OGDEN-TYPE ENERGIES FOR NEMATIC ELASTOMERS

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Abstract. Ogden-type extensions of the free–energy densities currently used to model the mechanical behavior of nematic elastomers are proposed and analyzed. Based on a multiplicative decomposition of the deformation gradient into an elastic and a spontaneous or remanent part, they provide a suitable framework to study the stiffening response at high imposed stretches. Geometrically linear versions of the models (Taylor expansions at order two) are provided and discussed. These small strain theories provide a clear illustration of the geometric structure of the underlying energy landscape (the energy grows quadratically with the distance from a non–convex set of spontaneous strains or energy wells). The comparison between small strain and finite deformation theories may also be useful in the opposite direction, inspiring finite deformation generalizations of small strain theories currently used in the mechanics of active and phase-transforming materials. The energy well structure makes the free–energy densities non–convex. Explicit quasi–convex envelopes are provided, and applied to compute the stiffening response of a specimen tested in plane strain extension experiments (pure shear).

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1. Introduction

Nematic elastomers are rubbery elastic solids made of cross-linked polymeric chains with embedded nematic mesogens. Their mechanical response is governed by the coupling of rubber elasticity with the orientational order of a liquid crystalline phase. In particular, nematic elastomers exhibit large spontaneous deformations which can be triggered and controlled by temperature, applied electric fields, irradiation by UV light. These properties make them interesting as materials for fast soft actuators and justify the considerable attention that they have attracted in recent years. The reader is referred to the monograph by Warner and Terentjev [26] for a thorough introduction to the physics of nematic elastomers, and for an extensive list of references.

Theoretical modeling of the mechanical response of nematic elastomers has concentrated on the occurrence of equilibrium configurations exhibiting fine domain patterns (stripe domains), and the stress plateau associated with rearrangement of stripe domains in stretching experiments (soft elasticity). Starting from the pioneering work of Warner, Terentjev, and their collaborators [5, 26], several models have been proposed [1, 7, 16, 17, 19, 27, 28]. The model based on the free–energy density put forward in [5] is particularly worth mentioning, both for its fundamental nature and for its success at reproducing (and even predicting) essential features

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of experimental observations. In fact, energy minimizing states computed with this model replicate experimental evidence with a remarkable degree of accuracy. Examples include the highly nontrivial spatially dependent domain structures observed in [29] and simulated numerically in [10, 11], the existence of a plateau in the stress–strain response in some uniaxial extension experiments [18, 10, 11], and the decay of shear moduli in stretching experiments when the imposed stretch reaches the ends of the stress plateau [4, 15, 21].

While the Warner-Terentjev model has been quite successful at reproducing observed material instabilities (stripe domains and soft elasticity, which are associated with the non-convexity of the proposed energies), it is unlikely that it will predict accurately stress-build-up at large imposed stretches. The reason is the Neo-Hookean form of the expression for the free–energy density, which results from the assumption of phantom gaussian chains made in its derivation from statistical mechanics. Just as in classical rubber elasticity, stress–strain curves showing the typical hardening response of rubbers at high strains and stresses requires the use of functional forms richer than the Neo-Hookean template. Inspired by the seminal work of Ogden [20], we provide here Ogden-type extensions of the Warner-Terentjev model to the regime of very high strains, and also include finite compressibility effects.

The main new results contained in this paper are the following. By exploiting a multiplicative decomposition of the deformation gradient into an elastic and a remanent or spontaneous part, we propose in Section 3 some new Ogden-type expressions for the free–energy density of nematic elastomers, and provide a template for further extensions. In Section 4 we compute the geometrically linear version (Taylor expansion at order two) of the new models, which shows the geometric structure of the underlying energy landscape in a very transparent fashion: the energy grows quadratically with the distance from the non-convex set of spontaneous strains (energy wells). Energies of this type are very common in the theoretical and computational mechanics community, especially in the context of active and phase-transforming materials [3]. Our discussion of their relation with a parent fully nonlinear theory may have the additional side benefit of inspiring generalizations in the opposite direction, namely, finite deformation generalizations of existing small strain theories for active materials.

Because of their "energy well" structure with multiple energy wells, the energies we deal with are invariably non–convex. In Section 5 we provide explicit formulas for their quasi–convex envelopes, and apply them to a simple thought experiment (pure–shear) to demonstrate their use and their potential at reproducing the stiffening behavior at very large imposed strains that is typical of elastomeric materials.

2. Classical expressions for the energy density

Let n be a unit vector denoting the current orientation of the nematic director, and let n_r be a reference orientation (e. g., the first basis vector of a given cartesian frame). The expression for the energy density proposed by Warner and Terentjev [5, 26] to model incompressible nematic elastomers is

$$\overline{W}_n(\overline{F}) = \frac{c}{2}\left[\mathrm{tr}\left(L_{n_r}\overline{F}^T L_n^{-1}\overline{F}\right) - 3\right], \quad \det\overline{F} = 1, \tag{2.1}$$

where $c > 0$ is a material parameter (controlling the rubber energy scale), tr denotes the trace operator, and

$$L_n := \alpha_\parallel^2 n\otimes n + \alpha_\perp^2 (I - n\otimes n), \qquad |n| = 1, \tag{2.2}$$

where

$$\alpha_{\parallel} = a^{\frac{1}{3}}, \quad \alpha_{\perp} = a^{-\frac{1}{6}}, \quad a = \left(\frac{\alpha_{\parallel}}{\alpha_{\perp}}\right)^2 > 1, \tag{2.3}$$

with a a material parameter (the step-length anisotropy quantifying the magnitude of the spontaneous stretch along n accompanying the isotropic-nematic phase transformation). Moreover, in (2.1), $\overline{F} = \nabla\overline{y}$ is the gradient of the deformation $\overline{y}$ mapping the minimum energy configuration associated with n_r into the current configuration, and $\overline{F}^T$ is the transpose of $\overline{F}$. Notice that, in view of (2.3), we have

$$\alpha_{\parallel}^2\alpha_{\perp}^4 = \det L_n = 1. \tag{2.4}$$

Following [12, 13] (see also the discussion in [15, Section 3]), we choose as reference configuration the minimum energy configuration associated with the high-temperature isotropic state, see Figure 1.

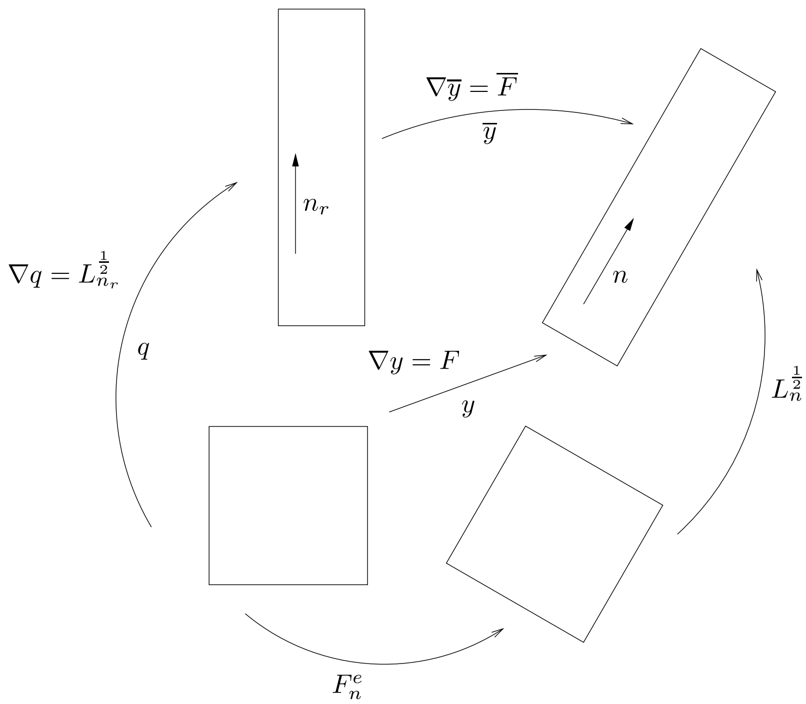

Figure 1. Schematic diagram illustrating two possible choices of reference configuration (the one for y and the other for $\overline{y}$) and the elastic part F_n^e of the deformation gradient F.

