Γ-CONVERGENCE OF ENERGIES FOR NEMATIC ELASTOMERS IN THE SMALL STRAIN LIMIT

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Abstract. We study two variational models recently proposed in the literature to describe the mechanical behaviour of nematic elastomers either in the fully nonlinear regime or in the framework of a geometrically linear theory. We show that, in the small strain limit, the energy functional of the first one Γ-converges to the relaxation of the second one, a functional for which an explicit representation formula is available.

1. Introduction

Nematic elastomers show a very rich and intriguing mechanical response, with a great potential for new technological applications. The properties of these materials, which were synthesized at the end of the 80s, arise from the interaction of electro-optical effects typical of nematic liquid crystals with the elasticity of a rubbery matrix (see [14]). Nematic elastomers exhibit reversible distortions as the material is heated and cooled through the nematic to isotropic phase transition temperature. A uniaxial contraction occurs parallel to the nematic director as a consequence of the ordering of the mesogenic units that are incorporated into a cross-linked polymer network.

The mathematical modelling of the mechanical response of nematic elastomers is already well established, see, e. g., [4], [5], [7]. Here we focus on some model elastic energies: those discussed in [8] and some variants. We work in the framework of a Frank-type theory, in which the liquid crystal order is supposed to be uniaxial with fixed degree of orientation. To describe the mechanical implications of such an order, the following tensor is introduced:

$$L_{\varepsilon,n} := (1+\varepsilon)^2 n\otimes n + (1+\varepsilon)^{-1}(I - n\otimes n), \tag{1.1}$$

where n is a unit vector (nematic director) and $\varepsilon > 0$ is a non-dimensional material parameter. Tensor (1.1) models the spontaneous deformation one can observe in a nematic elastomer as a consequence of the isotropic to nematic phase transition: $(1+\varepsilon)$ is the elongation in the direction along which the nematic director aligns, $(1+\varepsilon)^{-\frac{1}{2}}$ is the contraction along all the orthogonal directions.

Using the notation of Section 4, the energy for isotropic and incompressible nematic elastomers is written as

$$\frac{\mu}{2}\min_{n\in S^2}\left(FF^T\cdot L^{-1}_{\varepsilon,n} - 3\right), \tag{1.2}$$

where $F \in \mathbb{R}^{3\times 3}$ is the deformation gradient. This is a classical expression, studied, e. g., in [5] and [7], and obtained from an earlier proposal by Bladon, Terentjev and Warner (see [1]) by an affine change of variables, first introduced in [6]. This energy is non-negative and attains its minimum value of zero precisely if FF^T is of the form (1.1). The fact these states of deformation are those observed experimentally (under sufficiently small applied loads) is one of the main justifications for the physical soundness of the model.

Moving to the compressible case ($\det F \neq 1$), we consider the expression

$$W_\varepsilon(F) = \min_{n\in S^2} W_{\varepsilon,n}(F), \tag{1.3}$$

where

$$W_{\varepsilon,n}(F) = \begin{cases} \frac{\mu}{2}\left[FF^T \cdot L_{\varepsilon,n}^{-1} - 3 - 2\ln(\det F)\right] + \frac{\lambda}{2}(\det F - 1)^2, & \text{if } \det F > 0 \\ +\infty, & \text{if } \det F \leq 0, \end{cases} \tag{1.4}$$

and μ, $\lambda > 0$ are material constants. This is a natural generalization of (1.2). Indeed, observe that for $\det F = 1$ (1.3) reduces to (1.2). Moreover, W_ε attains its minimum value zero on the set of energy wells

$$\bigcup_{n\in S^2}\left\{RL_{\varepsilon,n}^{\frac{1}{2}} : \ R \in SO(3)\right\} = \left\{RL_{\varepsilon,\hat{n}}^{\frac{1}{2}}Q : \ Q, R \in SO(3)\right\},$$

where $\hat{n}$ is some fixed unit vector. Matrices F in this set are such that FF^T is of the form (1.1). The term in square brackets in (1.4) is motivated by Flory's work on polymer elasticity [9]. The presence of the term $\frac{\lambda}{2}(\det F - 1)^2$ guarantees that the Taylor expansion at order two coincides with isotropic elasticity with two independent natural parameters (shear modulus and bulk modulus, see (1.8) below).

We are interested in providing a justification, via Γ-convergence, of the linearized elasticity theory proposed in [8] on the basis of Taylor expansion, and of its relaxation obtained in [3]. The following theorem achieves this aim.

Theorem 1.1. *Let Ω be a bounded and Lipschitz domain, Γ_D a subset of $\partial\Omega$ of positive surface measure, $h \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ and $H^1_{h,\Gamma_D}(\Omega, \mathbb{R}^3)$ the closure of $\{v \in W^{1,\infty}(\Omega, \mathbb{R}^3) \, : \, v = h \text{ on } \Gamma_D\}$ in $H^1(\Omega, \mathbb{R}^3)$. Consider the energy functionals*

$$\mathscr{E}_\varepsilon(u) = \frac{1}{\varepsilon^2}\int_\Omega W_\varepsilon(I + \varepsilon\nabla u) - \int_\Omega lu,$$

with W_ε defined by (1.3) and (1.4). Then $\{\mathscr{E}_\varepsilon\}$ Γ-converges to

$$\overline{\mathscr{E}}(u) = \int_\Omega V^{qc}(sym\nabla u) - \int_\Omega lu \tag{1.5}$$

with respect to both the strong L^2- and the weak H^1- topology on $H^1_{h,\Gamma_D}(\Omega, \mathbb{R}^3)$. Here, V^{qc} is defined on $Sym(3)$ as

$$V^{qc}(E) = \mu \min_{Q\in\mathscr{Q}} |E_d - Q|^2 + \frac{k}{2}\mathrm{tr}^2 E, \tag{1.6}$$

where $k = \lambda + \frac{2}{3}\mu$,

$$\mathscr{Q} := \{M \in Sym(3) \text{ with eigenvalues in } [-1/2, 1] \text{ and } \mathrm{tr} M = 0\},$$

and

$$E_d = E - \frac{1}{3}\mathrm{tr}(E)I. \tag{1.7}$$

We remark (see [3]) that V^{qc} is the quasiconvex envelope (on linear strains) of

$$V(E) = \mu \min_{n\in S^2} |E_d - U_n|^2 + \frac{k}{2}\mathrm{tr}^2 E, \quad E \in Sym(3), \tag{1.8}$$

where

$$U_n = \frac{3}{2}\left(n \otimes n - \frac{1}{3}I\right), \tag{1.9}$$

and $\overline{\mathscr{E}}$ is the relaxation of

$$\mathscr{E}(u) = \int_\Omega V(sym\nabla u) - \int_\Omega lu. \tag{1.10}$$

Expressions (1.6) and (1.8) show that the parameters μ and $k = \lambda + \frac{2}{3}\mu$ have the physical meaning of a shear modulus and a bulk modulus, respectively.

In the engineering literature, it is customary to write small strain theories using the leading order term of the deviation of the strain from the identity. In other words, one considers $F = I + \nabla v + o(\varepsilon)$, where $|\nabla v| = \varepsilon$, and then writes the energy as a function of v. One easily sees (cfr. Remark 2.2) that this energy is related to (1.10) by a simple scaling and, modulo terms of order higher than two in ε, one obtains

$$\mathscr{E}(v) = \int_\Omega \left\{\mu \min_{n\in S^2} |(sym\nabla v)_d - E_0(n)|^2 + \frac{k}{2}\mathrm{tr}^2(\nabla v)\right\} - \int_\Omega lv, \tag{1.11}$$

where

$$E_0(n) = \frac{3}{2}\varepsilon\left(n \otimes n - \frac{1}{3}I\right),$$

and the corresponding relaxation

$$\overline{\mathscr{E}}(v) = \int_\Omega \left\{\mu \min_{Q\in\mathscr{Q}} |(sym\nabla v)_d - \varepsilon Q|^2 + \frac{k}{2}\mathrm{tr}^2(\nabla v)\right\} - \int_\Omega lv.$$

This relaxed functional may prove very useful to set up effective numerical schemes in applications where one is interested in the behaviour of global energy minimizers, similarly to what has been done in [4], [5]. When, instead, local minimizers or dynamics are studied (see, e. g., [2] and [10]), (1.11) describes the correct energetics.

