}_h]\big\rangle dx \quad \mathbf{Q}_h \rightharpoonup \mathbf{Q} \ w\text{-}L^2(\Omega, \mathbb{M}^{3\times 3})\Big\}$$

with $\{\mathbf{Q}_h\} \subset L^2(\Omega, \mathcal{Q}_X)$, $X = Fr, U, B$, can be obtained only for special sequences of matrices, while in the general case is unknown [22, Chapters 24 and 25], [47].

Chapter 4

Relaxation of anisotropic energies for nematic elastomers

4.1 Introduction

In this chapter we introduce non-convex functionals for nematic elastomers which have to be interpreted as the anisotropic versions of the models studied in Chapter 2, and we find explicitly the relaxations. We show that the relaxation of an incompressible model is obtained as the pointwise limit of the relaxation of the compressible energies. The result is obtained letting $\mathbf{v} : S \mapsto \mathbb{R}^2$ be the mechanical displacement constrained in the *plane-strain* geometry (see below).

4.1.1 The mechanical model

Let $\mathbf{F} \in \mathbb{M}^{3\times 3}$, $\mathbf{Q} \in \mathcal{Q}_X$ where X stands either for Fr or B and define

$$
\begin{aligned}
f^{\beta}_{mec}(\mathbf{Q},\mathbf{F}) &:= \frac{1}{2}\mathbb{C}\big(\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}\big) : (\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}) + \beta\mu|\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}_o|^2 = \\
&\mu|\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}|^2 + \beta\mu|\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}_o|^2 + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2 = \\
&\mu|\mathbb{E}_0(\mathbf{F})-\gamma\mathbf{Q}|^2 + \beta\mu|\mathbb{E}_0(\mathbf{F})-\gamma\mathbf{Q}_o|^2 + \Big(\frac{\lambda}{2}+\frac{\mu}{3}+\beta\frac{\mu}{3}\Big)(\operatorname{tr}\mathbf{F})^2.
\end{aligned}
\tag{4.1.1}
$$

The matrix $\mathbf{Q}_o$, which is given in the form $\mathbf{Q}_o = \mathbf{n}_o \otimes \mathbf{n}_o - (1/3)\mathbf{I}$, with $\mathbf{n}_o \in \mathbb{S}^2$, represents the order tensor at the moment of the formation of the crosslinks, that is when the nematic molecules are oriented along the direction $\mathbf{n}_o$ and the topology of the chains is frozen. Then, β is a non-negative parameter which is responsible for anisotropy. In fact, we note that the energy density f^{β}_{mec} obtained for $\beta = 0$, which has already been investigated in Chapters 2 and 3, is *isotropic*, in the sense that

$$
\begin{aligned}
f^{0}_{mec}(\mathbf{RQR}^T,\mathbf{RFR}^T) &= \frac{1}{2}\mathbb{C}\big(\mathbb{E}(\mathbf{RFR}^T)-\gamma\mathbf{RQR}^T\big) : \big(\mathbb{E}(\mathbf{RFR}^T)-\gamma\mathbf{RQR}^T\big) \\
&= \frac{1}{2}\mathbb{C}\big(\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}\big) : \big(\mathbb{E}(\mathbf{F})-\gamma\mathbf{Q}\big) = f^{0}_{mec}(\mathbf{Q},\mathbf{F}),
\end{aligned}
\tag{4.1.2}
$$

for every $\mathbf{R} \in \mathbb{SO}(3)$. It is immediate to verify (4.1.2) by noticing that $\mathbb{E}(\mathbf{R}\mathbf{F}\mathbf{R}^T) = \mathbf{R}\mathbb{E}(\mathbf{F})\mathbf{R}^T$. In particular, f^0_{mec} is a non-negative function which is equal to zero only if $\mathbb{E}(\mathbf{F}) = \gamma\mathbf{Q}$, with $\mathbf{Q} \in \mathcal{Q}_X$ where X stands either for Fr or B.

On the other hand, if $\beta > 0$, then (4.1.2) does not hold and f^β_{mec} is an anisotropic function. We notice that, in this case, f^β_{mec} is a non-negative function which is equal to zero only if $\mathbf{Q} = \mathbf{Q}_o$ and $\mathbb{E}(\mathbf{F}) = \gamma\mathbf{Q}_o$, i.e. if the mechanical strain can reproduce the order tensor $\mathbf{Q}_o$ at the moment of the formation of the crosslinks. The presence of the *microscopic* variable $\mathbf{Q}$ can be averaged out in order to obtain a *macroscopic* model (see Paragraph 2.1.1) where the order tensor is directly imposed by the strain. If we minimize (4.1.1) in $\mathbf{Q}$, we obtain

$$f^\beta_X(\mathbf{F}) := \inf_{\mathbf{Q}\in\mathcal{Q}_X} f^\beta_{mec}(\mathbf{F}) = \mu\, dist^2\big(\mathbb{E}(\mathbf{F}), \gamma\mathcal{Q}_X\big) + \beta\mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}_o|^2 + \frac{\lambda}{2}(\operatorname{tr}\mathbf{F})^2, \tag{4.1.3}$$

where X stands either for Fr or B.

As above, f^0_X is an isotropic function, in the sense that $f^0_X(\mathbf{R}\mathbf{F}\mathbf{R}^T) = f^0_X(\mathbf{F})\ \forall\mathbf{R} \in \mathbb{SO}(3)$, while f^β_X is anisotropic for $\beta > 0$. Moreover, f^β_B is a convex function, since the anisotropic correction $\mathbf{F} \mapsto \beta\mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}_o|^2$ is convex. On the other hand, f^β_{Fr} is not convex.