Introducing the affine change of variables q, with $\nabla q = L_{n_r}^{\frac{1}{2}}$, we set

$$y = \overline{y} \circ q,$$

where $\circ$ denotes the composition of the maps $\overline{y}$ and q, and let $F := \nabla y$. We have

$$\overline{F} = F L_{n_r}^{-\frac{1}{2}}$$

and can rewrite energy (2.1) as

$$W_n(F) := \frac{c}{2}\left\{\mathrm{tr}\left[(L_n^{-\frac{1}{2}}F)(L_n^{-\frac{1}{2}}F)^T\right] - 3\right\}, \quad \det F = 1.$$

Note that

$$\begin{aligned} L_n^{-\frac{1}{2}} &= \alpha_\parallel^{-1} n\otimes n + \alpha_\perp^{-1}(I - n\otimes n) \\ &= a^{-\frac{1}{3}} n\otimes n + a^{\frac{1}{6}}(I - n\otimes n). \end{aligned} \tag{2.5}$$

As we will see later, it is often useful to see W_n as a function of FF^T. By defining, for a positive symmetric matrix B,

$$\tilde{W}_n(B) := \frac{c}{2}\left[\mathrm{tr}\left(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}}\right) - 3\right], \quad \det B = 1, \tag{2.6}$$

we have that $W_n(F) = \tilde{W}_n(FF^T)$. Finally, denoting by $0 < \lambda_1(F) \le \lambda_2(F) \le \lambda_3(F)$ the singular values of F (so that $\lambda_1^2(F) \le \lambda_2^2(F) \le \lambda_3^2(F)$ are the ordered eigenvalues of $B = FF^T$), one easily shows (see the proof of Proposition 5.1 for details) that

$$\tilde{W}(B) := \min_{|n|=1} \tilde{W}_n(B) = \frac{c}{2\alpha_\perp^2}\left[\mathrm{tr}B - \left(1 - \frac{\alpha_\perp^2}{\alpha_\parallel^2}\right)\lambda_3^2 - 3\alpha_\perp^2\right],$$

or, equivalently, that

$$\begin{aligned} W(F) := \min_{|n|=1} W_n(F) &= \frac{c}{2\alpha_\perp^2}\left[\lambda_1^2(F) + \lambda_2^2(F) + \left(\frac{\alpha_\perp}{\alpha_\parallel}\right)^2 \lambda_3^2(F) - 3\alpha_\perp^2\right] \\ &= \frac{c}{2} a^{\frac{1}{3}}\left[\lambda_1^2(F) + \lambda_2^2(F) + \frac{1}{a}\lambda_3^2(F) - 3a^{-\frac{1}{3}}\right]. \end{aligned}$$

The foregoing algebraic manipulations can be summarized by the schematic graph of Figure 1, which naturally suggests to introduce the matrices

$$F_n^e := L_n^{-\frac{1}{2}} F, \quad B_n^e := F_n^e (F_n^e)^T = L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}} \tag{2.7}$$

arising from the decomposition

$$F = L_n^{\frac{1}{2}} F_n^e$$

of the deformation gradient F into an elastic part F_n^e and a spontaneous part $L_n^{\frac{1}{2}}$. The matrix $L_n^{\frac{1}{2}}$ describes the stress-free strain of the material corresponding to the current orientation n of the nematic director. Using (2.7), expression (2.6) assumes the classical Neo-Hookean form

$$\tilde{W}_n(B) = \frac{c}{2}(\mathrm{tr}B_n^e - 3), \quad \det B = 1. \tag{2.8}$$

3. Ogden-type expressions for the energy density

We use the following notation: $Sym(3)$, $Psym(3)$, $Orth(3)$ and $SO(3)$ denote the set of matrices in $\mathbb{R}^{3\times 3}$ which are symmetric, positive definite and symmetric, orthogonal, rotations, respectively. As usual, we label with $sym(M)$ the symmetric part $\frac{M+M^T}{2}$ of a matrix $M \in \mathbb{R}^{3\times 3}$.

Following Ciarlet [9, Chapter 4], and motivated by formula (2.8), we use the same notation used for the classical expression of the energies (W_n, W, $\tilde{W}_n$, and $\tilde{W}$) and propose the following natural generalization of (2.8):

$$W_n(F) := \tilde{W}_n(FF^T), \qquad \det F = 1, \tag{3.1}$$

where

$$\tilde{W}_n(B) := \sum_{i=1}^{N} \frac{c_i}{\gamma_i} \left[\operatorname{tr}(B_n^e)^{\frac{\gamma_i}{2}} - 3 \right] + \sum_{j=1}^{M} \frac{d_j}{\delta_j} \left[\operatorname{tr} \operatorname{Cof}(B_n^e)^{\frac{\delta_j}{2}} - 3 \right], \quad \det B = 1, \tag{3.2}$$

B_n^e is given by (2.7), Cof$F$ is the cofactor of F, and c_i, γ_i, d_j and δ_j are constants such that

$$\gamma_i,\ \delta_j \in \mathbb{R} \setminus \{0\}, \qquad \frac{c_i}{\gamma_i}, \frac{d_j}{\delta_j} \geq 0, \quad i = 1, ..., N, \quad j = 1, ..., M.$$

We recall that the p-th power A^p of a matrix $A \in Psym(3)$ is well-defined by the formula

$$A^p := Q\mathrm{Diag}(\lambda_i^p)Q^T, \quad p \in \mathbb{R},$$

where $Q \in Orth(3)$ is a matrix which diagonalizes A. Observe that, choosing $N = M = 1$ and $\gamma_1 = \delta_1 = 2$, $\tilde{W}_n$ takes the Mooney-Rivlin form

$$\tilde{W}_n(B) = \frac{c_1}{2} (\operatorname{tr} B_n^e - 3) + \frac{d_1}{2} (\operatorname{tr} \operatorname{Cof} B_n^e - 3), \quad \det B = 1,$$

and we obtain the Neo-Hookean model (2.8) if $d_1 = 0$. Moreover, setting $d_j = 0$ for $j = 1, ..., M$ in (3.2) and taking the minimum with respect to $|n| = 1$, we obtain energies in "separable form" of the type discussed by Ogden in [20, Chapter 4] (see Section 5).

A common practice to pass from an incompressible model, with associated energy density W_{dev} defined on $\{F \in \mathbb{R}^{3\times3} :\ \det F = 1\}$, to a corresponding compressible model W^{comp} is to define

$$W^{comp}(F) := W_{dev}((\det F)^{-\frac{1}{3}} F) + W_{vol}(\det F), \quad \det F > 0,$$

where W_{vol} is such that

$$W_{vol} \geq 0 \quad \text{ and } \quad W_{vol}(t) = 0 \ \text{ if and only if } t = 1. \tag{3.3}$$

Here, we choose W_{vol} of the form

$$W_{vol}(t) = c(t^2 - 1) - d \log t,$$

for some $c, d > 0$ such that (3.3) is satisfied. By imposing condition (3.3), we obtain the function

$$W_{vol}(t) = c\left(t^2 - 1 - 2\log t\right), \quad t > 0. \tag{3.4}$$

W_{vol} defined by (3.4) has also the following properties:

(i) W_{vol} is a convex function;
(ii) $W_{vol}(t) \to +\infty$, as $t \to 0^+$;
(iii) $W_{vol}(t) \to +\infty$, as $t \to +\infty$.

By choosing $W_{dev} = W_n$, where W_n is defined by (3.1) and (3.2), we define for $\det F > 0$

$$W_n^{comp}(F) := W_n((\det F)^{-\frac{1}{3}} F) + W_{vol}(\det F),$$

so that

$$W_n^{comp}(F) = \sum_{i=1}^{N} \frac{c_i}{\gamma_i} \left[(\det F)^{-\frac{\gamma_i}{3}} \mathrm{tr}(L_n^{-\frac{1}{2}} F F^T L_n^{-\frac{1}{2}})^{\frac{\gamma_i}{2}} - 3 \right] + \sum_{j=1}^{M} \frac{d_j}{\delta_j} \left[(\det F)^{-\frac{2\delta_j}{3}} \mathrm{tr}\,\mathrm{Cof}(L_n^{-\frac{1}{2}} F F^T L_n^{-\frac{1}{2}})^{\frac{\delta_j}{2}} - 3 \right] + W_{vol}(\det F). \quad (3.5)$$