2. Proof of Theorem 1.1

Our result is an application of the abstract theory developed by B. Schmidt in [13]. In this work, linearized theories are derived from nonlinear elasticity theory for multi-well energies. More precisely, the author considers a family of frame indifferent multi-well energies W_ε, defined on the space of the deformation gradients $\mathbb{R}^{d\times d}$, which are minimized and equal to zero at $SO(d)U_1(\varepsilon), ..., SO(d)U_N(\varepsilon)$. Here, for $i = 1, ..., N$, $U_i(\varepsilon)$ is a symmetric matrix of the form

$$U_i(\varepsilon) = I + \varepsilon U_i + o(\varepsilon).$$

Notice that, for ε small enough, $U_i(\varepsilon)$ is positive definite. Moreover, standard regularity conditions and orientation preserving are assumed, together with the hypothesis that

$$W_\varepsilon(F) \geq C\mathrm{dist}^2(F, SO(d)\mathscr{U}_\varepsilon)$$

for every $F \in \mathbb{R}^{d\times d}$, where $\mathscr{U}_\varepsilon = \bigcup_{i=1}^N \{U_i(\varepsilon)\}$.

Under these natural assumptions on the (nonlinear) energy densities, suitable rescalings of the energy functionals are considered:

$$\mathscr{E}_\varepsilon(u) = \frac{1}{\varepsilon^2}\int_\Omega W_\varepsilon(I + \varepsilon\nabla u) - \int_\Omega lu.$$

Theorem 2.1 in [13] states what follows: define $V_\varepsilon : Sym(d) \to \mathbb{R}$ as

$$V_\varepsilon(E) = \frac{1}{\varepsilon^2} W_\varepsilon(I + \varepsilon E),$$

and suppose that $\{V_\varepsilon\}$ converges uniformly on compact sets of $Sym(d)$ to a function V satisfying

$$V(E) \leq \alpha(1 + |E|^2) \tag{2.1}$$

(in this case, V is called the "linear limit" of W_ε). Then $\{\mathscr{E}_\varepsilon\}$ Γ-converges, with respect to both the strong L^2- and the weak H^1- topology on $H^1_{h,\Gamma_D}(\Omega, \mathbb{R}^3)$ (see Theorem 1.1 for a definition), to the relaxation of

$$\mathscr{E}(u) = \int_\Omega V(sym\nabla u) - \int_\Omega lu,$$

which is given by

$$\overline{\mathscr{E}}(u) = \int_\Omega V^{qc}(sym\nabla u) - \int_\Omega lu,$$

where V^{qc} is the quasiconvexification on linear strains of V (see [13] for a definition). One class of energy densities which is explicitly analysed in [13] is of the form

$$W_\varepsilon(F) = \min_{i=1,\dots N} W_{\varepsilon,i}(F), \tag{2.2}$$

where, for $i = 1, ..., N$, $W_{\varepsilon,i}$ are admissible single-well energies, minimized and equal to zero, respectively, at $SO(d)U_i(\varepsilon)$. In [13, Proposition 3.3] it is shown that the linear limit of such a family of energy densities is

$$V(E) = \frac{1}{2} \min_{i=1,\dots,N} < a_i(E - U_i), E - U_i >,$$

where $a_i = d^2 W_{\varepsilon,i}(U_i(\varepsilon))$. The double-well case $N = 2$ with $a_1 = a_2$ is of particular interest since, in this case, an explicit formula for the quasiconvex envelope of V is available [12].

The energy densities (1.3) we consider in this paper can be viewed as an infinite-dimensional analogue of (2.2). To handle this case, an extension of the theory for energy densities with wells which vary on a compact is required. For this purpose, we generalize the results in [13] to the following class of "admissible" energy densities.

Definition 2.1. *We say that W_ε is an* admissible *family of energy densities if, for every ε small enough, it satisfies:*

(i) $W_\varepsilon : \mathbb{R}^{d\times d} \to [0, +\infty]$ *is frame indifferent;*
(ii) $W_\varepsilon(F) = 0 = \min_{\mathbb{R}^{d\times d}} W_\varepsilon$ *for every* $F \in SO(d)\mathscr{U}_\varepsilon$*, with*

$$\mathscr{U}_\varepsilon := \{U \in Sym(d) \ : \ U = I + \varepsilon\hat{U} + o(\varepsilon), \ \hat{U} \in \mathscr{M}\}, \tag{2.3}$$

where $\mathscr{M}$ is a compact in $\mathbb{R}^{d\times d}$;
(iii) W_ε *is measurable and continuous in a ε-independent neighbourhood of I;*
(iv) *there exists a constant C not depending on ε and F such that*

$$W_\varepsilon(F) \geq C\mathrm{dist}^2(F, SO(d)\mathscr{U}_\varepsilon); \tag{2.4}$$

(v) $W_\varepsilon(F) = +\infty$*, if* $\det F \leq 0$.

The generalization of [13, Theorem 2.1] to this class of energies does not require any change in its proof. Indeed, for such a proof, condition (ii) and (iv) of the previous definition can be replaced by the condition

$$W_\varepsilon(F) \geq c\,\mathrm{dist}^2(F, SO(d)) - C\varepsilon^2,$$

for some c, $C > 0$, see [13, Remark 2.9]. Observe that this condition is implied by (2.3) and (2.4): let

$$\mathrm{dist}(F, SO(d)\mathscr{U}_\varepsilon) = |F - RU|,$$

for some $R \in SO(d)$ and $U = I + \varepsilon\hat{U} + o(\varepsilon)$, $\hat{U} \in \mathscr{M}$. Since $\hat{U}$ varies in the compact $\mathscr{M}$, we have that

$$|F - R| \leq |F - RU| + |U - I| \leq \mathrm{dist}(F, SO(d)\mathscr{U}_\varepsilon) + K\varepsilon,$$

and therefore

$$\mathrm{dist}(F, SO(d)) \leq \mathrm{dist}(F, SO(d)\mathscr{U}_\varepsilon) + K\varepsilon,$$

for some $K > 0$ and every $\varepsilon > 0$ small enough.
We now move to the specific energies for nematic elastomers and focus on the three-dimensional case $d = 3$. Let us introduce

$$\mathscr{U}_\varepsilon = \{U_{\varepsilon,n} := L_{\varepsilon,n}^{\frac{1}{2}} \ : \ n \in S^2\}, \tag{2.5}$$

and observe that, expanding (1.1) in ε around zero, we obtain

$$L_{\varepsilon,n} = I + \varepsilon L_n + o(\varepsilon), \quad \text{with} \ \ L_n = 3\left(n \otimes n - \frac{1}{3}I\right). \tag{2.6}$$

Similarly, from

$$U_{\varepsilon,n} = (1+\varepsilon)n \otimes n + (1+\varepsilon)^{-\frac{1}{2}}(I - n \otimes n),$$

we have that

$$U_{\varepsilon,n} = I + \varepsilon U_n + o(\varepsilon), \tag{2.7}$$

with $U_n = \frac{1}{2}L_n$ defined as in (1.9). This shows that $\mathscr{U}_\varepsilon$ is a class of type (2.3).

In order to apply [13, Theorem 2.1], we have to check that $\{W_\varepsilon\}$ is an admissible family of energy densities in the sense of Definition 2.1 and then compute the limit which defines V and verify that this limit is uniform on compact sets of $Sym(3)$. Once the expression of V is known, it is easy to check that it satisfies the growth condition (2.1). Finally, we use the results in [3] to obtain the explicit characterization (1.6) of the quasiconvex hull (on linear strains) of V. Throughout this section, we label with $\lambda_1(M) \geq \lambda_2(M) \geq \lambda_3(M)$ the ordered eigenvalues of the 3×3 symmetric matrix M.

Proof of Theorem 1.1. We start by verifying the admissibility of $\{W_\varepsilon\}$. By the definition of W_ε as a minimum over S^2, it is easy to check that W_ε is frame-indifferent, while (iii) and (v) of Definition 2.1 clearly hold. To prove (ii), notice that, if $\det F > 0$, then

$$W_\varepsilon(F) = \frac{\mu}{2} f_\varepsilon^{opt}(FF^T) + \frac{\lambda}{2}(\det F - 1)^2,$$

where f_ε^{opt} is defined as in (4.3) (specialized to dimension 3). By Proposition 4.1, this is minimal at the value 0 on $SO(3)\mathscr{U}_\varepsilon$. Notice that $SO(3)\mathscr{U}_\varepsilon = \mathscr{U}_\varepsilon SO(3)$. To prove that (iv) holds for W_ε, we restrict attention to the non-trivial case $\det F > 0$ and look separately at three regimes: the case F far from $SO(3)$, the case F close to $SO(3)$ and the intermediate regime. Thus, we divide the proof into three steps.