4.2 The two-dimensional plane-strain model

Let us consider a domain $\Omega \subset \mathbb{R}^3$ in the form $\Omega = S \times (-\delta, \delta)$ with $\delta > 0$ and $S \subset \mathbb{R}^2$. In view of the orthogonal decomposition (0.1.52), we write any matrix $\mathbf{F} \in \mathbb{M}^{3\times3}$ in the form $\mathbf{F} = \mathbf{E} + \mathbf{F}^{sk}$. We make the assumption that the mechanical displacement and the director have fixed components in the direction $\mathbf{i}_3$ (plane-strain model). Precisely, we assume that the strain field and the order tensor are constant along the direction $\mathbf{i}_3$. We write the director in the form $\mathbf{n} = (\widehat{\mathbf{n}}, 0)$, where $\widehat{\mathbf{n}} = (n_1, n_2) \in \mathbb{S}^1$ and we take the original orientation of the molecules in the sample in the form $\mathbf{n}_o = (\widehat{\mathbf{n}}_o, 0)$, where $\widehat{\mathbf{n}}_o = (n_{o1}, n_{o2}) \in \mathbb{S}^1$. It is not restrictive to write $\widehat{\mathbf{n}}_o = (1, 0)$: if this is not the case, it is always possible to change the reference frame so that this becomes true.

We adopt the following parameterization for $\mathbf{E} \in \mathbb{M}^{3\times3}_{sym}$, $\mathbf{Q} \in \mathcal{Q}_{Fr}$ and $\mathbf{Q}_o$

$$\mathbf{E} = \begin{pmatrix} e_{11} & e_{12} & 0 \\ e_{12} & e_{22} & 0 \\ 0 & 0 & e_0 \end{pmatrix}, \mathbf{Q} = \begin{pmatrix} n_1^2 - \frac{1}{3} & n_1n_2 & 0 \\ n_1n_2 & n_2^2 - \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{pmatrix}, \mathbf{Q}_o = \begin{pmatrix} \frac{2}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{pmatrix}, \tag{4.2.1}$$

where $e_0 = -\gamma/3$. For convenience we define the sub-matrices

$$\widehat{\mathbf{E}} := \begin{pmatrix} e_{11} & e_{12} \\ e_{12} & e_{22} \end{pmatrix}, \quad \widehat{\mathbf{Q}} := \begin{pmatrix} n_1^2 - \frac{1}{3} & n_1n_2 \\ n_1n_2 & n_2^2 - \frac{1}{3} \end{pmatrix} = \begin{pmatrix} n_1^2 - \frac{1}{2} & n_1n_2 \\ n_1n_2 & n_2^2 - \frac{1}{2} \end{pmatrix} + \frac{1}{6}\mathbf{I}, \tag{4.2.2}$$

$$\widehat{\mathbf{Q}}_o := \begin{pmatrix} \frac{2}{3} & 0 \\ 0 & -\frac{1}{3} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} + \frac{1}{6}\mathbf{I}. \tag{4.2.3}$$

We introduce the two-dimensional version of the set of Frank tensors

$$\begin{aligned}\mathcal{Q}_{Fr}^{2dim} &:= \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} + \frac{1}{6}\mathbf{I} : \text{spectrum}(\mathbf{Q}) = \Big\{-\frac{1}{3}, \frac{2}{3}\Big\}\Big\} \\ &= \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} + \frac{1}{6}\mathbf{I} : \text{spectrum}(\mathbb{E}_0(\mathbf{Q})) = \Big\{-\frac{1}{2}, \frac{1}{2}\Big\}\Big\},\end{aligned} \tag{4.2.4}$$

and the two-dimensional version of the set of de Gennes tensors

$$\begin{aligned}\mathcal{Q}_{B}^{2dim} &:= \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} + \frac{1}{6}\mathbf{I} : \text{spectrum}(\mathbf{Q}) \in \Big[-\frac{1}{3}, \frac{2}{3}\Big]\Big\} \\ &= \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} + \frac{1}{6}\mathbf{I} : \text{spectrum}(\mathbb{E}_0(\mathbf{Q})) \in \Big[-\frac{1}{2}, \frac{1}{2}\Big]\Big\}.\end{aligned} \tag{4.2.5}$$

If we introduce the deviators of the sets $\mathcal{Q}_{Fr}^{2dim}$, $\mathcal{Q}_{B}^{2dim}$

$$\mathbb{E}_0\big(\mathcal{Q}_{Fr}^{2dim}\big) := \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} : \text{spectrum}(\mathbb{E}(\mathbf{Q})) = \Big\{-\frac{1}{2}, \frac{1}{2}\Big\}\Big\},$$

$$\mathbb{E}_0\big(\mathcal{Q}_{B}^{2dim}\big) := \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} : \text{spectrum}(\mathbb{E}(\mathbf{Q})) \in \Big[-\frac{1}{2}, \frac{1}{2}\Big]\Big\},$$

then $\mathcal{Q}_{Fr}^{2dim}$, $\mathcal{Q}_{B}^{2dim}$ can be written also as

$$\mathcal{Q}_{Fr}^{2dim} = \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} + \frac{1}{6}\mathbf{I} : \text{spectrum}\big(\mathbb{E}_0(\mathbf{Q})\big) \in \mathbb{E}_0\big(\mathcal{Q}_{Fr}^{2dim}\big)\Big\},$$

$$\mathcal{Q}_{B}^{2dim} = \Big\{\mathbf{Q} \in \mathbb{M}^{2\times 2}_{0sym} + \frac{1}{6}\mathbf{I} : \text{spectrum}\big(\mathbb{E}_0(\mathbf{Q})\big) \in \mathbb{E}_0\big(\mathcal{Q}_{B}^{2dim}\big)\Big\}.$$