Also in this case it is useful to express the energy density as function of $B = FF^T$:

$$W_n^{comp}(F) = \tilde{W}_n^{comp}(FF^T), \quad \det F > 0,$$

where for every $B \in Psym(3)$

$$\tilde{W}_n^{comp}(B) = \sum_{i=1}^{N} \frac{c_i}{\gamma_i} \left[(\det B)^{-\frac{\gamma_i}{6}} \mathrm{tr}(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}})^{\frac{\gamma_i}{2}} - 3 \right] + \sum_{j=1}^{M} \frac{d_j}{\delta_j} \left[(\det B)^{-\frac{\delta_j}{3}} \mathrm{tr}\,\mathrm{Cof}(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}})^{\frac{\delta_j}{2}} - 3 \right] + W_{vol}(\sqrt{\det B}). \quad (3.6)$$

Proposition 3.1. *W_n^{comp} is a non-negative function on $\{F \in \mathbb{R}^{3\times3} : \det F > 0\}$ and*

$$W_n^{comp}(F) = 0 \quad \text{if and only if} \quad FF^T = L_n.$$

Observe that, by left polar decomposition, the condition $FF^T = L_n$ (together with $\det F > 0$) is equivalent to

$$F \in \{F \in \mathbb{R}^{3\times3} : \ F = U_n R \ \text{ for some } \ R \in SO(3)\}, \quad U_n := L_n^{\frac{1}{2}}.$$

Proof. For $F \in \mathbb{R}^{3\times3}$ with $\det F > 0$, we denote by ν_1, ν_2, ν_3 the (positive) eigenvalues of $L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}}$, where $B = FF^T \in Psym(3)$. Then, by using the standard inequality between geometric and arithmetic mean and (2.4), for $i = 1, ..., N$ and $j = 1, ..., M$ we have that

$$\begin{aligned} (\det B)^{-\frac{\gamma_i}{6}} \mathrm{tr}(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}})^{\frac{\gamma_i}{2}} &= (\det B)^{\frac{-\gamma_j}{6}} \sum_{k=1}^{3} \nu_k^{\frac{\gamma_i}{2}} \geq 3 (\det B)^{\frac{-\gamma_i}{6}} \left(\prod_{k=1}^{3} \nu_k^{\frac{\gamma_i}{2}} \right)^{\frac{1}{3}} \\ &= 3 (\det B)^{\frac{-\gamma_i}{6}} \left[\det \left(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}} \right) \right]^{\frac{\gamma_i}{6}} = 3, \end{aligned} \quad (3.7)$$

and

$$\begin{aligned} (\det B)^{-\frac{\delta_j}{3}} \mathrm{trCof}(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}})^{\frac{\delta_j}{2}} &= (\det B)^{\frac{-\delta_j}{3}} \left[(\nu_1\nu_2)^{\frac{\delta_j}{2}} + (\nu_1\nu_3)^{\frac{\delta_j}{2}} + (\nu_2\nu_3)^{\frac{\delta_j}{2}} \right] \\ &\geq 3 (\det B)^{\frac{-\delta_j}{3}} \left[(\nu_1\nu_2)^{\frac{\delta_j}{2}} (\nu_1\nu_3)^{\frac{\delta_j}{2}} (\nu_2\nu_3)^{\frac{\delta_j}{2}} \right]^{\frac{1}{3}} = 3, \end{aligned} \quad (3.8)$$

so that, looking at (3.6) and recalling (3.3), W_n^{comp} is non-negative. The equality holds in (3.7) if and only if $\nu_1 = \nu_2 = \nu_3 = \nu$, that is

$$L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}} = \nu I, \quad \text{for some } \nu > 0, \quad (3.9)$$

and in (3.8) if and only if $\nu_1\nu_2 = \nu_1\nu_3 = \nu_2\nu_3 = \alpha^2$, that is

$$\mathrm{Cof}(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}}) = \alpha^2 I, \quad \text{for some } \alpha > 0. \quad (3.10)$$

By (3.9) and (3.10) and by property (3.3) of W_{vol}, we obtain that $W_n^{comp}(F) = \tilde{W}_n^{comp}(B) = 0$ if and only if $L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}} = I$. □

4. Behavior for small strains

In order to obtain the geometrically linear approximation of the Ogden-type model introduced in the previous section, we consider the small strain regime $|\nabla u| = \varepsilon$, where u is the displacement associated with the deformation y through $y(x) = x + u(x)$, and matrices L_n that scale with ε as

$$L_n = L_{n,\varepsilon} := (1+\varepsilon)^2 n \otimes n + (1+\varepsilon)^{-1}(I - n \otimes n). \tag{4.1}$$

This scaling is necessary to ensure that the stress-free strains described by L_n are reachable within a small strain theory, see [22] and [15, Appendix B.1]. Using the notation introduced in Section 2 and based on the material parameter a, we have that $a^{\frac{1}{3}} = 1 + \varepsilon$. By expanding (4.1) in ε around $\varepsilon = 0$, we obtain

$$L_{n,\varepsilon} = I + \varepsilon \hat{L}_n + o(\varepsilon), \quad \text{with} \quad \hat{L}_n := 3\left(n \otimes n - \frac{1}{3} I\right). \tag{4.2}$$

Similarly, from

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

we have that

$$U_{n,\varepsilon} = I + \varepsilon \hat{U}_n + o(\varepsilon), \quad \text{with} \quad \hat{U}_n = \frac{1}{2}\hat{L}_n. \tag{4.3}$$

Now, we define

$$W_{n,\varepsilon}^{comp}(F) := \tilde{W}_{n,\varepsilon}^{comp}(FF^T), \quad \det F > 0,$$

where $\tilde{W}_{n,\varepsilon}^{comp}$ is given by (3.6) with $L_{n,\varepsilon}$ in place of L_n. More explicitly,

$$\begin{aligned} \tilde{W}_{n,\varepsilon}^{comp}(B) = &\sum_{i=1}^{N} \frac{c_i}{\gamma_i}\left[(\det B)^{-\frac{\gamma_i}{6}} \operatorname{tr}(L_{n,\varepsilon}^{-\frac{1}{2}} B L_{n,\varepsilon}^{-\frac{1}{2}})^{\frac{\gamma_i}{2}} - 3\right] \\ &+ \sum_{j=1}^{M} \frac{d_j}{\delta_j}\left[(\det B)^{-\frac{\delta_j}{3}} \operatorname{tr}\operatorname{Cof}(L_{n,\varepsilon}^{-\frac{1}{2}} B L_{n,\varepsilon}^{-\frac{1}{2}})^{\frac{\delta_j}{2}} - 3\right] + W_{vol}(\sqrt{\det B}), \end{aligned} \tag{4.4}$$

for every $B \in Psym(3)$.

Proposition 4.1. *In the small strain regime $|\nabla u| = \varepsilon$, we have that, modulo terms of order higher than two in ε,*

$$W_{n,\varepsilon}^{comp}(I + \nabla u) = \mu \left|[e(u)]_d - \varepsilon \hat{U}_n\right|^2 + \frac{k}{2}\operatorname{tr}^2(\nabla u), \tag{4.5}$$

where $e(u) = sym(\nabla u)$, $[e(u)]_d$ denotes the deviatoric part of the matrix $e(u)$, $\hat{U}_n$ is the traceless matrix defined in (4.3) and

$$k = 4c, \qquad \mu = \frac{1}{2}\left(\sum_{i=1}^{N} c_i \gamma_i + \sum_{j=1}^{M} d_i \delta_j\right), \tag{4.6}$$

c, c_i, γ_i, d_j and δ_j being the constants defining $W_{n,\varepsilon}^{comp}$ in (3.4), (4.4).