In what follows, we use the standard convention and denote by C a generic positive constant whose exact value may change from line to line.
Step 1. We prove that there exist $\alpha > 0$ and $C_1 > 0$ such that, for every ε small enough and for every $F \in \mathbb{R}^{3\times 3}$,

$$\text{if } \operatorname{dist}(F, SO(3)) \le \alpha, \text{ then } W_\varepsilon(F) \ge C_1 \operatorname{dist}^2(F, SO(3)\mathscr{U}_\varepsilon).$$

We can write $W_{\varepsilon,n}(F) = \tilde{W}_{\varepsilon,n}(FF^T)$, where $\tilde{W}_{\varepsilon,n}$ is defined on $Psym(3)$ by

$$\tilde{W}_{\varepsilon,n}(B) = \frac{\mu}{2} f(B, L_{\varepsilon,n}) + \frac{\lambda}{2}(\sqrt{\det B} - 1)^2, \tag{2.8}$$

and f defined as in (4.1) with $d = 3$. Let $\operatorname{dist}(F, SO(3)) \le \alpha$, with $\alpha > 0$ to be chosen later. Then $|FF^T - I| \le \alpha^2 + 2\alpha$ and FF^T belongs to the closed ball centered in $L_{\varepsilon,n}$ and with radius $2\alpha^2 + 4\alpha$, for every ε small enough. Thus, for α small enough, we can expand $\tilde{W}_{\varepsilon,n}$ around $L_{\varepsilon,n}$:

$$\tilde{W}_{\varepsilon,n}(FF^T) = \tilde{W}_{\varepsilon,n}(L_{\varepsilon,n}) + d\tilde{W}_{\varepsilon,n}(L_{\varepsilon,n})[FF^T - L_{\varepsilon,n}] + \\ + \frac{1}{2} d^2\tilde{W}_{\varepsilon,n}(L_{\varepsilon,n})[FF^T - L_{\varepsilon,n}]^2 + R_\alpha, \tag{2.9}$$

where

$$|R_\alpha| \le C_\alpha |FF^T - L_{\varepsilon,n}|^3, \tag{2.10}$$

for a certain positive constant C_α, which depends on α but not on ε and n. From Proposition (4.1), both $\tilde{W}_{\varepsilon,n}$ and its differential $d\tilde{W}_{\varepsilon,n}$ vanish at $L_{\varepsilon,n}$. Moreover, simple calculations give

$$d\tilde{W}_{\varepsilon,n}(B)[H] = \frac{\mu}{2}[H \cdot L_{\varepsilon,n}^{-1} - B^{-T} \cdot H] + \frac{\lambda}{2}(\sqrt{\det B} - 1)\sqrt{\det B} B^{-T} \cdot H,$$

and in turn

$$d^2\tilde{W}_{\varepsilon,n}(L_{\varepsilon,n})[H]^2 = \frac{\mu}{2}\operatorname{tr}(L_{\varepsilon,n}^{-1}H)^2 + \frac{\lambda}{4}\operatorname{tr}^2 L_{\varepsilon,n}^{-1} H, \tag{2.11}$$

for every $B \in Psym(3)$ and $H \in Sym(3)$. Observe that

$$d^2\tilde{W}_{\varepsilon,n}(L_{\varepsilon,n})[H]^2 \ge \frac{\mu}{2}\operatorname{tr}(L_{\varepsilon,n}^{-1}H)^2 \ge \frac{\mu}{4}|H|^2, \tag{2.12}$$

for every ε sufficiently small and every n. Thus, from (2.9), (2.10) and (2.12) it turns out that

$$\begin{aligned} W_{\varepsilon,n}(F) &= \frac{1}{2} d^2\tilde{W}_{\varepsilon,n}(L_{\varepsilon,n})[FF^T - L_{\varepsilon,n}]^2 + R_\alpha \\ &\ge \frac{\mu}{8}|FF^T - L_{\varepsilon,n}|^2 + R_\alpha \\ &\ge \frac{\mu}{8}|FF^T - L_{\varepsilon,n}|^2 \left(1 - \frac{8C_\alpha}{\mu}|FF^T - L_{\varepsilon,n}|\right), \end{aligned}$$

for every ε small enough. Now, it is possible to choose $\alpha > 0$ such that the parenthesis in the last inequality is arbitrarily close to one and hence

$$W_{\varepsilon,n}(F) \ge C|FF^T - L_{\varepsilon,n}|^2.$$

Therefore, since $|\sqrt{G} - \sqrt{H}| \le C|G - H|$ for every G, $H \in Psym(3)$, if H is sufficiently near I, then there exists a constant $C_1 > 0$, not depending on F, ε and n, such that

$$W_{\varepsilon,n}(F) \ge C_1 |\sqrt{FF^T} - U_{\varepsilon,n}|^2.$$

Then, we can conclude by using the following inequalities:

$$W_\varepsilon(F) := \min_{n\in S^2} W_{\varepsilon,n}(F) \geq C_1 \min_{n\in S^2} |\sqrt{FF^T} - U_{\varepsilon,n}|^2 \geq C_1 \mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon).$$

Step 2. Let α be the constant found in the first step. We now show that there exists $C_2 > 0$ such that, for every ε small enough,

$$\text{if } \mathrm{dist}(F, SO(3)) > \alpha, \text{ then } W_\varepsilon(F) \geq C_2.$$

Recall that, by polar decomposition, $|\sqrt{FF^T} - I| = \mathrm{dist}(F, SO(3))$ (see [11, Ex. 7, p. 17] for more details). Thus, if $\mathrm{dist}(F, SO(3)) > \alpha$, by Lemma 4.3 with $B = FF^T$ and $d = 3$, there exists $\delta \in (0, 1)$ such that, if

$$\det FF^T \in [1 - \delta, 1 + \delta],$$

then $f^\varepsilon_{opt} > \frac{\alpha^2}{2}$ for every ε small enough and therefore

$$W_\varepsilon(F) = \frac{\mu}{2} f^\varepsilon_{opt}(FF^T) + \frac{\lambda}{2}(\det F - 1)^2 > \frac{\mu\alpha^2}{4} > 0.$$

On the other hand, if $\det FF^T \in \mathbb{R} \setminus [1 - \delta, 1 + \delta]$, then

$$W_\varepsilon(F) \geq \frac{\lambda}{2}(\det F - 1)^2 \geq \frac{\lambda}{2} \min\{1, \delta^2\} > 0.$$

Step 3. Finally, we prove that there exists β large enough such that,

$$\text{if } \mathrm{dist}(F, SO(3)) > \beta, \text{ then } W_\varepsilon(F) \geq C_3 \mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon)$$

for a certain $C_3 > 0$ and for every ε small enough.
By using Proposition (4.1) with $d = 3$ and writing $\lambda_i = \lambda_i(\sqrt{FF^T})$, we have that

$$W_\varepsilon(F) \geq \frac{\mu}{2}[(1 + \varepsilon)^{-2}\lambda_1^2 + (1 + \varepsilon)(\lambda_2^2 + \lambda_3^2) - 3 - 2\ln(\lambda_1\lambda_2\lambda_3)].$$

Therefore, since $(1 + \varepsilon)^{-2}$, $(1 + \varepsilon)$ tend to 1 as ε tends to zero, we have that, for ε small enough,

$$W_\varepsilon(F) \geq \frac{\mu}{2}\left[\frac{|F|^2}{2} - 3 - \ln(\lambda_1\lambda_2\lambda_3)^2\right]. \tag{2.13}$$

By using the inequality between arithmetic and geometric mean, we obtain from (2.13)

$$\begin{aligned} W_\varepsilon(F) &\geq \frac{\mu}{2}\left[\frac{|F|^2}{2} - 3 - 3\ln\frac{|F|^2}{3}\right] \\ &> \frac{\mu}{2}\left[\frac{|F|^2}{2} - 3\ln|F|^2\right], \end{aligned}$$

so that, if $|F|$ is sufficiently large, we have that $W_\varepsilon(F) \geq \frac{\mu}{8}|F|^2$. Thus, if β is large enough, we have that

$$W_\varepsilon(F) \geq C|FF^T - I|, \tag{2.14}$$

for a certain constant $C > 0$. Now, observe that

$$|\sqrt{FF^T} - I|^2 = \sum_{i=1}^3(\lambda_i - 1)^2 \leq \sqrt{3\sum_{i=1}^3(\lambda_i^2 - 1)^2} + 6 = \sqrt{3}|FF^T - I| + 6. \tag{2.15}$$