In view of the parameterization (4.2.1), the mechanical energy density in (4.1.1) reads

$$f_{mec}^{\beta}(\mathbf{Q}, \mathbf{F}) = \mu|\widehat{\mathbf{E}} - \gamma\widehat{\mathbf{Q}}|^2 + \beta\mu|\widehat{\mathbf{E}} - \gamma\widehat{\mathbf{Q}}_o|^2 + \frac{\lambda}{2}\Big(\text{tr}\,\widehat{\mathbf{E}} - \frac{\gamma}{3}\Big)^2. \tag{4.2.6}$$

For simplicity, in what follows we drop all the superscripts and we write (4.2.6) as

$$f_{mec}^{\beta}(\mathbf{Q}, \mathbf{F}) = \mu\big|\mathbb{E}_0\big(\mathbf{E} - \gamma\mathbf{Q}\big)\big|^2 + \beta\mu\big|\mathbb{E}_0\big(\mathbf{E} - \gamma\mathbf{Q}_o\big)\big|^2 + K_{II}\Big(\text{tr}\,\mathbf{E} - \frac{\gamma}{3}\Big)^2, \tag{4.2.7}$$

where

$$K_{II} := \Big(\frac{\lambda}{2} + \frac{\mu}{2} + \beta\frac{\mu}{2}\Big). \tag{4.2.8}$$

As in (4.1.3), we introduce new macroscopic models by minimizing (4.2.7) in $\mathbf{Q}$

$$\begin{aligned}g_X^{\beta}(\mathbf{F}) := \inf_{\mathbf{Q}\in\mathcal{Q}_X^{2dim}} f_{mec}^{\beta}(\mathbf{Q}, \mathbf{F}) = \\ \Big(\inf_{\mathbf{Q}\in\mathcal{Q}_X^{2dim}} \mu|\mathbf{E} - \gamma\mathbf{Q}|^2\Big) + \beta\mu|\mathbf{E} - \gamma\mathbf{Q}_o|^2 + \frac{\lambda}{2}\Big(\text{tr}\,\mathbf{E} - \frac{\gamma}{3}\Big)^2,\end{aligned} \tag{4.2.9}$$

where X stands either for Fr or B. In the case $X = Fr$, we can express the dependence of g^{β}_{Fr} on the components of the 2×2 strain matrix introducing the new function

$$g^{\beta}_{Fr}(\mathbf{F}) = \widetilde{g}^{\beta}_{Fr}(e_{11}, e_{22}, e_{12}) = \mu\Big\{2\Big(\frac{e_{11}-e_{22}}{2}\Big)^2 + 2e_{12}^2 + \frac{\gamma^2}{2} - 2\gamma\,\theta_M\big(\mathbb{E}_0(\mathbf{E})\big)\Big\} \tag{4.2.10}$$
$$+\beta\mu\Big\{2\Big(\frac{e_{11}-e_{22}}{2}\Big)^2 + 2e_{12}^2 + \frac{\gamma^2}{2} - 2\gamma\Big(\frac{e_{11}-e_{22}}{2}\Big)\Big\} + K_{II}\Big(e_{11}+e_{22}-\frac{\gamma}{3}\Big)^2,$$

where θ_M is the largest eigenvalue of $\mathbb{E}_0(\mathbf{F})$, equal to

$$\theta_M\big(\mathbb{E}_0(\mathbf{E})\big) = \sqrt{\Big(\frac{e_{11}-e_{22}}{2}\Big)^2 + e_{12}^2}. \tag{4.2.11}$$

It is straightforward to write $\widetilde{g}^{\beta}_{Fr}$ and g^{β}_{Fr} as

$$\widetilde{g}^{\beta}_{Fr}(e_{11}, e_{22}, e_{12}) = (\mu+\beta\mu)\Big\{2\Big(\frac{e_{11}-e_{22}}{2}\Big)^2 + 2e_{12}^2 + \frac{\gamma^2}{2}\Big\} - \tag{4.2.12}$$
$$2\mu\gamma\sqrt{\Big(\frac{e_{11}-e_{22}}{2}\Big)^2 + e_{12}^2} - 2\gamma\beta\mu\Big(\frac{e_{11}-e_{22}}{2}\Big) + K_{II}\Big(e_{11}+e_{22}-\frac{\gamma}{3}\Big)^2,$$

$$g^{\beta}_{Fr}(\mathbf{F}) = (\mu+\beta\mu)dist^2\Big(\mathbb{E}_0(\mathbf{F}), 2R\,\mathbb{E}_0\big(\mathcal{Q}^{2dim}_{Fr}\big)\Big) + \tag{4.2.13}$$
$$K_{II}\Big(\operatorname{tr}\mathbf{F} - \frac{\gamma}{3}\Big)^2 + \mu\frac{\gamma^2}{2}\Big(\beta + \frac{\beta}{1+\beta}\Big) - 2\beta\mu\gamma\Big(\frac{e_{11}(\mathbf{F}) - e_{22}(\mathbf{F})}{2}\Big),$$

where

$$R := \frac{\gamma}{2+2\beta} \tag{4.2.14}$$

and $e_{ij}(\mathbf{F})$ $(i,j \in \{1,2\})$ are the components of the symmetric part of $\mathbf{F}$, that is $e_{ij}(\mathbf{F}) = (F_{ij} + F_{ji})/2$. As anticipated, we calculate explicitly the quasiconvex envelope of g^{β}_{X}. Since g^{β}_{B} is convex, the result in the case $X = B$ is trivial. We are left with g^{β}_{Fr}. In the following, we may adopt the notation $\big(g^{\beta}_{Fr}(\mathbf{F})\big)^{qc} \equiv \big(g^{\beta}_{Fr}\big)^{qc}(\mathbf{F})$ and similarly for the other envelopes.