Notice that the incompressible version of the large and small strain theories can be obtained by considering the formal limit $c \to +\infty$ and $k \to +\infty$ in (3.5) (where c is inside W_{vol}) and in (4.5), respectively: in the large strain regime we obtain again W_n defined in (3.1) and (3.2); in the small strain regime we obtain

$$W^{comp}_{n,\varepsilon}(I + \nabla u) = \mu \left| e(u) - \varepsilon \hat{U}_n \right|^2, \qquad \mathrm{tr}[e(u)] = 0.$$

Proof. In order to obtain (4.5), we follow [22] and define for every $E \in Sym(3)$ the linear limit

$$V(E) := \lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon^2} W^{comp}_{n,\varepsilon}(I + \varepsilon E) = \lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon^2} \tilde{W}^{comp}_{n,\varepsilon}\left((I + \varepsilon E)^2\right).$$

Since 0 is the minimum value attained by $\tilde{W}^{comp}_{n,\varepsilon}$ at $L_{n,\varepsilon}$ (see Proposition 3.1), the linear terms of the Taylor expansions vanish and we have

$$\begin{aligned} V(E) &= \lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon^2} \left\{ \frac{1}{2} d^2 \tilde{W}^{comp}_{n,\varepsilon}(L_{n,\varepsilon})[(I + \varepsilon E)^2 - L_{n,\varepsilon}]^2 + o\left(|(I + \varepsilon E)^2 - L_{n,\varepsilon}|^2 \right) \right\} \\ &= \frac{1}{2} d^2 \tilde{W}^{comp}_{n,0}(I)[2E - \hat{L}_n]^2 = 2 d^2 \tilde{W}^{comp}_{n,0}(I)[E - \hat{U}_n]^2, \end{aligned} \tag{4.7}$$

where the last two equalities are obtained using (4.2)-(4.3). Here, $d^2\tilde{W}(L)[M]^2$ denotes the second differential of the function $\tilde{W}$ evaluated at L and then applied to $[M, M]$. Notice that, for every $B \in Psym(3)$,

$$\begin{aligned} \tilde{W}^{comp}_{n,0}(B) = \sum_{i=1}^{N} \frac{c_i}{\gamma_i} &\left[(\det B)^{-\frac{\gamma_i}{6}} \mathrm{tr} B^{\frac{\gamma_i}{2}} - 3 \right] \\ &+ \sum_{j=1}^{M} \frac{d_j}{\delta_j} \left[(\det B)^{-\frac{\delta_j}{3}} \mathrm{tr}\, \mathrm{Cof} B^{\frac{\delta_j}{2}} - 3 \right] + W_{vol}(\sqrt{\det B}). \end{aligned}$$

Simple rules of tensor calculus give that, for every symmetric matrix H,

$$\begin{aligned} d^2 \tilde{W}^{comp}_{n,0}(I)[H]^2 = \sum_{i=1}^{N} c_i \gamma_i &\left\{ -\frac{1}{12} \mathrm{tr}^2 H + \frac{1}{4} |H|^2 \right\} \\ &+ \sum_{j=1}^{M} d_j \delta_j \left\{ -\frac{1}{12} \mathrm{tr}^2 H + \frac{1}{4} |H|^2 \right\} + c\, \mathrm{tr}^2 H, \end{aligned}$$

so that, from (4.7) and from the fact that $\hat{U}_n$ is traceless, we have

$$V(E) = \frac{1}{2} \left(\sum_{i=1}^{N} c_i \gamma_i + \sum_{j=1}^{M} d_i \delta_j \right) |E - \hat{U}_n|^2 + \left[-\frac{1}{6} \left(\sum_{i=1}^{N} c_i \gamma_i + \sum_{j=1}^{M} d_i \delta_j \right) + 2c \right] \mathrm{tr}^2 E.$$

Writing now $V(E)$ in terms of $E_d := E - \frac{1}{3}(\mathrm{tr} E)\, I$, since

$$|E - \hat{U}_n|^2 = |E_d - \hat{U}_n|^2 + \frac{1}{3} \mathrm{tr}^2 E,$$

we obtain that

$$V(E) = \frac{1}{2} \left(\sum_{i=1}^{N} c_i \gamma_i + \sum_{j=1}^{M} d_i \delta_j \right) |E_d - \hat{U}_n|^2 + 2c\, \mathrm{tr}^2 E. \tag{4.8}$$

It remains to observe that, since $W^{comp}_{n,\varepsilon}(F)$ can be expressed in terms of FF^T (through $\tilde{W}^{comp}_{n,\varepsilon}$), it turns out that

$$\lim_{\varepsilon\to 0^+} \frac{1}{\varepsilon^2} W^{comp}_{n,\varepsilon}(I+\varepsilon M) = \lim_{\varepsilon\to 0^+} \frac{1}{\varepsilon^2} W^{comp}_{n,\varepsilon}(I+\varepsilon sym(M)) =: V(sym(M)),$$

for every $M \in \mathbb{R}^{3\times 3}$. In particular, we have that, modulo terms of order higher than two,

$$W^{comp}_{n,\varepsilon}\left(I+\varepsilon\frac{\nabla u}{|\nabla u|}\right) = \varepsilon^2 V\left(sym\left(\frac{\nabla u}{|\nabla u|}\right)\right) = \varepsilon^2 V\left(\frac{e(u)}{|\nabla u|}\right).$$

Thus, considering ∇u with the proper scale $|\nabla u| = \varepsilon$ and using (4.8), we obtain

$$W^{comp}_{n,\varepsilon}\left(I+\nabla u\right) = \frac{1}{2}\left(\sum_{i=1}^{N} c_i\gamma_i + \sum_{j=1}^{M} d_i\delta_j\right)\left|[e(u)]_d - \varepsilon\hat{U}_n\right|^2 + 2c\,\mathrm{tr}^2\left(\nabla u\right).$$

□

Energy densities like (4.5) have been used in the study of nematic elastomers in the small strain regime in [2, 6, 7, 8, 15, 17]. One reason to derive small strain theories from the fully nonlinear ones is to obtain the expressions for the initial shear and bulk moduli in terms of the constants and exponents of the fully nonlinear models, as done in (4.6). While our main interest here has been to derive the small strain limit of fully nonlinear Ogden-type models, also the opposite path is interesting. In fact, energies of the form (4.5) are quite common in the modeling of active and phase-transforming materials, where geometrically linear theories are often used [3]. Our discussion of their relation with parent (fully nonlinear) theories such as (3.1) provides several templates to generalize these small strain theories to the regime of large deformations.

5. Applications: stress-strain response through quasiconvex envelopes

In this section we focus on the purely mechanical response of an incompressible material governed by the Ogden-type energies introduced in Section 3, in the large deformation regime. This means to consider the stored elastic energies obtained, for each fixed F, by minimizing the energy density (3.1) with respect to n, and to use the resulting expressions to compute stable equilibria and associated stresses arising in the material as a consequence of prescribing its state of deformation.

Minimization with respect to n leads to non-convex stored elastic energies and, in turn, loss of stability of homogeneously deformed states with respect to configurations exhibiting shear bands (stripe domains, which are indeed observed experimentally). The tool we will use to predict global features of the material response, such as stress–strain curves, is to replace these expressions with their quasiconvex envelopes (see the discussion in [8], where a similar study has been performed in the small strain regime).

Referring to the expressions (3.1)-(3.2) which define the energy density W_n, let us restrict the attention to the case $c_i > 0$, $\gamma_i \geq 2$ for $i = 1, ..., N$ and $d_j = 0$ for $j = 1, ..., M$, so that $W_n(F) = \tilde{W}_n(FF^T)$, where

$$\tilde{W}_n(B) = \sum_{i=1}^{N} \frac{c_i}{\gamma_i}\left[\mathrm{tr}(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}})^{\frac{\gamma_i}{2}} - 3\right], \qquad \det B = 1. \tag{5.1}$$

In order to minimize (5.1) with respect to $|n| = 1$, we need the following proposition.

Proposition 5.1. *Let $B \in Psym(3)$ and let $0 < \lambda_1^2 \le \lambda_2^2 \le \lambda_3^2$ be its ordered eigenvalues and $\{b_1, b_2, b_3\}$ an orthonormal basis of eigenvectors with $Bb_i = \lambda_i^2 b_i$, $i = 1, 2, 3$.*

For every $\gamma \ge 2$, we have that

$$\min_{|n|=1} \operatorname{tr}\left(L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}}\right)^{\frac{\gamma}{2}} = a^{\frac{\gamma}{6}} \left[\left(\lambda_1^2\right)^{\frac{\gamma}{2}} + \left(\lambda_2^2\right)^{\frac{\gamma}{2}} + \left(\frac{\lambda_3^2}{a}\right)^{\frac{\gamma}{2}} \right]. \tag{5.2}$$

The minimum is achieved by n aligned with b_3.