Thus, if ε is small enough, from (2.7) and (2.15) we have that

$$\begin{aligned}\frac{1}{2}|\sqrt{FF^T}-U_{\varepsilon,n}|^2 &\leq |\sqrt{FF^T}-I|^2+|I-U_{\varepsilon,n}|^2\\ &\leq \sqrt{3}|FF^T-I|+6+|\varepsilon U_n+o(\varepsilon)|^2\\ &\leq \sqrt{3}|FF^T-I|+7\frac{C}{\beta}\frac{\beta}{C}\\ &< \left(\sqrt{3}+7\frac{C}{\beta}\right)|FF^T-I|, \qquad (2.16)\end{aligned}$$

for every $n\in S^2$. From (2.14) and (2.16), by choosing $\beta>0$ sufficiently large, we can conclude that there exists $C_3>0$ such that for every $\varepsilon>0$ small enough

$$W_\varepsilon(F)\geq C_3|\sqrt{FF^T}-U_{\varepsilon,n}|^2,$$

and in turn

$$W_\varepsilon(F)\geq C_3\mathrm{dist}^2(F,SO(3)\mathscr{U}_\varepsilon).$$

The quadratic growths established by steps 1 and 3, together with the estimate in step 2, show that we can bound W_ε with a single function, growing with the square of the distance, so that (2.4) holds.

Next, we compute the linear limit

$$V(E)=\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^2}W_\varepsilon(I+\varepsilon E),\quad E\in Sym(3).$$

Observe that

$$V(E)=\min_{n\in S^2}\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^2}\tilde{W}_{\varepsilon,n}((I+\varepsilon E)(I+\varepsilon E)^T),$$

where $\tilde{W}_{\varepsilon,n}$ is defined as in (2.8). Since $\tilde{W}_{\varepsilon,n}$ and its gradient vanish at $L_{\varepsilon,n}$, we have that

$$\begin{aligned}V(E)=\min_{n\in S^2}\lim_{\varepsilon\to 0}\Big\{&\frac{1}{2\varepsilon^2}d^2\tilde{W}_{\varepsilon,n}(L_{\varepsilon,n})[(I+\varepsilon E)(I+\varepsilon E)^T-L_{\varepsilon,n}]^2\\ &+\frac{1}{\varepsilon^2}o(|(I+\varepsilon E)(I+\varepsilon E)^T-L_{\varepsilon,n}|^2)\Big\},\end{aligned}$$

and then, from (2.6),

$$V(E)=\frac{1}{2}\min_{n\in S^2}d^2\tilde{W}_{0,n}(I)[2E-L_n]^2.$$

Observe that the limit is uniform on compact subsets of $Sym(3)$. From (2.11), it turns out that

$$\begin{aligned}V(E) &= \frac{1}{2}\min_{n\in S^2}\frac{\mu}{2}\mathrm{tr}(2E-L_n)^2+\frac{\lambda}{4}\mathrm{tr}^2(2E-L_n)\\ &= \frac{1}{2}\min_{n\in S^2}2\mu\mathrm{tr}(E-U_n)^2+\lambda\mathrm{tr}^2(E-U_n)\\ &= \mu\min_{n\in S^2}|E-U_n|^2+\frac{\lambda}{2}\mathrm{tr}^2E, \qquad (2.17)\end{aligned}$$

where in the second identity we used the fact that $L_n=2U_n$, with U_n defined as in (1.9). Clearly, V satisfies the growth condition (2.1).

Finally, we establish (1.5) and (1.6). Since U_n is traceless, we prefer to write the second summand of (2.17) in terms of the deviatoric part E_d of E, as defined in (1.7). Thus, since

$$|E-U_n|^2=|E_d-U_n|^2+\frac{\mathrm{tr}^2 E}{3} \tag{2.18}$$

and $\lambda=k-\frac{2}{3}\mu$, we obtain (1.8) and in turn

$$\mathscr{E}(u)=\int_\Omega\left\{\mu\min_{n\in S^2}|(sym\nabla u)_d-U_n|^2+\frac{k}{2}\mathrm{tr}^2(\nabla u)\right\}-\int_\Omega lu, \tag{2.19}$$

which is the functional that has to be relaxed in order to obtain (1.5). This can be done by using [3, Theorem 1] with $\gamma=1$, $\mathscr{Q}$ in place of $\mathscr{Q}_B$ and the set

$$\left\{U_n=\frac{3}{2}\left(n\otimes n-\frac{1}{3}I\right)\ :\ n\in S^2\right\}$$

of 3×3 traceless matrices with eigenvalues $1,-\frac{1}{2},-\frac{1}{2}$, in place of $\mathscr{Q}_{Fr}$. Observe that in [3] the relaxation of (2.19) is obtained by the quasiconvexification of the integrand seen as a function of $F=\nabla u\in\mathbb{R}^{3\times3}$. This is equivalent to the quasiconvexification on linear strains of the integrand seen as a function of $E=sym\nabla u\in Sym(3)$.
The proof of Theorem 1.1 is thus concluded. □

Remark 2.2. *By frame indifference,*

$$\lim_{\varepsilon\to0}\frac{W_\varepsilon(I+\varepsilon\nabla u)}{\varepsilon^2}=\lim_{\varepsilon\to0}\frac{W_\varepsilon\left(\sqrt{(I+\varepsilon\nabla u)(I+\varepsilon\nabla u)^T}\right)}{\varepsilon^2}. \tag{2.20}$$

Thus, by Taylor expansion,

$$V(sym\nabla u):=\lim_{\varepsilon\to0}\frac{W_\varepsilon(I+\varepsilon sym\nabla u)}{\varepsilon^2}=\lim_{\varepsilon\to0}\frac{W_\varepsilon(I+\varepsilon\nabla u)}{\varepsilon^2}.$$

At the same time, again from (2.20), we have that

$$V(sym\nabla u)=\lim_{\varepsilon\to0}\frac{\tilde{W}_\varepsilon(I+2\varepsilon sym\nabla u)}{\varepsilon^2},$$

for a certain $\tilde{W}_\varepsilon$ defined on $Sym(3)$. Notice that, while W_ε is defined as a function of F, $\tilde{W}_\varepsilon$ is defined as a function of $B=FF^T$. Observe also that, from the definition of V, we have

$$W_\varepsilon\left(I+\varepsilon\frac{E}{|E|}\right)=\varepsilon^2V\left(\frac{E}{|E|}\right),\quad E\in Sym(3)\setminus\{0\},$$

modulo terms of order higher than two in ε. Therefore, if $|E|=\varepsilon$,

$$\begin{aligned}W_\varepsilon\left(I+\varepsilon\frac{E}{|E|}\right)&=\varepsilon^2\left\{\mu\min_{n\in S^2}\left|\frac{E_d}{\varepsilon}-U_n\right|^2+\frac{k}{2\varepsilon^2}\mathrm{tr}^2E\right\}\\&=\mu\min_{n\in S^2}|E_d-\varepsilon U_n|^2+\frac{k}{2}\mathrm{tr}^2E.\end{aligned}$$

We can recognize in the last expression the formula for the energy in the small deformations regime obtained in [8].