Proposition 14 *Let* $\mathbf{F} \in \mathbb{M}^{2\times 2}$ *and denote with* $e_{ij} = e_{ij}(\mathbf{F})$ *the components of* $\mathbf{E} = \mathbb{E}(\mathbf{F})$, $i,j \in \{1,2\}$. *Let* g^{β}_{Fr} *as in* (4.2.9) *(*$X = Fr$*) and define*

$$g^{\beta}_{A}(\mathbf{F}) = (\mu+\beta\mu)dist^2\Big(\mathbb{E}_0(\mathbf{F}), 2R\,\mathbb{E}_0\big(\mathcal{Q}^{2dim}_{B}\big)\Big) + \tag{4.2.15}$$
$$K_{II}\Big(\operatorname{tr}\mathbf{F} - \frac{\gamma}{3}\Big)^2 + \mu\frac{\gamma^2}{2}\Big(\frac{\beta^2+2\beta}{1+\beta}\Big) - 2\beta\mu\gamma\Big(\frac{e_{11}(\mathbf{F}) - e_{22}(\mathbf{F})}{2}\Big).$$

Then

$$\Big(g^{\beta}_{Fr}\Big)^{qc}(\mathbf{F}) = g^{\beta}_{A}(\mathbf{F}). \tag{4.2.16}$$

Remark 24 *We write the function* g_A^β *introduced in* (4.2.15) *in components. Let* $\widetilde{g}_A^\beta(e_{11}, e_{22}, e_{12}) = g_A^\beta(\mathbf{F})$ *defined as*

$$\widetilde{g}_A^\beta(e_{11}, e_{22}, e_{12}) = \begin{cases} \widetilde{g}_{Fr}^\beta(e_{11}, e_{22}, e_{12}) & \text{if } \left(\frac{e_{11}-e_{22}}{2}\right)^2 + e_{12}^2 > R^2, \\ \mu\frac{\gamma^2}{2}\Big(\frac{\beta^2+2\beta}{1+\beta}\Big) - 2\beta\mu\gamma\Big(\frac{e_{11}-e_{22}}{2}\Big) + K_{II}\Big(e_{11}+e_{22}-\frac{\gamma}{3}\Big)^2 & \\ & \text{if } \left(\frac{e_{11}-e_{22}}{2}\right)^2 + e_{12}^2 \le R^2. \end{cases} \quad (4.2.17)$$

Proof. To find the quasiconvex envelope of g_{Fr}^β it is enough to prove that the rank-one convex envelope of g_{Fr}^β coincides with its convex envelope and to apply (0.1.58). We show that

$$\left(g_{Fr}^\beta(\mathbf{F})\right)^{rc} \le g_A^\beta(\mathbf{F}) \le \left(g_{Fr}^\beta(\mathbf{F})\right)^c \le \left(g_{Fr}^\beta(\mathbf{F})\right)^{rc}. \quad (4.2.18)$$

The last inequality follows by definition (see (0.1.58)). To prove the second inequality, we recall equations (4.2.13) and (4.2.15). Since $\mathcal{Q}_{Fr}^{2dim} \subset \mathcal{Q}_B^{2dim}$, then $g_A^\beta \le g_{Fr}^\beta$ and, since $\mathcal{Q}_B^{2dim}$ is convex, g_A^β is convex (because it is the sum of convex functions). By taking the convex envelope of g_{Fr}^β we obtain $g_A^\beta \le (g_{Fr}^\beta)^c$. The proof of the first inequality requires an explicit construction. Let us write the orthogonal decomposition of any matrix $\mathbb{M}^{2\times 2} \ni \mathbf{F} = \mathbb{E}_0(\mathbf{E}) + \mathbf{F}^{sk} + \frac{(\mathrm{tr}\,\mathbf{F})}{2}\mathbf{I}$, and let us parameterize the symmetric and the deviatoric part as follows

$$\mathbb{E}(\mathbf{F}) = \begin{pmatrix} e_{11} & e_{12} \\ e_{12} & e_{22} \end{pmatrix}, \quad \mathbb{E}_0(\mathbf{F}) = \gamma\begin{pmatrix} \alpha & \delta \\ \delta & -\alpha \end{pmatrix}, \quad \gamma\alpha = \frac{e_{11}-e_{22}}{2}, \ \gamma\delta = e_{12}. \quad (4.2.19)$$

Notice that if $(\frac{e_{11}-e_{22}}{2})^2 + e_{12}^2 > R^2$, then there is nothing to prove because $g_{Fr}^\beta \equiv g_A^\beta$. Now, suppose that $(\frac{e_{11}-e_{22}}{2})^2 + e_{12}^2 \le R^2$, namely

$$(\alpha^2 + \delta^2) \le \frac{1}{(2+2\beta)^2}. \quad (4.2.20)$$

We employ a *lamination* construction, that is we find two matrices $\mathbf{F}_1, \mathbf{F}_2$ with $rank(\mathbf{F}_1 - \mathbf{F}_2) \le 1$ such that $\mathbf{F} = (1-\nu)\mathbf{F}_1 + \nu\mathbf{F}_2$ with $\nu \in [0,1]$ and $g_A^\beta(\mathbf{F}) = (1-\nu)g_{Fr}^\beta(\mathbf{F}_1) + \nu g_{Fr}^\beta(\mathbf{F}_2)$, thus realizing the minimum in (0.1.57). In order to obtain such matrices, we define

$$\mathbf{E}_{0,1} = \gamma\begin{pmatrix} \alpha & \overline{\delta} \\ \overline{\delta} & -\alpha \end{pmatrix}, \quad \mathbf{E}_{0,2} = \gamma\begin{pmatrix} \alpha & -\overline{\delta} \\ -\overline{\delta} & -\alpha \end{pmatrix}, \quad \mathbf{W}_1 := \gamma\begin{pmatrix} 0 & \overline{\delta} \\ -\overline{\delta} & 0 \end{pmatrix}, \quad (4.2.21)$$

with

$$\overline{\delta} := \sqrt{\frac{1}{(2+2\beta)^2} - \alpha^2}. \quad (4.2.22)$$