We recall that $a > 1$, that L_n is defined in (2.2), and that $L_n^{-\frac{1}{2}}$ is given by (2.5). In order to simplify the notation for the proof of Proposition 5.1, let us set

$$\alpha := \frac{\gamma}{2}, \qquad \mu_i := \lambda_i^2, \qquad i = 1, 2, 3, \tag{5.3}$$

and

$$M_n := a^{-\frac{1}{2}} n \otimes n + (I - n \otimes n) = (a^{-\frac{1}{2}} - 1) n \otimes n + I, \tag{5.4}$$

so that

$$L_n^{-\frac{1}{2}} = a^{\frac{1}{6}} M_n. \tag{5.5}$$

By using the positions (5.3)-(5.5), the thesis (5.2) to be proved is equivalent to

$$\min_{|n|=1} \operatorname{tr}(M_n B M_n)^\alpha = \mu_1^\alpha + \mu_2^\alpha + \left(\frac{\mu_3}{a}\right)^\alpha, \tag{5.6}$$

for every $\alpha \ge 1$, where $0 < \mu_1 \le \mu_2 \le \mu_3$ are the ordered eigenvalues of B. To prove Proposition 5.1, we need the following two lemmas whose proofs are postponed to Section 6.

Lemma 5.2. *For every unit vector $n \in \mathbb{R}^3$, the maximum eigenvalue of $M_n B M_n$ is greater than or equal to* $\max\{\mu_2, \mu_3/a\}$.

Lemma 5.3. *Let $0 < \overline{x} \le \overline{y} \le \overline{z}$ and $0 < x \le y \le z$ be such that*

$$\text{(i)}\ \ xyz = \overline{x}\,\overline{y}\,\overline{z}, \quad \text{(ii)}\ \ x + y + z \ge \overline{x} + \overline{y} + \overline{z}, \quad \text{(iii)}\ \ z \ge \overline{z}. \tag{5.7}$$

Then, for every $\alpha > 1$ we have that

$$x^\alpha + y^\alpha + z^\alpha \ge \overline{x}^\alpha + \overline{y}^\alpha + \overline{z}^\alpha.$$

Proof of Proposition 5.1. Recall that we want to prove (5.6) and that M_n is defined in (5.4). We first note that (5.6) is true for $\alpha = 1$. Indeed,

$$\begin{aligned} \operatorname{tr}(M_n B M_n) = B \cdot M_n^2 &= B \cdot \left[\left(\frac{1}{a} - 1 \right) n \otimes n + I \right] \\ &= \left(\frac{1}{a} - 1 \right) (Bn) \cdot n + \operatorname{tr} B \end{aligned}$$

and, as $\left(\frac{1}{a} - 1\right) < 0$, the minimum is obtained when $(Bn) \cdot n$ equals the maximum eigenvalue of B. This happens if n is parallel to b_3 and we have

$$\min_{|n|=1} \operatorname{tr}(M_n B M_n) = \left(\frac{1}{a} - 1 \right) \mu_3 + \operatorname{tr} B = \mu_1 + \mu_2 + \frac{\mu_3}{a}. \tag{5.8}$$

Now, by using the definition of the α-power of a positive definite and symmetric matrix, we write our minimum problem as

$$\min_{|n|=1} \operatorname{tr}(M_n B M_n)^\alpha = \min_{(x,y,z)\in\mathscr{A}} (x^\alpha + y^\alpha + z^\alpha), \tag{5.9}$$

where

$$\mathscr{A} := \big\{(x,y,z)\in\mathbb{R}^3 \,:\, 0<x\le y\le z, \text{ and } x,y,z \text{ eigenvalues of } M_nBM_n \text{ for some } |n|=1\big\}.$$

It is easy to check that μ_1, μ_2 and μ_3/a are eigenvalues of $M_{b_3}BM_{b_3}$, so that, by relabeling them $\overline{x}$, $\overline{y}$ and $\overline{z}$ in such a way that $\overline{x}\le\overline{y}\le\overline{z}$, we have that

$$(\overline{x},\overline{y},\overline{z})\in\mathscr{A}, \tag{5.10}$$

with $\overline{z}\in\{\mu_2,\frac{\mu_3}{a}\}$. Finally, observe that for every $(x,y,z)\in\mathscr{A}$,

$$xyz = \det(M_nBM_n) = \det B\det M_n^2 = \frac{\mu_1\mu_2\mu_3}{a} = \overline{x}\,\overline{y}\,\overline{z}. \tag{5.11}$$

We now apply Lemma 5.3. Take $(x,y,z)\in\mathscr{A}$: since (5.7) (i) is assured by (5.11), (5.7) (ii) by (5.8), and (5.7) (iii) by Lemma 5.2, we have that

$$x^\alpha+y^\alpha+z^\alpha \ge \overline{x}^\alpha+\overline{y}^\alpha+\overline{z}^\alpha,$$

for every $\alpha>1$. Thus, by considering also (5.9) and (5.10), we have obtained that

$$\min_{|n|=1}\operatorname{tr}(M_nBM_n)^\alpha = \overline{x}^\alpha+\overline{y}^\alpha+\overline{z}^\alpha,$$

that is (5.6). □

By considering $\tilde{W}_n$ given by (5.1), we define

$$\begin{aligned}\tilde{W}(B) &:= \min_{|n|=1}\tilde{W}_n(B)\\ &= \sum_{i=1}^N \frac{c_i}{\gamma_i}\min_{|n|=1}\left[\operatorname{tr}(L_n^{-\frac12}BL_n^{-\frac12})^{\frac{\gamma_i}{2}}-3\right], \quad \det B=1.\end{aligned} \tag{5.12}$$

In view of Proposition 5.1 and by recalling (2.3), we have that

$$\tilde{W}(B) = \sum_{i=1}^N \frac{c_i}{\gamma_i\alpha_\perp^{\gamma_i}}\left[\lambda_1^{\gamma_i}+\lambda_2^{\gamma_i}+\left(\frac{\alpha_\perp}{\alpha_\parallel}\right)^{\gamma_i}\lambda_3^{\gamma_i}-3\alpha_\perp^{\gamma_i}\right], \tag{5.13}$$

where $0<\lambda_1^2\le\lambda_2^2\le\lambda_3^2$ are the ordered eigenvalues of B (and $\lambda_i>0$, $i=1,2,3$). Then, we set

$$W(F) := \tilde{W}(FF^T), \quad \det F = 1. \tag{5.14}$$

We remark that in all the terms of the sum in (5.12), the minimum is achieved by n aligned with the eigenvector of B corresponding to its largest eigenvalue λ_3^2. Therefore, within this model, the nematic director is always aligned with the direction of maximal principal stretch.

Energies of the type above are not quasiconvex, and exhibit material instabilities that reproduce, up to a surprising level of accuracy, those that are observed experimentally (stripe domain instabilities, [25]). The quasiconvex envelope W^{qc} of the energy density W is defined by

$$W^{qc}(F) := \inf_w \frac{1}{|\Omega|}\int_\Omega W\left(F+\nabla w(x)\right)dx\,, \tag{5.15}$$

where Ω is an arbitrary (Lipschitz) domain (it can be shown that definition (5.15) does not depend on shape and size of the test region Ω), $|\Omega|$ is its volume, and w is an arbitrary perturbation (a Lipschitz-continuous displacement field perturbing the affine state $y(x) = Fx$) vanishing on $\partial\Omega$. Stable materials are characterized by $W^{qc} \equiv W$. If, for some F, $W^{qc}(F) < W(F)$, then the state of homogeneous deformation F is unstable: the material shows an energetic preference to develop spatially modulated deformations with gradient $F + \nabla w(x)$ (typically, shear bands) at fixed average deformation F. The minimal energy cost to maintain the state of average deformation F is $W^{qc}(F)$, rather than $W(F)$, and this is achieved through domain patterns with length scales which are very small compared to the size of the domain Ω.

For energies such as (5.14), an explicit formula for their quasiconvex envelope is available. Figure 2 gives a sketch of the sets L, I, and S appearing in the following proposition.