3. An alternative model

It is natural to explore the small strain behaviour of another class of model energies, discussed in [8], and obtained from the Warner-Terentjev incompressible template (1.2), by a procedure which is quite common in rubber elasticity and computational mechanics. This is based on the additive split of the energy density into a distortional term (invariant under the transformation $F \to \alpha F$, with α a positive scalar), obtained from (1.2) by replacing F with $(\det F)^{-\frac{1}{3}}F$, and a volumetric term (which only depends on $\det F$). Using the notation of Section 4, the resulting energy is of the form

$$W_{1,\varepsilon}(F) = \min_{n\in S^2} W_{1,\varepsilon,n}(F), \tag{3.1}$$

where

$$W_{1,\varepsilon,n}(F) = \begin{cases} \frac{\mu}{2}(\det F)^{-\frac{2}{3}}FF^T \cdot L_{\varepsilon,n}^{-1} - \frac{3}{2}\mu + \frac{k}{2}(\det F - 1)^2, & \text{if } \det F > 0, \\ +\infty, & \text{if } \det F \leq 0, \end{cases} \tag{3.2}$$

and $L_{\varepsilon,n}$ is given by (1.1) for $\varepsilon > 0$ and $n \in S^2$. $W_{1,\varepsilon}$ is again a natural generalization of (1.2) because it coincides with it for $\det F = 1$, it has the same set of energy wells

$$SO(3)\mathscr{U}_\varepsilon = \bigcup_{n\in S^2} \left\{ RL_{\varepsilon,n}^{\frac{1}{2}} : \quad R \in SO(3) \right\}$$

as (1.3) and the same behaviour near the energy wells (same linear limit (1.8) or, equivalently, same Taylor expansion at order two). However, $W_{1,\varepsilon}$ violates the hypothesis of quadratic growth with respect to $\mathrm{dist}(F, SO(3)\mathscr{U}_\varepsilon)$ (see Remark 3.2). Therefore, we cannot apply to it the abstract theory of [13]: the characterization of the Γ-limit of the functionals

$$\mathscr{E}_{1,\varepsilon}(u) = \frac{1}{\varepsilon^2}\int_\Omega W_{1,\varepsilon}(I + \varepsilon\nabla u) - \int_\Omega lu \tag{3.3}$$

requires an extension of Schmidt's theory.

While Schmidt's theory does not apply to (3.1), it does apply to energies with quadratic growth that are obtained from (3.1) by changing its functional form only for matrices F such that, simultaneously, $\mathrm{dist}(F, SO(3))$ and $\det F$ are large. More in detail, we define, for $\beta > 0$,

$$W_\varepsilon^\beta(F) = \begin{cases} W_{1,\varepsilon}(F), & \text{if either } \ \mathrm{dist}(F, SO(3)) \leq \beta \ \text{ or } \ \det F \leq \beta \\ W_2(F), & \text{otherwise,} \end{cases} \tag{3.4}$$

where W_2 is any function of F such that $W_2(F) \geq C\mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon)$ for some constant $C > 0$, whenever $\det F > \beta$ and $\mathrm{dist}(F, SO(3)) > \beta$. W_ε^β has the same set of energy wells $SO(3)\mathscr{U}_\varepsilon$ of (3.1), for every $\beta > 0$. Moreover, $W_{1,\varepsilon}$ and W_ε^β have the same linear limit (1.8). Since the threshold β can be made arbitrarily large, (3.4) modifies energy (3.1) only in a regime in which $|F|$ and $\det F$ are very large. It is well-known from rubber elasticity that, in such extreme regimes, neohookean-type energies such as (1.2), in which the energy depends linearly on FF^T, are unable to reproduce the experimentally observed behaviour. In fact, expression (1.2) is best regarded as a conceptual tool to explore the behaviour of nematic elastomers under small applied forces, i. e., near the energy wells. The correction W_2 in (3.4) can thus be seen as a technical device with no mechanical significance, since it alters the values of the energy in a regime of deformations where expression (1.2), and hence (3.1), is no longer reliable.

Once the legitimacy of the correction (3.4) is accepted, we can compute the small strain Γ-limit of all energies of this type for every β sufficiently large. They all share the same Γ-limit, which is independent of β. This is not surprising since, looking at the proof of Theorem 1.1, it is clear that the important features of the energy densities involved are their behaviour near the energy wells (the only part which is involved in the computation of the linear limit: this is given by (1.8), which is independent of β), and the growth condition (2.4) (which is true for every β large enough). We thus have the following theorem.

Theorem 3.1. *Under the same assumptions of Theorem 1.1, consider the energy functionals*

$$\mathscr{E}_\varepsilon^\beta(u) = \frac{1}{\varepsilon^2}\int_\Omega W_\varepsilon^\beta(I+\varepsilon\nabla u) - \int_\Omega lu, \tag{3.5}$$

with W_ε^β defined by (3.1), (3.2) and (3.4) for $\beta > 0$. Then, for every β sufficiently large, $\{\mathscr{E}_\varepsilon^\beta\}$ Γ-converges to $\overline{\mathscr{E}}$, where $\overline{\mathscr{E}}$ is given by (1.5) and (1.6), with respect to both the strong L^2- and the weak H^1- topology on $H^1_{h,\Gamma_D}(\Omega,\mathbb{R}^3)$.

Proof of Theorem 3.1. Let us verify the admissibility of $\{W_\varepsilon^\beta\}$ in the sense of Definition 2.1. It is clear that (i), (iii) and (v) of Definition 2.1 hold. To prove (ii), consider the non-trivial case $\det F > 0$, and notice that, if $\operatorname{dist}(F, SO(3)) > \beta$ and $\det F > \beta$, $W_\varepsilon^\beta(F)$ is non-negative, otherwise

$$W_\varepsilon^\beta(F) = \frac{\mu}{2} g_\varepsilon^{opt}(FF^T) + \frac{k}{2}(\det F - 1)^2, \tag{3.6}$$

where g_ε^{opt} is defined as in (4.8) with $d = 3$. By Proposition 4.2, expression (3.6) is minimal at the value 0 on $SO(3)\mathscr{U}_\varepsilon$, where $\mathscr{U}_\varepsilon$ is defined in (2.5). Next, we prove that (iv) holds for W_ε^β, for every β large enough. More precisely, we want to prove that for every β sufficiently large there exists a constant $C_\beta > 0$ such that $W_\varepsilon^\beta(F) \geq C_\beta \operatorname{dist}^2(f, SO(3)\mathscr{U}_\varepsilon)$ for every F and every $\varepsilon > 0$ small enough. In view of the definition of W_ε^β, it is enough to prove that there exists $\beta_1 > 0$ such that, for every $\beta \geq \beta_1$,

$$W_\varepsilon^1(F) \geq C_\beta \operatorname{dist}^2(f, SO(3)\mathscr{U}_\varepsilon),$$

whenever $\operatorname{dist}(F, SO(3)) \leq \beta$ or $\det F \leq \beta$, and $\varepsilon > 0$ is sufficiently small. We divide the proof of this in the following three steps and restrict attention to the non-trivial case $\det F > 0$.
Step 1. We prove that there exist $\alpha > 0$ and $C_1 > 0$ such that, for every ε small enough and for every $F \in \mathbb{R}^{3\times 3}$,

$$\text{if } \operatorname{dist}(F, SO(3)) \leq \alpha, \text{ then } W_{1,\varepsilon}(F) \geq C_1 \operatorname{dist}^2(F, SO(3)\mathscr{U}_\varepsilon).$$

This can be shown as done in step 1 of the proof of Theorem 1.1: we use the expansion of $\tilde{W}_{1,\varepsilon,n}$ around $L_{\varepsilon,n}$, where $\tilde{W}_{1,\varepsilon,n}$ is defined in (4.14) and $W_{1,\varepsilon,n}(F) = \tilde{W}_{1,\varepsilon,n}(FF^T)$, and we use Lemma 4.5 to conclude.
Step 2. Let α be the constant found in the first step. We want to show that there exists $C_2 > 0$ such that, for every ε small enough,

$$\text{if } \operatorname{dist}(F, SO(3)) > \alpha, \text{ then } W_{1,\varepsilon}(F) \geq C_2.$$

Again, the proof is the same of step 2 of the proof of Theorem 1.1, by using Lemma 4.4 in place of Lemma 4.3.
Step 3. Finally, we prove that there exists β_1 large enough such that, for every $\beta \geq \beta_1$,

$$\text{if } \mathrm{dist}(F, SO(3)) > \beta \text{ and } \det F \leq \beta, \text{ then } W_{1,\varepsilon}(F) \geq C_\beta \mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon),$$

for every ε small enough.
By using Proposition (4.2) and writing $\lambda_i = \lambda_i(\sqrt{FF^T})$, we have that

$$\begin{aligned} W_{1,\varepsilon}(F) &\geq \frac{\mu}{2}(\det F)^{-\frac{2}{3}}[\lambda_1^2(1+\varepsilon)^{-2} + \lambda_2^2(1+\varepsilon) + \lambda_3^2(1+\varepsilon)] - \frac{3}{2}\mu \\ &\geq \frac{\mu}{2\beta^{\frac{2}{3}}}[\lambda_1^2(1+\varepsilon)^{-2} + \lambda_2^2(1+\varepsilon) + \lambda_3^2(1+\varepsilon)] - \frac{3}{2}\mu. \end{aligned}$$