Let

$$\nu := \frac{1}{2}\Big(1 - \frac{\delta}{\overline{\delta}}\Big). \tag{4.2.23}$$

Notice that, in view of (4.2.20), then $0 \leq \nu \leq 1$ and $(1-\nu)\overline{\delta} + \nu(-\overline{\delta}) = \delta$, and $\mathbb{E}_0(\mathbf{F}) = (1-\nu)\mathbf{E}_{0,1} + \nu\mathbf{E}_{0,2}$. Define

$$\widetilde{\mathbf{W}} := \mathbf{F}^{sk} - (1-2\nu)\mathbf{W}_1 \tag{4.2.24}$$

and, finally,

$$\mathbf{F}_1 := \mathbf{E}_{0,1} + \mathbf{W}_1 + \widetilde{\mathbf{W}} + \frac{(\operatorname{tr}\mathbf{F})}{2}\mathbf{I}, \qquad \mathbf{F}_2 := \mathbf{E}_{0,2} - \mathbf{W}_1 + \widetilde{\mathbf{W}} + \frac{(\operatorname{tr}\mathbf{F})}{2}\mathbf{I}. \tag{4.2.25}$$

It is straightforward to verify that $\mathbf{F} = (1-\nu)\mathbf{F}_1 + \nu\mathbf{F}_2$ and, since

$$\mathbf{E}_{0,1} + \mathbf{W}_1 = \gamma\begin{pmatrix} \alpha & 2\overline{\delta} \\ 0 & -\alpha \end{pmatrix}, \quad \mathbf{E}_{0,2} - \mathbf{W}_1 = \gamma\begin{pmatrix} \alpha & -2\overline{\delta} \\ 0 & -\alpha \end{pmatrix}, \tag{4.2.26}$$

that $rank(\mathbf{F}_1 - \mathbf{F}_2) \leq 1$. Then, a direct computation shows that the eigenvalues of $\mathbf{E}_{0,1}$ and $\mathbf{E}_{0,2}$ belong to $2R\mathbb{E}_0\big(\mathcal{Q}^{2dim}_{Fr}\big)$ and hence we have

$$g^{\beta}_{Fr}(\mathbf{F}_1) = g^{\beta}_{Fr}(\mathbf{F}_2) = \tag{4.2.27}$$
$$\mu\frac{\gamma^2}{2}\Big(\frac{\beta^2+2\beta}{1+\beta}\Big) - 2\beta\mu\gamma\Big(\frac{e_{11}(\mathbf{F}) - e_{22}(\mathbf{F})}{2}\Big) + K_{II}\Big(\operatorname{tr}\mathbf{F} - \frac{\gamma}{3}\Big)^2 = g^{\beta}_{A}(\mathbf{F}).$$

Now, thanks to the representation formula (0.1.57), it follows that

$$\big(g^{\beta}_{Fr}\big)^{rc}(\mathbf{F}) \leq (1-\nu)g^{\beta}_{Fr}(\mathbf{F}_1) + \nu g^{\beta}_{Fr}(\mathbf{F}_2) = g^{\beta}_{A}(\mathbf{F}). \tag{4.2.28}$$

□

4.2.1 The compressible elastomers: relaxation theorem

Theorem 21 *Let $S \subset \mathbb{R}^2$ be a Lipschitz domain and denote with ∂S_D an open subset of ∂S with positive surface measure. Let g^{β}_{Fr}, g^{β}_{B} as in* (4.2.9) *and g^{β}_{A} as in* (4.2.15)*. Let $\mathbf{v}_o(x) \in H^1(S,\mathbb{R}^2)$. Let us define (here X stands either for Fr, A or B)*

$$\mathrm{G}^{\beta}_{X}(\mathbf{v}) := \int_S g^{\beta}_{X}(\nabla\mathbf{v})dx, \quad \forall\, \mathbf{v} \in H^1(S,\mathbb{R}^2) \tag{4.2.29}$$

$$\mathrm{G}^{\beta,v_o,\partial S_D}_{X}(\mathbf{v}) := \begin{cases} \displaystyle\int_S g^{\beta}_{X}(\nabla\mathbf{v})dx & \text{on } H^1_{\partial S_D}(S,\mathbb{R}^2) + \mathbf{v}_o(x), \\ +\infty & \text{otherwise in } H^1(S,\mathbb{R}^2) \end{cases} \tag{4.2.30}$$

Then,

$$\overline{\mathrm{G}}^{\beta}_{Fr} = \mathrm{G}^{\beta}_{A}, \quad \overline{\mathrm{G}}^{\beta,v_o,\partial S_D}_{Fr} = \mathrm{G}^{\beta,v_o,\partial S_D}_{A}, \quad \overline{\mathrm{G}}^{\beta}_{B} = \mathrm{G}^{\beta}_{B}, \quad \overline{\mathrm{G}}^{\beta,v_o,\partial S_D}_{B} = \mathrm{G}^{\beta,v_o,\partial S_D}_{B}. \tag{4.2.31}$$

It then follows

$$\inf_{H^1(S,\mathbb{R}^2)} \mathrm{G}^{\beta,v_o,\partial S_D}_{Fr}(\mathbf{v}) = \min_{H^1(S,\mathbb{R}^2)} \mathrm{G}^{\beta,v_o,\partial S_D}_{A}(\mathbf{v}). \tag{4.2.32}$$