Proposition 5.4. *Let W be the energy density given by (5.14) and (5.13) with $\alpha_\perp$, $\alpha_\parallel$, $a = \left(\frac{\alpha_\parallel}{\alpha_\perp}\right)^2$ defined by (2.3), and $c_i > 0$, $\gamma_i \geq 2$. Consider the following sets of $3{\times}3$-matrices:*

$$L := \left\{ F \in \mathbb{R}^{3\times 3} : \det F = 1,\ \frac{1}{\lambda_{\min}(F)} \leq a^{\frac{1}{6}} \right\}, \tag{5.16}$$

$$I := \left\{ F \in \mathbb{R}^{3\times 3} : \det F = 1,\ \frac{1}{\lambda_{\min}(F)} \geq a^{\frac{1}{6}},\ \frac{1}{\lambda_{\min}(F)} \geq a^{-\frac{1}{2}} \lambda^2_{max}(F) \right\}, \tag{5.17}$$

$$S := \left\{ F \in \mathbb{R}^{3\times 3} : \det F = 1,\ \frac{1}{\lambda_{\min}(F)} \leq a^{-\frac{1}{2}} \lambda^2_{max}(F) \right\}, \tag{5.18}$$

where $0 < \lambda_{min} = \lambda_1 \leq \lambda_{mid} = \lambda_2 \leq \lambda_{max} = \lambda_3$ are the ordered singular values of F. Then, the quasiconvex envelope W^{qc} of W is given by

$$W^{qc}(F) = \begin{cases} 0, & \text{for } F \in L \\ W(F), & \text{for } F \in S \\ \displaystyle\sum_{i=1}^{N} \frac{c_i}{\gamma_i} \left[\left(a^{\frac{1}{6}} \lambda_{min}(F) \right)^{\gamma_i} + 2 \left(\frac{1}{a^{\frac{1}{6}} \lambda_{min}(F)} \right)^{\frac{\gamma_i}{2}} - 3 \right], & \text{for } F \in I. \end{cases} \tag{5.19}$$

Proof. We observe that each summand in W is of the form

$$\frac{c_i}{\gamma_i} \left[\left(\frac{\lambda_1(F)}{a^{-\frac{1}{6}}} \right)^{\gamma_i} + \left(\frac{\lambda_2(F)}{a^{-\frac{1}{6}}} \right)^{\gamma_i} + \left(\frac{\lambda_3(F)}{a^{\frac{1}{3}}} \right)^{\gamma_i} - 3 \right],$$

and apply the arguments in [14] to conclude that (5.19) holds. □

Consider now

$$W_2(F) := \tilde{W}_2(FF^T), \qquad \det F = 1,$$

where, for every $B \in Psym(3)$ with $\det B = 1$,

$$\begin{aligned} \tilde{W}_2(B) &:= \min_{|n|=1} \tilde{W}_n(B) \qquad (5.20) \\ &= \min_{|n|=1} \left\{ \sum_{i=1}^{N} \frac{c_i}{\gamma_i} \left[\operatorname{tr}(B_n^e)^{\frac{\gamma_i}{2}} - 3 \right] + \sum_{j=1}^{M} \frac{d_j}{\delta_j} [\operatorname{tr} \operatorname{Cof}(B_n^e)^{\frac{\delta_j}{2}} - 3] \right\}, \end{aligned}$$

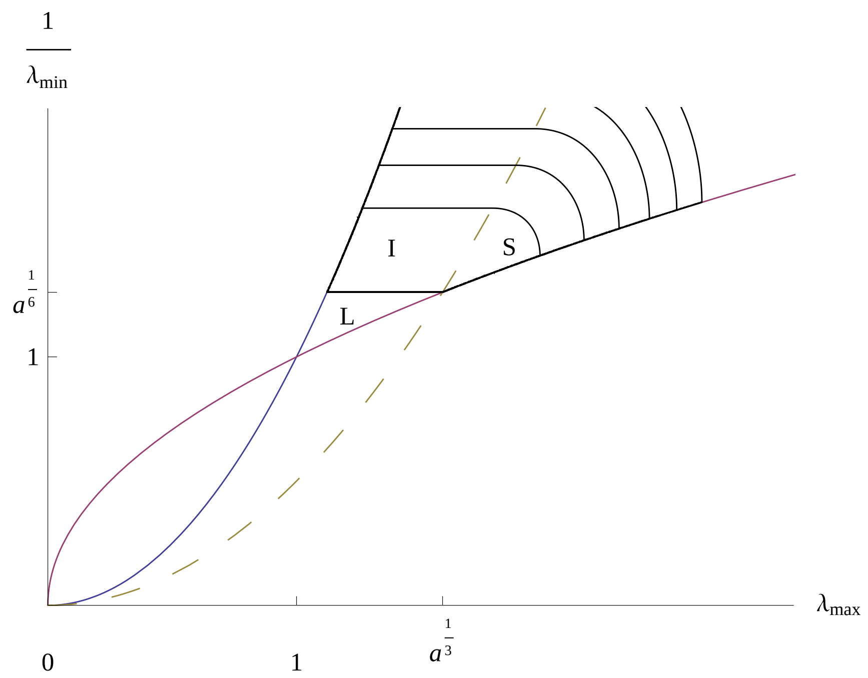

FIGURE 2. Level curves of the quasiconvex envelopes of the Ogden-type energies (5.19), (5.22), and illustration of the sets L, I, and S appearing in their definitions ($a = 4$).

and B_n^e is given by (2.7). If $d_j > 0$ for some $j = 1, ..., M$, these expressions may be not separable in the sense discussed in [20, Chapter 4], and the characterization of their quasiconvex envelopes is an open problem, except in the Mooney-Rivlin case $N = M = 1$ and $\gamma_1 = \delta_1 = 2$ (and c_1, $d_1 \geq 0$). In this case, $\tilde{W}_n$ is of the form

$$\tilde{W}_n(B) = \frac{c_1}{2}[B{\cdot}L_n^{-1} - 3] + \frac{d_1}{2}\left[B^{-1}{\cdot}L_n - 3\right].$$

Recalling that

$$L_n = a^{\frac{2}{3}} n{\otimes}n + a^{-\frac{1}{3}}(I - n{\otimes}n), \qquad a > 1, \tag{5.21}$$

it is easy to show that

$$W_2(F) = \frac{c_1}{2}\left\{a^{\frac{1}{3}}\left[\mathrm{tr}(FF^T) + \left(\frac{1}{a} - 1\right)\lambda_{max}(FF^T)\right] - 3\right\} + \frac{d_1}{2}\left\{\frac{1}{a^{\frac{1}{3}}}\left[\mathrm{tr}(FF^T)^{-1} + (a-1)\frac{1}{\lambda_{max}(FF^T)}\right] - 3\right\},$$

where $\lambda_{max}(FF^T)$ is the maximum eigenvalue of FF^T. Equivalently,

$$W_2(F) = \frac{c_1}{2}\left[\left(\frac{\lambda_1}{a^{-\frac{1}{6}}}\right)^2 + \left(\frac{\lambda_2}{a^{-\frac{1}{6}}}\right)^2 + \left(\frac{\lambda_3}{a^{\frac{1}{3}}}\right)^2 - 3\right] + \frac{d_1}{2}\left[\left(\frac{\lambda_2\lambda_3}{a^{\frac{1}{6}}}\right)^2 + \left(\frac{\lambda_1\lambda_3}{a^{\frac{1}{6}}}\right)^2 + \left(\frac{\lambda_1\lambda_2}{a^{-\frac{1}{3}}}\right)^2 - 3\right].$$

Notice that here, again, the n that achieves the minimum in (5.20) is the eigenvector of B associated with its largest eigenvalue, just as in the case of (5.13). Using results obtained by Šilhavý in [23], we have that

$$W_2^{qc}(F) = \begin{cases} 0, & \text{for } F \in L \\ W_2(F), & \text{for } F \in S \\ \hat{W}_2(\lambda_{min}), & \text{for } F \in I \end{cases} \tag{5.22}$$

where L, S and I are the sets defined in (5.16)-(5.18), and

$$\hat{W}_2(s) := \frac{c_1}{2}\left[\left(a^{\frac{1}{6}}s\right)^2 + \frac{2}{a^{\frac{1}{6}}s} - 3\right] + \frac{d_1}{2}\left[\left(\frac{1}{a^{\frac{1}{6}}s}\right)^2 + 2a^{\frac{1}{6}}s - 3\right].$$

From now on, we focus on the incompressible model W defined in (5.13)-(5.14). We will use the knowledge of the quasiconvex envelope W^{qc} of W to examine the mechanical response of a sample tested in pure shear. This is a plane strain condition (plane strain extension) often used in classical rubber elasticity to assess the performance of constitutive models, see [20, 24] and Figure 5 for a sketch illustrating these laoding conditions.