Therefore, since $(1+\varepsilon)^{-2}$, $(1+\varepsilon)$ tend to 1 as ε tends to zero, we have that, for ε small enough,

$$W_{1,\varepsilon}(F) \geq \frac{\mu}{4\beta^{\frac{2}{3}}}[\lambda_1^2 + \lambda_2^2 + \lambda_3^2] - \frac{3}{2}\mu = \frac{\mu}{4\beta^{\frac{2}{3}}}|FF^T| - \frac{3}{2}\mu. \tag{3.7}$$

Observe that $\beta < |\sqrt{FF^T} - I| \leq C|FF^T - I|$. Thus, if β_1 is large enough, on one hand, from (3.7), we have that for every $\beta \geq \beta_1$

$$W_{1,\varepsilon}(F) \geq \tilde{C}_\beta |FF^T - I|; \tag{3.8}$$

on the other hand, proceeding as in (2.15)-(2.16), we obtain again that, for every ε small enough,

$$\frac{1}{2}|\sqrt{FF^T} - U_{\varepsilon,n}|^2 < \left(\sqrt{3} + 7\frac{C}{\beta}\right)|FF^T - I|, \tag{3.9}$$

for every $n \in S^2$. From (3.8) and (3.9) we can conclude that for every $\beta \geq \beta_1$ and every $\varepsilon > 0$ sufficiently small,

$$W_{1,\varepsilon}(F) \geq C_\beta |\sqrt{FF^T} - U_{\varepsilon,n}|^2,$$

for a certain $C_\beta > 0$, from which

$$W_{1,\varepsilon}(F) \geq C_\beta \mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon).$$

The quadratic growths established by steps 1 and 3, together with the estimate in step 2, show that we can bound $W_{1,\varepsilon}$ with a single function, growing with the square of the distance, in the case $\mathrm{dist}(F, SO(3)) \leq \beta$ or $\det B \leq \beta$.

Now, let us compute the linear limit

$$\hat{V}(E) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} W_\varepsilon^\beta(I + \varepsilon E), \quad E \in Sym(3).$$

It is clear that

$$\begin{aligned} \hat{V}(E) &= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} W_{1,\varepsilon}(I + \varepsilon E) \\ &= \min_{n \in S^2} \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} W_{1,\varepsilon,n}(I + \varepsilon E) \\ &= \min_{n \in S^2} \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \tilde{W}_{1,\varepsilon,n}((I + \varepsilon E)(I + \varepsilon E)^T), \end{aligned}$$

where $\tilde{W}_{1,\varepsilon,n}$ is defined as in (4.14). Since $\tilde{W}_{1,\varepsilon,n}$ and its gradient vanish at $L_{\varepsilon,n}$, we have that

$$\hat{V}(E) = \min_{n\in S^2}\lim_{\varepsilon\to 0}\left\{\frac{1}{2\varepsilon^2}d^2\tilde{W}_{1,\varepsilon,n}(L_{\varepsilon,n})[(I+\varepsilon E)(I+\varepsilon E)^T - L_{\varepsilon,n}]^2 \right.$$
$$\left. + \frac{1}{\varepsilon^2}o(|(I+\varepsilon E)(I+\varepsilon E)^T - L_{\varepsilon,n}|^2)\right\},$$

and then, from (2.6),

$$\hat{V}(E) = \frac{1}{2}\min_{n\in S^2} d^2\tilde{W}_{1,0,n}(I)[2E - L_n]^2.$$

From (4.17) and from the fact that $L_n = 2U_n$, it turns out that

$$\hat{V}(E) = \mu\min_{n\in S^2}|E-U_n|^2 + \left(\frac{k}{2}-\frac{\mu}{3}\right)\mathrm{tr}^2 E = V(E), \quad E\in Sym(3),$$

where V is given by (1.8). As done in the proof of Theorem 3.1, by using (2.18) and [3, Theorem 1], we obtain (1.6) and then the thesis. □

We remark again that, even if the Γ-limits of (3.5) are all the same, independent of β, this says nothing about the Γ-limit of (3.3). In fact, $W_{1,\varepsilon}(F) \geq C\,\mathrm{dist}^{\frac{3}{2}}(F, SO(3)\mathscr{U}_\varepsilon)$ for $|F|$ large enough (as can be seen using Young's inequality) and $W_{1,\varepsilon}$ violates the hypothesis of quadratic growth on $\mathbb{R}^{3\times 3}$ (see the following remark), while Schmidt's theory requires quadratic growth. Characterizing the Γ-limit of (3.3), and establishing whether this coincides with the Γ-limit of (3.5) requires an extension of Schmidt's theory. These are interesting questions, and will be addressed in future work.

Remark 3.2. *$W_{1,\varepsilon}$ does not have a quadratic growth in $\mathrm{dist}(F, SO(3)\mathscr{U}_\varepsilon)$ in the regime of large determinant and norm. By Proposition 4.2, we have that*

$$W_{1,\varepsilon}(F) = \frac{\mu}{2}(\det F)^{-\frac{2}{3}}[\lambda_1^2(1+\varepsilon)^{-2} + \lambda_2^2(1+\varepsilon) + \lambda_3^2(1+\varepsilon)] - \frac{3}{2}\mu + \frac{k}{2}(\det F - 1)^2,$$

where $\lambda_i = \lambda_i(\sqrt{FF^T})$. More generally, consider an energy of the form

$$G_\varepsilon(F) = \frac{\mu}{2}(\det F)^{-\frac{2}{3}}[\lambda_1^2(1+\varepsilon)^{-2} + \lambda_2^2(1+\varepsilon) + \lambda_3^2(1+\varepsilon)] + g(\det F),$$

with g any scalar-valued function which goes to $+\infty$ as $\det F \to +\infty$. We observe that G_ε cannot satisfy

$$G_\varepsilon(F) \geq C\mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon) \quad \textit{for every } F\in\mathbb{R}^{3\times 3},$$

for a certain $C>0$ and for any ε small enough. Indeed, G_ε doesn't satisfy this growth condition if F has both norm and determinant arbitrarily large.

In order to prove this, given a fixed arbitrary constant $C>0$, we have to show that for every $\hat{\varepsilon}>0$ there exists $\varepsilon<\hat{\varepsilon}$ and $F\in\mathbb{R}^{3\times 3}$ such that

$$G_\varepsilon(F) < C\mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon).$$

Indeed, let F be of the form

$$\begin{bmatrix} \lambda g(\lambda)(1+\varepsilon) & 0 & 0 \\ 0 & \frac{(1+\varepsilon)^{-\frac{1}{2}}}{\lambda g(\lambda)} & 0 \\ 0 & 0 & \lambda(1+\varepsilon)^{-\frac{1}{2}} \end{bmatrix}$$

with $\varepsilon < \hat{\varepsilon}$ and $\lambda \in \mathbb{R}$ to be chosen later. It turns out that

$$G_\varepsilon(F) = \frac{\mu}{2}\lambda^{-\frac{2}{3}}\left[\lambda^2 g^2(\lambda) + \frac{1}{\lambda^2 g^2(\lambda)} + \lambda^2\right] + g(\lambda),$$

which behaves as $\lambda^{2-\frac{2}{3}} g^2(\lambda)$ for λ large. At the same time, when $\varepsilon \to 0$,

$$\mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon) \longrightarrow (\lambda g(\lambda) - 1)^2 + \left(\frac{1}{\lambda g(\lambda)} - 1\right)^2 + (\lambda - 1)^2.$$

Thus, for any $\delta > 0$, we can find $\varepsilon < \hat{\varepsilon}$ such that

$$\mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon) > (\lambda g(\lambda) - 1)^2 + \left(\frac{1}{\lambda g(\lambda)} - 1\right)^2 + (\lambda - 1)^2 - \delta. \tag{3.10}$$

Now, if we choose λ large enough such that

$$G_\varepsilon(F) \leq C\left[(\lambda g(\lambda) - 1)^2 + \left(\frac{1}{\lambda g(\lambda)} - 1\right)^2 + (\lambda - 1)^2 - \delta\right],$$

we can conclude from (3.10) that

$$G_\varepsilon(F) < C\mathrm{dist}^2(F, SO(3)\mathscr{U}_\varepsilon),$$

as claimed.