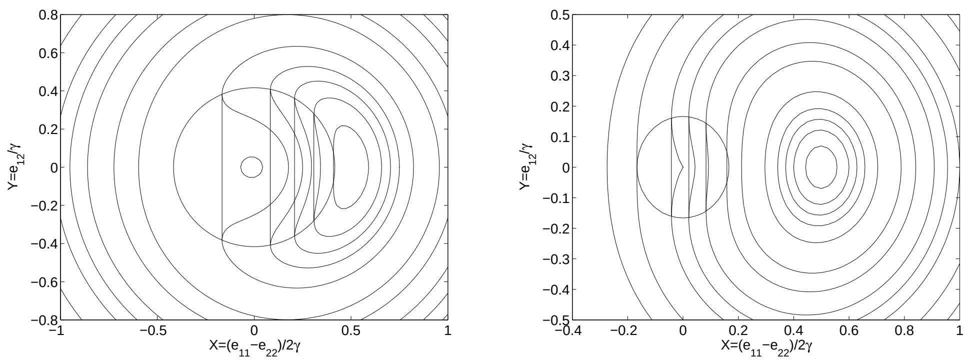

Figure 4.1: Level-curves of $\frac{1}{\gamma^2\mu}\{\widetilde{g}^{\beta}_{Fr} - K_{II}(e_{11}+e_{22}-\gamma/3)^2\}$ and the circumference of coordinates $X^2+Y^2=R^2$. The vertical lines correspond to the level curves of the laminated energy. LEFT: $\beta = 0.2$, RIGHT: $\beta = 2$.

Proof. In the case $X = B$ there is nothing to prove because the functionals are convex. For $X = Fr$, the result is an applications of well-known theorems (see [1] and [8, Theorem 2.3]). The relaxation is the integral of the quasiconvex envelope. By Proposition 14, we have that $(g^{\beta}_{Fr})^{qc} = g^{\beta}_{A}$. □

4.2.2 The incompressible elastomers: relaxation theorem

Theorem 22 *Let $S \subset \mathbb{R}^2$ be a Lipschitz domain and denote with ∂S_D an open subset of ∂S with positive surface measure. Let g^{β}_{Fr}, g^{β}_{B} as in* (4.2.9) *and g^{β}_{A} as in* (4.2.15). *Let $\mathbf{v}_o(x) \in H^1(S,\mathbb{R}^2)$ with $\operatorname{div}\mathbf{v}_o = \gamma/3$ a.e. in S. Let us define (here X stands either for Fr, A or B)*

$$\mathcal{G}^{\beta}_{X}(\mathbf{v}) := \begin{cases} \int_S g^{\beta}_{X}(\nabla\mathbf{v})dx & \text{on } H^1(S,\mathbb{R}^2), \operatorname{div}\mathbf{v} = \gamma/3 \\ +\infty & \text{otherwise in } H^1(S,\mathbb{R}^2) \end{cases} \tag{4.2.33}$$

$$\mathcal{G}^{\beta,v_o,\partial S_D}_{X}(\mathbf{v}) := \begin{cases} \int_S g^{\beta}_{X}(\nabla\mathbf{v})dx & \text{on } H^1_{\partial S_D}(S,\mathbb{R}^2) + \mathbf{v}_o(x), \operatorname{div}\mathbf{v} = \gamma/3 \\ +\infty & \text{otherwise in } H^1(S,\mathbb{R}^2) \end{cases} \tag{4.2.34}$$

Then,

$$\overline{\mathcal{G}}^{\beta}_{Fr} = \mathcal{G}^{\beta}_{A}, \quad \overline{\mathcal{G}}^{\beta,v_o,\partial S_D}_{Fr} = \mathcal{G}^{\beta,v_o,\partial S_D}_{A}, \quad \overline{\mathcal{G}}^{\beta}_{B} = \mathcal{G}^{\beta}_{B}, \quad \overline{\mathcal{G}}^{\beta,v_o,\partial S_D}_{B} = \mathcal{G}^{\beta,v_o,\partial S_D}_{B}. \tag{4.2.35}$$

It then follows

$$\inf_{H^1(S,\mathbb{R}^2)} \mathcal{G}^{\beta,v_o,\partial S_D}_{Fr}(\mathbf{v}) = \min_{H^1(S,\mathbb{R}^2)} \mathcal{G}^{\beta,v_o,\partial S_D}_{A}(\mathbf{v}). \tag{4.2.36}$$

Proof. Again, for $X = B$ there is nothing to prove because the functionals are convex. We prove that $\overline{\mathcal{G}}^{\beta}_{Fr} = \mathcal{G}^{\beta}_{A}$. We employ an idea due to Braides[8] and already used in Chapters 2 and 3. To start, we prove that $\overline{\mathcal{G}}^{\beta}_{Fr} \geq \mathcal{G}^{\beta}_{A}$. Let us define

$$g^{\beta,h}_{Fr}(\mathbf{F}) := g^{\beta}_{Fr}(\mathbf{F}) + h\Big(\operatorname{tr}\mathbf{F} - \frac{\gamma}{3}\Big)^2 = \inf_{\mathbf{Q}\in\mathcal{Q}^{2dim}_{Fr}} \mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}|^2 + \beta\mu|\mathbb{E}(\mathbf{F}) - \gamma\mathbf{Q}_o|^2 + \Big(\frac{\lambda}{2} + h\Big)\Big(\operatorname{tr}\mathbf{F} - \frac{\gamma}{3}\Big)^2,\ h \in \mathbb{N} \tag{4.2.37}$$

and

$$\mathrm{G}^{\beta,h}_{Fr}(\mathbf{v}) := \int_S g^{\beta,h}_{Fr}(\nabla\mathbf{v})dx, \quad \forall\,\mathbf{v} \in H^1(S,\mathbb{R}^2). \tag{4.2.38}$$