Plane strain conditions lead to a simplified expression for W (which becomes a function of λ_{max} alone) and to a very transparent representation of the quasi-convex envelope in (λ, δ)-plane, where λ and δ denote applied stretch and shear, respectively. We start by rewriting the energy given in (5.13) as

$$W(F) = \sum_{i=1}^{N} \frac{c_i}{\gamma_i}\left[\left(\frac{\lambda_{min}}{a^{-\frac{1}{6}}}\right)^{\gamma_i} + \left(\frac{\lambda_{mid}}{a^{-\frac{1}{6}}}\right)^{\gamma_i} + \left(\frac{\lambda_{max}}{a^{\frac{1}{3}}}\right)^{\gamma_i} - 3\right] \geq 0. \tag{5.23}$$

It is easy to check that in the plane strain conditions defined by

$$F(\lambda, \delta) = \begin{bmatrix} a^{-\frac{1}{6}} & 0 & 0 \\ 0 & \lambda & \delta \\ 0 & 0 & \frac{a^{\frac{1}{6}}}{\lambda} \end{bmatrix},$$

expression (5.23) simplifies to

$$W(F(\lambda, \delta)) = \sum_{i=1}^{N} \frac{c_i}{\gamma_i}\left[1 + \left(\frac{a^{\frac{1}{3}}}{\lambda_{max}}\right)^{\gamma_i} + \left(\frac{\lambda_{max}}{a^{\frac{1}{3}}}\right)^{\gamma_i} - 3\right] \geq 0, \tag{5.24}$$

with equality holding if and only if $\lambda_{max} = a^{\frac{1}{3}}$. The same arguments (based on a lamination construction, see below) used in [8] for the small, plane strain case or in [14] for large strains in three dimensions show that the quasi-convex envelope of (5.24) is given by

$$W^{qc}(F(\lambda, \delta)) = \begin{cases} 0, & \text{if } \lambda_{max}(F(\lambda, \delta)) \leq a^{\frac{1}{3}} \\ W(F(\lambda, \delta)), & \text{if } \lambda_{max}(F(\lambda, \delta)) \geq a^{\frac{1}{3}}. \end{cases}$$

Observe that, since

$$\lambda_{max}^2(F(\lambda, \delta)) = \frac{1}{2}\left(\lambda^2 + \delta^2 + \frac{a^{\frac{1}{3}}}{\lambda^2}\right) + \frac{1}{2}\sqrt{\left(\lambda^2 + \delta^2 + \frac{a^{\frac{1}{3}}}{\lambda^2}\right)^2 - 4a^{\frac{1}{3}}},$$

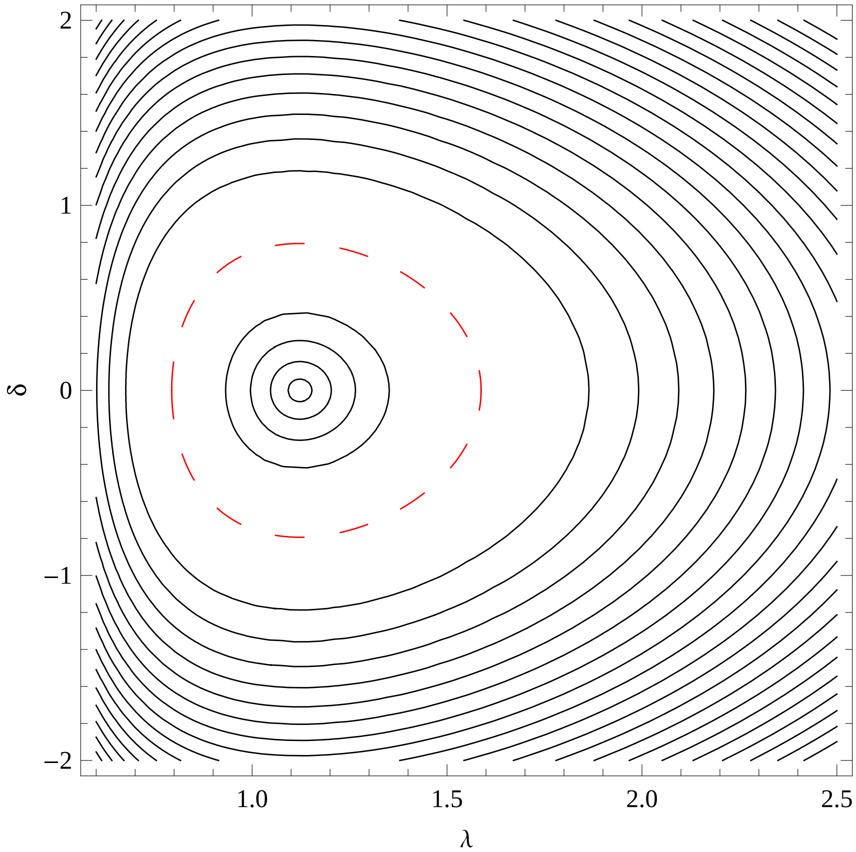

FIGURE 3. Level curves of the Ogden-type energy (5.13) ($a = 4$, $c_1 = 1.5$, $\gamma_1 = 1.5$, $c_2 = 0.01$, $\gamma_2 = 5.0$, arbitrary units). The dashed (red) line gives the zero level set describing the spontaneous deformations that minimize the energy density.

we have that $\lambda_{max} \leq a^{\frac{1}{3}}$ if and only if $\lambda \in \left[a^{-\frac{1}{6}}, a^{\frac{1}{3}}\right]$ and $|\delta| \leq \delta^*(\lambda)$, where

$$\delta^*(\lambda) := \frac{1}{\lambda}\left(\lambda^2 - \frac{1}{a^{\frac{1}{3}}}\right)^{\frac{1}{2}}\left(a^{\frac{2}{3}} - \lambda^2\right)^{\frac{1}{2}}. \tag{5.25}$$

This allows us to write W^{qc} as

$$W^{qc}(F(\lambda,\delta)) = \begin{cases} 0, & \text{if } \lambda \in \left[a^{-\frac{1}{6}}, a^{\frac{1}{3}}\right] \text{ and } |\delta| \leq \delta^*(\lambda) \\ W(F(\lambda,\delta)), & \text{otherwise.} \end{cases} \tag{5.26}$$

Level curves of energy (5.24) and of its quasi-convex envelope (5.26) are shown in Figure 3 and 4. These plots clearly illustrate that, in fact,

$$W^{qc}(F(\lambda,\delta)) = f^c(\lambda,\delta),$$

where f^c is the convex envelope of the function

$$f(\lambda,\delta) := W(F(\lambda,\delta)).$$

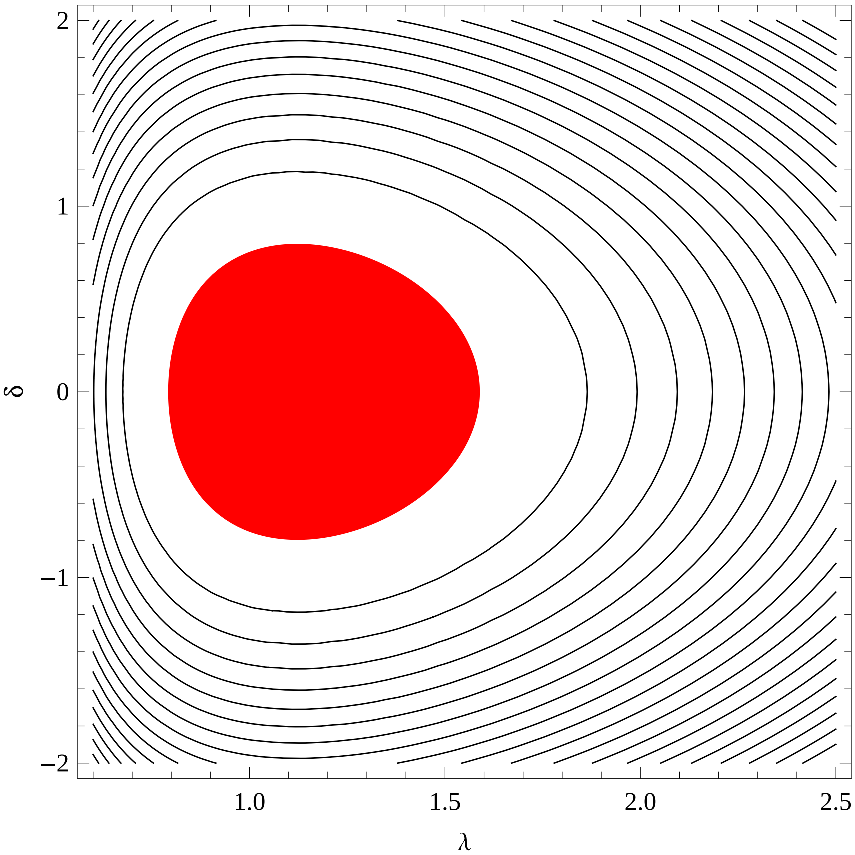

FIGURE 4. Level curves of the quasiconvex envelope of the Ogden-type energy (5.13) ($a = 4$, $c_1 = 1.5$, $\gamma_1 = 1.5$, $c_2 = 0.01$, $\gamma_2 = 5.0$, arbitrary units). The shaded (red) region gives the set of macroscopic strains that can be accommodated at zero energy.