4. Appendix: some results from tensor calculus

We use the following notation: $Sym(d)$, $Psym(d)$, $Orth(d)$ and $SO(d)$ denote the set of matrices in $\mathbb{R}^{d\times d}$ which are symmetric, positive definite and symmetric, orthogonal, rotations, respectively. We label with $\lambda_1(M) \geq \lambda_2(M) \geq ... \geq \lambda_d(M)$ the ordered eigenvalues of a matrix $M \in Sym(d)$, and with $B \cdot L = \mathrm{tr}(BL^T)$ the scalar product between two matrices B, $L \in \mathbb{R}^{d\times d}$.

The next proposition is a slight variant of [8, Proposition 1].

Proposition 4.1. *Let B, $L \in \mathbb{R}^{d\times d}$ and consider, where defined, the scalar-valued function*

$$f(B, L) = B \cdot L^{-1} - d - \ln(\det B). \tag{4.1}$$

The following properties hold:

(i) *for every $L \in Psym(d)$ with $\det L = 1$, we have that*

$$\min_{B\in Psym(d)} f(B, L) = f(L, L) = 0;$$

(ii) *assume that L is of the form*

$$L_{\varepsilon,n} := (1+\varepsilon)^2 n \otimes n + (1+\varepsilon)^{-\frac{2}{(d-1)}}(I - n \otimes n), \tag{4.2}$$

for $\varepsilon > 0$ and n belonging to the unitary sphere S^{d-1}. Then, for every $B \in Psym(d)$, we have that

$$f^\varepsilon_{opt}(B) := \min_{n\in S^{d-1}} f(B, L_{\varepsilon,n}) = (1+\varepsilon)^{-2}\lambda_1(B) + (1+\varepsilon)^{\frac{2}{d-1}}\left[\mathrm{tr}B - \lambda_1(B)\right] - d - \ln(\det B); \tag{4.3}$$

(iii) *for every* $\varepsilon > 0$,

$$\min_{B \in Psym(d)} f^{\varepsilon}_{opt}(B) = 0$$

and this minimum is obtained by any matrix in $Psym(d)$ *whose largest eigenvalue is* $(1+\varepsilon)^2$ *and whose other eigenvalues are all equal to* $(1+\varepsilon)^{-\frac{2}{(d-1)}}$.

Proof. To prove (i), let $\{b_1, ..., b_d\}$ and $\{l_1, ..., l_d\}$ be the orthonormal bases of eigenvectors of B, $L \in Psym(d)$, respectively. Then

$$\begin{aligned} B \cdot L^{-1} &= \left(\sum_{i=1}^{d} \lambda_i(B) b_i \otimes b_i \right) \cdot \left(\sum_{j=1}^{d} \lambda_j(L^{-1}) l_j \otimes l_j \right) \\ &= \sum_{i,j=1}^{d} \lambda_i(B)\lambda_j(L^{-1})(b_i l_j)^2 \geq \sum_{i=1}^{d} \lambda_i(B)\lambda_i(L^{-1})(b_i l_i)^2. \end{aligned}$$

Observe that the equality holds if and only if $b_i l_j = 0$ for all $i \neq j$; thus, in order to minimize $f(\cdot, L)$, we restrict our attention to the case in which both B and L are in diagonal form. Then, by using the well-known inequality between arithmetic and geometric mean and the fact that $\det L = 1$, we have that

$$\begin{aligned} f(B, L) &= \sum_{i=1}^{d} \lambda_i(B)\lambda_i(L^{-1}) - d - \ln(\det B) && (4.4) \\ &\geq d(\det BL^{-1})^{\frac{1}{d}} - d - \ln(\det B) && (4.5) \\ &= d\psi(\alpha), && (4.6) \end{aligned}$$

where $\psi(\alpha) := \alpha - 1 - \ln \alpha$ and $\alpha := (\det B)^{\frac{1}{d}}$. Since $\psi \geq 0$ and $\psi(\alpha) = 0$ if and only if $\alpha = 1$, we have, from (4.4)-(4.6), that $f(B, L) = 0$ if and only if $\lambda_i(B)\lambda_i(L^{-1}) = \lambda_j(B)\lambda_j(L^{-1})$ for every i, $j \in \{1, ..., d\}$ and $\alpha = 1$. These conditions are equivalent to

$$1 = \det B \det L^{-1} = \prod_{i=1}^{d} \lambda_i(B)\lambda_i(L^{-1}) = \left[\lambda_i(B)\lambda_i(L^{-1})\right]^d, \quad \text{for every } i = 1, ..., d,$$

which gives $B = L$.
To prove (ii), let us fix $\hat{n} \in S^{d-1}$ and observe that

$$L^{-1}_{\varepsilon,\hat{n}} = (1+\varepsilon)^{\frac{2}{d-1}} \left[I - \left(1 - (1+\varepsilon)^{-\frac{2d}{d-1}} \right) \hat{n} \otimes \hat{n} \right].$$

Clearly,

$$f^{\varepsilon}_{opt}(B) = \min_{R \in Orth(d)} f(B, RL_{\varepsilon,\hat{n}}R^T),$$

thus

$$\begin{aligned} f^{\varepsilon}_{opt}(B) &= (1+\varepsilon)^{\frac{2}{d-1}} \min_{R \in Orth(d)} B \cdot \left[I - \left(1 - (1+\varepsilon)^{-\frac{2d}{d-1}} \right) R\hat{n} \otimes R\hat{n} \right] - d - \ln(\det B) \\ &= (1+\varepsilon)^{\frac{2}{d-1}} \min_{R \in Orth(d)} \left[\mathrm{tr} B - \left(1 - (1+\varepsilon)^{-\frac{2d}{d-1}} \right) BR\hat{n} \cdot R\hat{n} \right] - d - \ln(\det B). \end{aligned}$$

From the last equality we deduce that the minimum is attained when R maps $\hat{n}$ onto the maximum eigenvalue of B and thus the thesis follows.

To prove (iii), observe that

$$\begin{aligned}\min_{B\in Psym(d)} f^{\varepsilon}_{opt}(B) &= \min_{n\in S^{d-1}}\min_{B\in Psym(d)} f(B,L_{\varepsilon,n})\\ &= \min_{n\in S^{d-1}} f(L_{\varepsilon,n},L_{\varepsilon,n})=0,\end{aligned}$$

where the last equality follows from (i). □

We also use the following result, which we state without proof.

Proposition 4.2. *Let $B,\ L\in\mathbb{R}^{d\times d}$ and consider, where defined, the scalar-valued function*

$$g(B,L)=(\det B)^{-\frac{1}{d}}B\cdot L^{-1}-d. \tag{4.7}$$

The following statements hold:

(i) *for every $L\in Psym(d)$ with $\det L=1$, we have that*

$$\min_{B\in Psym(d)} g(B,L)=g(\alpha L,L)=0,\quad \textit{for every } \alpha>0;$$

(ii) *assume that $L=L_{\varepsilon,n}$, for some $\varepsilon>0$ and $n\in S^{d-1}$, where $L_{\varepsilon,n}$ is defined in (4.2). Then, for every $B\in Psym(d)$, we have that*

$$\begin{aligned}g^{\varepsilon}_{opt}(B):=\min_{n\in S^{d-1}} g(B,L_{\varepsilon,n})=(\det B)^{-\frac{1}{d}}\Big\{&(1+\varepsilon)^{-2}\lambda_1(B)\\ &+(1+\varepsilon)^{\frac{2}{(d-1)}}\left[\mathrm{tr}B-\lambda_1(B)\right]\Big\}-d;\end{aligned} \tag{4.8}$$

(iii) *for every $\varepsilon>0$,*

$$\min_{B\in Psym(d)} g^{\varepsilon}_{opt}(B)=0$$

and this minimum is obtained by any matrix in $Psym(d)$ whose largest eigenvalue is $\alpha(1+\varepsilon)^2$ and whose other eigenvalues are all equal to $\alpha(1+\varepsilon)^{-\frac{2}{(d-1)}}$, for some $\alpha>0$.

We now collect some results from tensor calculus that we used in the Section 2 and 3.

Lemma 4.3. *Let $B\in Psym(d)$ and suppose that $|\sqrt{B}-I|>\alpha>0$. There exists $\delta\in(0,1)$ such that, if*

$$\det B\in[1-\delta,1+\delta],$$

then, for every ε small enough,

$$f^{\varepsilon}_{opt}(B)>\frac{\alpha^2}{2}>0,$$

where f^{ε}_{opt} is the function defined in (4.3).