By Proposition 14, the relaxation of $\mathrm{G}^{\beta,h}_{Fr}$ is $\mathrm{G}^{\beta,h}_{A}$, that is the functional obtained by integrating in S the energy density defined as

$$g^{\beta,h}_{A}(\mathbf{F}) := g^{\beta}_{A}(\mathbf{F}) + h\Big(\operatorname{tr}\mathbf{F} - \frac{\gamma}{3}\Big)^2 = (\mu+\beta\mu)dist^2\Big(\mathbb{E}_0(\mathbf{F}), 2R\,\mathbb{E}_0\big(\mathcal{Q}^{2dim}_{B}\big)\Big) + \mu\frac{\gamma^2}{2}\Big(\beta + \frac{\beta}{1+\beta}\Big) - 2\beta\gamma\mu\Big(\frac{e_{11}(\mathbf{F}) - e_{22}(\mathbf{F})}{2}\Big) + (K_{II}+h)\Big(\operatorname{tr}\mathbf{F} - \frac{\gamma}{3}\Big)^2. \tag{4.2.39}$$

By applying a well-known property of the Gamma-convergence (see Proposition 2), we observe that

$$\Gamma\text{-}\lim_{h\to+\infty} \mathrm{G}^{\beta,h}_{Fr} = \Gamma\text{-}\lim_{h\to+\infty} \overline{\mathrm{G}}^{\beta,h}_{Fr} = \Gamma\text{-}\lim_{h\to+\infty} \mathrm{G}^{\beta,h}_{A} = \sup_h \mathrm{G}^{\beta,h}_{A}. \tag{4.2.40}$$

Then, by Beppo-Levi's Theorem, we can compute the supremum in (4.2.40) by taking the pointwise limit of the energy densities

$$\lim_{h\to+\infty}\Big[\big(g^{\beta,h}_{Fr}(\mathbf{F})\big)^{qc}\Big] = \sup_h\Big[g^{\beta,h}_{A}(\mathbf{F})\Big] = \begin{cases} g^{\beta}_{A}(\mathbf{F}) & \text{if } \operatorname{tr}\mathbf{F} = \gamma/3, \\ +\infty & \text{otherwise,} \end{cases}$$

and hence

$$\sup_h \mathrm{G}^{\beta,h}_{A} = \mathcal{G}^{\beta}_{A}. \tag{4.2.41}$$

We note that the Gamma-convergence in the weak topology of H^1 is equivalent to the Gamma-convergence in the strong L^2-topology by Korn's inequality (0.1.53). Then, by definition we have

$$\mathcal{G}^{\beta}_{Fr} \geq \mathrm{G}^{\beta,h}_{A}, \quad \forall\, h \in \mathbb{N}. \tag{4.2.42}$$

By taking the supremum in h and taking the relaxation of both sides, we obtain, thanks to (4.2.41):

$$\overline{\mathcal{G}}^{\beta}_{Fr} \geq \mathcal{G}^{\beta}_{A}. \tag{4.2.43}$$

The second inequality $\overline{\mathcal{G}}^{\beta}_{Fr} \leq \mathcal{G}^{\beta}_{A}$ is trivial if $\operatorname{div} \mathbf{v} \neq \gamma/3$. Then, in what follows we suppose $\mathbf{v} \in H^1(S, \mathbb{R}^2)$ and $\operatorname{div} \mathbf{v} = \gamma/3$. We show that there exists a sequence $\{\mathbf{z}_h\}$ with $\operatorname{div} \mathbf{z}_h = \gamma/3$ and $\mathbf{z}_h \rightharpoonup \mathbf{v}$ weakly in $H^1(S, \mathbb{R}^2)$ such that

$$\overline{\mathcal{G}}^{\beta}_{Fr}(\mathbf{v}) \leq \liminf_{h\to+\infty} \mathcal{G}^{\beta}_{Fr}(\mathbf{z}_h) \leq \liminf_{h\to+\infty} \mathrm{G}^{\beta,h}_{Fr}(\mathbf{v}_h), \tag{4.2.44}$$

for any sequence $\{\mathbf{v}_h\}$ in $H^1(S, \mathbb{R}^2)$ weakly converging to $\mathbf{v}$. This yields the claim since, in view of Theorem 21, we have

$$\begin{aligned} \mathcal{G}^{\beta}_{A}(\mathbf{v}) &= \inf\big\{\liminf_{h\to+\infty} \mathrm{G}^{\beta,h}_{Fr}(\mathbf{v}_h), \mathbf{v}_h \rightharpoonup \mathbf{v}\ w\text{-}H^1(S, \mathbb{R}^2)\big\} \qquad (4.2.45)\\ &= \inf\big\{\liminf_{h\to+\infty} \mathrm{G}^{\beta,h}_{Fr}(\mathbf{v}_h), \mathbf{v}_h \rightharpoonup \mathbf{v}\ w\text{-}H^1(S, \mathbb{R}^2), \mathbf{v}_h - \mathbf{v} \in H^1_o(S, \mathbb{R}^2)\big\}. \end{aligned}$$

Moreover, we can assume that the right hand side in (4.2.44) is finite and also uniformly bounded by some constant, so that

$$\|\operatorname{div} \mathbf{v}_h - \gamma/3\|^2_{L^2(S)} \leq Const/h \Longrightarrow \operatorname{div} \mathbf{v}_h \overset{h\to\infty}{\longrightarrow} \gamma/3\ s\text{-}L^2(S). \tag{4.2.46}$$