Proof. From the expression of f^{ε}_{opt} given in point (ii) of Proposition 4.1, it is clear that for a parameter $\eta\in(0,1)$ to be chosen and for every ε small enough, we have that

$$f^{\varepsilon}_{opt}(B)>\eta\,\mathrm{tr}B-d-\ln(\det B). \tag{4.9}$$

Now, if we write $\lambda_i=\lambda_i(\sqrt{B})$, the hypothesis $|\sqrt{B}-I|^2>\alpha^2$ becomes

$$\sum_{i=1}^{d}(\lambda_i-1)^2>\alpha^2.$$

Expanding the squares and using again the inequality between arithmetic and geometric mean, we obtain

$$\begin{aligned} \mathrm{tr}B = \sum_{i=1}^{d} \lambda_i^2 &> \alpha^2 - d + 2\sum_{i=1}^{d} \lambda_i \\ &\geq \alpha^2 - d + 2d(\det B)^{\frac{1}{2d}}. \end{aligned} \tag{4.10}$$

From (4.9) and (4.10) it descends that

$$\begin{aligned} f_{opt}^{\varepsilon}(B) &> \eta\left[\alpha^2 - d + 2d(\det B)^{\frac{1}{2d}}\right] - d - \ln(\det B) \\ &\geq \eta\left[\alpha^2 - d + 2d(1-\delta)^{\frac{1}{2d}}\right] - d - \ln(1+\delta) := K, \end{aligned} \tag{4.11}$$

where in the last inequality we are supposing $\det B$ to vary in $[1-\delta, 1+\delta]$, with $\delta \in (0,1)$ a parameter to be chosen. Finally, since the right hand side of (4.11) tends to α^2 as $\eta \to 1^-$ and $\delta \to 0^+$, we can choose η sufficiently near 1 and δ sufficiently near 0 such that $K \geq \frac{\alpha^2}{2}$ and the thesis follows. □

Lemma 4.4. *Let $B \in Psym(d)$ and suppose that $|\sqrt{B} - I| > \alpha > 0$. There exists $\delta \in (0,1)$ such that, if*

$$\det B \in [1-\delta, 1+\delta],$$

then, for every ε small enough,

$$g_{opt}^{\varepsilon}(B) > \frac{\alpha^2}{2},$$

where g_{opt}^{ε} is the function defined in (4.8).

Proof. From the expression of g_{opt}^{ε}, we have that, for a parameter $\eta \in (0,1)$ to be chosen and for any ε small enough,

$$g_{opt}^{\varepsilon}(B) > \eta(\det B)^{-\frac{1}{d}}\mathrm{tr}B - d. \tag{4.12}$$

Now, as in the proof of Lemma 4.3, consider (4.10) (where $\lambda_i = \lambda_i(\sqrt{B})$), which descends from the hypothesis. From (4.12) and (4.10) we obtain that

$$\begin{aligned} g_{opt}^{\varepsilon}(B) &> \eta(\det B)^{-\frac{1}{d}}\left[\alpha^2 - d + 2d(\det B)^{\frac{1}{2d}}\right] - d \\ &\geq \frac{\eta}{(1+\delta)^{\frac{1}{d}}}\left[\alpha^2 - d + 2d(1-\delta)^{\frac{1}{2d}}\right] - d := K, \end{aligned} \tag{4.13}$$

where in the last inequality we are supposing $\det B$ to vary in $[1-\delta, 1+\delta]$, with $\delta \in (0,1)$ a parameter to be chosen. Since the right hand side of (4.13) tends to α^2 as $\eta \to 1^-$ and $\delta \to 0^+$, we can choose η sufficiently near 1 and δ sufficiently near 0 such that $K \geq \frac{\alpha^2}{2}$ and the thesis follows. □

Lemma 4.5. *Let μ and k be two positive constants. For $\varepsilon > 0$ and $n \in S^2$, let $\tilde{W}_{1,\varepsilon,n}$ be the scalar-valued function which, to each $B \in Psym(3)$, gives the value*

$$\tilde{W}_{1,\varepsilon,n}(B) = \frac{\mu}{2} g(B, L_{\varepsilon,n}) + \frac{k}{2}(\sqrt{\det B} - 1)^2, \tag{4.14}$$

where g and $L_{\varepsilon,n}$ are defined in (4.7) and (4.2), specialized to dimension 3, respectively. Then, there exists a positive constant C such that

$$d^2\tilde{W}_{1,\varepsilon,n}(L_{\varepsilon,n})[S]^2 \geq C|S|^2$$

for every $n \in S^2$, $S \in Sym(3)$, and for every ε small enough.

Proof. For $B \in Psym(3)$, let $h_1(B) = (\det B)^{-\frac{1}{3}} B$ and $h_2(B) = (\sqrt{\det B} - 1)^2$. Then, for every $S \in Sym(3)$, we have

$$dh_1(B)[S] = -\frac{1}{3}(\det B)^{-\frac{1}{3}}(B^{-1} \cdot S)B + (\det B)^{-\frac{1}{3}} S,$$

and

$$dh_2(B)[S] = (\det B - \sqrt{\det B})B^{-1} \cdot S.$$

By some computations, we obtain:

$$\begin{aligned} d^2 h_1(B)[S,H] = \frac{1}{9}(\det B)^{-\frac{1}{3}}(B^{-1} \cdot S)(B^{-1} \cdot H)B+ \\ + \frac{1}{3}(\det B)^{-\frac{1}{3}}[(B^{-1}HB^{-1}) \cdot S]B - \frac{1}{3}(\det B)^{-\frac{1}{3}}(B^{-1} \cdot S)H- \\ - \frac{1}{3}(\det B)^{-\frac{1}{3}}(B^{-1} \cdot H)S, \end{aligned}$$

and

$$\begin{aligned} d^2 h_2(B)[S,H] = \left(\det B - \frac{\sqrt{\det B}}{2}\right)(B^{-1} \cdot S)(B^{-1} \cdot H)- \\ - (\det B - \sqrt{\det B})(B^{-1}HB^{-1}) \cdot S, \end{aligned}$$

for every S, $H \in Sym(3)$. Thus, if $L = L_{\varepsilon,n}$ for some ε and n, we have that

$$d^2 h_1(L)[S]^2 = \frac{1}{9}(L^{-1} \cdot S)^2 L + \frac{1}{3}[(L^{-1}SL^{-1}) \cdot S]L - \frac{2}{3}(L^{-1} \cdot S)S, \tag{4.15}$$

and

$$d^2 h_2(L)[S]^2 = \frac{1}{2}(L^{-1} \cdot S)^2, \tag{4.16}$$

for every $S \in Sym(3)$. Since $g(B,L) = h_1(B) \cdot L^{-1} - 3$, by using (4.15) and (4.16) we obtain that

$$\begin{aligned} d^2 \tilde{W}_{1,\varepsilon,n}(L)[S]^2 &= \frac{\mu}{2} d^2 h_1(L)[S]^2 \cdot L^{-1} + \frac{k}{2} d^2 h_2(L)[S]^2 \\ &= \frac{\mu}{2}\left[-\frac{1}{3}(L^{-1} \cdot S)^2 + (L^{-1}SL^{-1}) \cdot S\right] + \frac{k}{4}(L^{-1} \cdot S)^2, \end{aligned}$$

and therefore, by the fact that $(L^{-1}SL^{-1}) \cdot S = \mathrm{tr}(L^{-1}S)^2$, that

$$2d^2 \tilde{W}_{1,\varepsilon,n}(L)[S]^2 = \left(\frac{k}{2} - \frac{\mu}{3}\right)\mathrm{tr}^2(L^{-1}S) + \mu\,\mathrm{tr}(L^{-1}S)^2. \tag{4.17}$$

Now, since for every $H \in Sym(3)$ one has that $\mathrm{tr}^2 H \le 3\mathrm{tr} H^2$, then

$$2d^2 \tilde{W}_{1,\varepsilon,n}(L_{\varepsilon,n})[S]^2 \ge \min\left\{\mu, \frac{3}{2}k\right\}\mathrm{tr}(L_{\varepsilon,n}^{-1}S)^2.$$

The conclusion follows from the fact that $\mathrm{tr}(L_{\varepsilon,n}^{-1}S)^2 \ge \frac{1}{4}|S|^2$ for every ε sufficiently small. □

Acknowledgments

We wish to thank G. Dal Maso and B. Schmidt for helpful discussions.

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