By Proposition 1 (with $p = n = 2$), there exists some $\mathbf{w}_h \in H^1_o(S, \mathbb{R}^2)$ such that

$$\begin{cases} \operatorname{div} \mathbf{w}_h = \operatorname{div} (\mathbf{v}_h - \mathbf{v}) = \operatorname{div} \mathbf{v}_h - \gamma/3, \\ \|\mathbf{w}_h\|_{H^1(S,\mathbb{R}^2)} \leq C_b \|\operatorname{div} \mathbf{v}_h - \gamma/3\|_{L^2(S)}, \end{cases} \tag{4.2.47}$$

and, in view of (4.2.46), we have that $\mathbf{w}_h \to 0\ s\text{-}H^1(S, \mathbb{R}^2)$ as $h \to +\infty$. Then, if we define

$$\mathbf{z}_h := \mathbf{v}_h - \mathbf{w}_h, \tag{4.2.48}$$

then $\mathbf{z}_h \rightharpoonup \mathbf{v}\ w\text{-}H^1(S, \mathbb{R}^2)$ as $h \to +\infty$, with $\mathbf{z}_h - \mathbf{v}_h \in H^1_o(S, \mathbb{R}^2)$ and $\operatorname{div} \mathbf{z}_h = \gamma/3$. Now, recalling that the distance is a Lipschitz function, the following inequality is straightforward

$$\big|g^{\beta}_{Fr}(\mathbf{F}_1) - g^{\beta}_{Fr}(\mathbf{F}_2)\big| \leq Const\big|\mathbb{E}(\mathbf{F}_1) - \mathbb{E}(\mathbf{F}_2)\big|\Big(|\mathbb{E}(\mathbf{F}_1)| + |\mathbb{E}(\mathbf{F}_2)| + 1\Big), \tag{4.2.49}$$

$\forall\, \mathbf{F}_1, \mathbf{F}_2 \in \mathbb{M}^{2\times 2}$. To conclude, we write

$$\begin{aligned} \overline{\mathcal{G}}^{\beta}_{Fr}(\mathbf{v}) \leq \liminf_{h\to+\infty} \overline{\mathcal{G}}^{\beta}_{Fr}(\mathbf{z}_h) \leq \liminf_{h\to+\infty} \mathcal{G}^{\beta}_{Fr}(\mathbf{z}_h) \leq \liminf_{h\to+\infty} \int_S g^{\beta}_{Fr}(\mathbf{v}_h) dx + \qquad (4.2.50)\\ \lim_{h\to+\infty} \Big|\int_S g^{\beta}_{Fr}(\mathbf{v}_h) dx - \int_S g^{\beta}_{Fr}(\mathbf{z}_h) dx\Big| \leq \liminf_{h\to+\infty} \mathrm{G}^{\beta,h}_{Fr}(\mathbf{v}_h) + 0. \end{aligned}$$

The third inequality in (4.2.50) holds because $\operatorname{div} \mathbf{z}_h = \gamma/3$ and the last inequality is due to (4.2.49).

This proof can be easily adapted also for the relaxation of functionals with slightly different boundary conditions. The relaxation result is immediate for the functional (4.2.34) with $X = Fr$ and where $\partial S_D \equiv \partial S$ that is

$$\mathcal{G}_{Fr}^{\beta,v_o,o}(\mathbf{v}) := \begin{cases} \displaystyle\int_S g_{Fr}^{\beta}(\nabla \mathbf{v})dx & \text{on } H_o^1(S,\mathbb{R}^2) + \mathbf{v}_o(x), \operatorname{div} \mathbf{v} = \gamma/3 \\ +\infty & \text{otherwise in } H^1(S,\mathbb{R}^2). \end{cases} \tag{4.2.51}$$

Then, the general case with $\partial S_D \neq \partial S$ is due to an abstract argument, since, for any $\mathbf{v} \in H^1(S,\mathbb{R}^2)$, we have

$$\mathcal{G}_X^{\beta,\widehat{v}_o,o}(\mathbf{v}) \geq \mathcal{G}_X^{\beta,\widehat{v}_o,\partial S_D}(\mathbf{v}) \geq \mathcal{G}_X^{\beta}(\mathbf{v}) \tag{4.2.52}$$

where $\widehat{\mathbf{v}}_o \equiv \mathbf{v}$. Hence, the relaxation of $\mathcal{G}_X^{\beta,\widehat{v}_o,\partial S_D}$ is equal to $\mathcal{G}_A^{\beta}$ on the subspace $H^1_{\partial S_D}(S,\mathbb{R}^2) + \widehat{\mathbf{v}}_o$ and $+\infty$ outside (because the subspace is weakly closed). $\square$

Discussion. The physical interpretation of this relaxation result is still under investigation[16]. In particular, we believe that a more explicit characterization of the microstructure developed by G_A^{β} and $\mathcal{G}_A^{\beta}$ may arise from the analysis of the family of energies

$$(\mathbf{Q},\mathbf{v}) \mapsto \begin{cases} \displaystyle\int_S \Big\{\varepsilon^2|\nabla \mathbf{Q}|^2 + \mu|\mathbb{E}(\nabla \mathbf{v}) - \gamma \mathbf{Q}|^2 + \beta\mu|\mathbb{E}(\nabla \mathbf{v}) - \gamma \mathbf{Q}_o|^2\Big\}dx \\ \qquad \text{on } H^1(S,\mathcal{Q}_{Fr}^{2dim}) \times H_o^1(S,\mathbb{R}^2) + \mathbf{v}_o(x), \operatorname{div} \mathbf{v} = \gamma/3 \\ +\infty \qquad \text{otherwise in } L^2(S,\mathbb{M}^{2\times 2}) \times H^1(S,\mathbb{R}^2). \end{cases}$$

as $\varepsilon \to 0$, which is left to a forthcoming paper[14].

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