Observe that at a macroscopic unsheared ($\delta = 0$) deformation with $\lambda \in \left(a^{-\frac{1}{6}}, a^{\frac{1}{3}}\right)$ the energy $W^{qc}(F(\lambda, 0)) = f^c(\lambda, 0) = 0$ can be obtained by combining the microscopic deformation states $(\lambda, \pm\delta^*(\lambda))$, with alternating equal and opposite shears of magnitude δ^* given by (5.25), in a stripe domain configuration with stripes of equal width and parallel to the direction x_2 of imposed stretch (see [13, 10, 11, 8] for further details and Figure 5 for a sketch).

Since $\frac{\partial}{\partial\delta} f(\lambda, 0) = 0$, $\delta = 0$ always gives a stationary point for $f(\lambda, \cdot)$. This equilibrium state is, however, unstable if $\lambda \in \left(a^{-\frac{1}{6}}, a^{\frac{1}{3}}\right)$ (the energy plots in Figures 3 and 6 show a local maximum at $\delta = 0$ along lines with constant λ, leading to a negative shear modulus). Since, as already mentioned, the macroscopic deformation state $(\lambda, \delta = 0)$ can be resolved by a stripe domain pattern alternating the states $(\lambda, \pm\delta^*(\lambda))$ in stripes of equal width at a smaller (in fact, zero) energy cost, we have $W^{qc}(F(\lambda, 0)) = W(F(\lambda, \pm\delta^*(\lambda)))$ (see Figure 4), and the quasi-convex envelope W^{qc} can be used to obtain a stable, macroscopically unsheared state of minimal energy for all imposed stretches $\lambda > 0$. The corresponding stresses can be computed

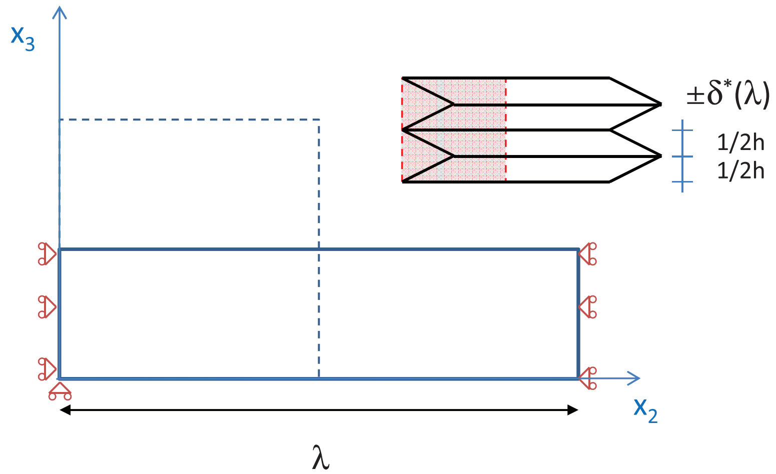

FIGURE 5. Sketch of the geometry for the pure shear experiment, and stripe domain patterns with alternating shears $\pm\delta^*(\lambda)$ on stripes of thickness $1/2h$, $h \gg 1$, providing the lowest energy configurations for stretches $\lambda \in \left(a^{-\frac{1}{6}}, a^{\frac{1}{3}}\right)$ in the plateau region.

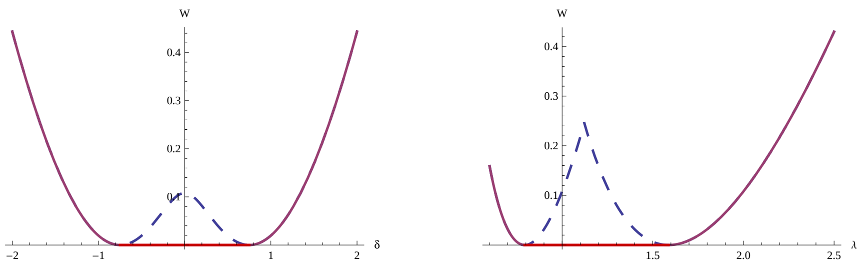

FIGURE 6. Sections of the Ogden-type energy (5.13) (dashed lines) and of its quasiconvex envelope (full lines) at constant $\lambda = 1$ (left) and at constant $\delta = 0$ (right). The energy is in arbitrary units, the material parameter values are $a = 4$, $c_1 = 1.5$, $\gamma_1 = 1.5$, $c_2 = 0.01$, $\gamma_2 = 5.0$.

from

$$\sigma(\lambda) := \frac{\partial}{\partial\lambda} f^c(\lambda, 0) = \begin{cases} 0, & \text{if } \lambda \le a^{\frac{1}{3}} \\ \displaystyle\sum_{i=1}^{N} c_i \left[-\frac{a^{\frac{\gamma_i}{3}}}{\lambda^{\gamma_i+1}} + \frac{\lambda^{\gamma_i-1}}{a^{\frac{\gamma_i}{3}}} \right], & \text{if } \lambda \ge a^{\frac{1}{3}} \end{cases} \tag{5.27}$$

In order to obtain the last equality we have used that, since

$$\lambda_{max}(F(\lambda,0)) = \begin{cases} \dfrac{a^{\frac{1}{6}}}{\lambda}, & \text{if } \lambda \le a^{\frac{1}{12}} \\ \lambda, & \text{if } \lambda \ge a^{\frac{1}{12}}, \end{cases}$$

we also have

$$f^c(\lambda,0) = \begin{cases} \displaystyle\sum_{i=1}^N \frac{c_i}{\gamma_i}\left[1 + \left(a^{\frac{1}{6}}\lambda\right)^{\gamma_i} + \left(\frac{1}{a^{\frac{1}{6}}\lambda}\right)^{\gamma_i} - 3\right], & \text{if } \lambda < a^{-\frac{1}{6}} \\ 0, & \text{if } \lambda \in \left[a^{-\frac{1}{6}}, a^{\frac{1}{3}}\right] \\ \displaystyle\sum_{i=1}^N \frac{c_i}{\gamma_i}\left[1 + \left(\frac{a^{\frac{1}{3}}}{\lambda}\right)^{\gamma_i} + \left(\frac{\lambda}{a^{\frac{1}{3}}}\right)^{\gamma_i} - 3\right], & \text{if } \lambda > a^{\frac{1}{3}}. \end{cases}$$

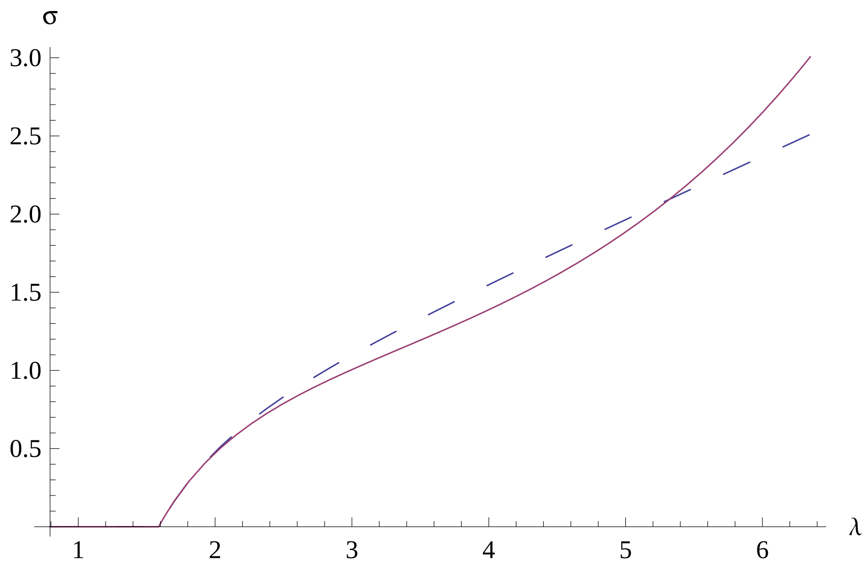

FIGURE 7. Stress-strain response in plane strain extension (pure shear). Dashed lines from Neo-Hookean expression obtained from (5.13) with $N = 1$, $c_1 = 1.0$, $\gamma_1 = 2$, full curves from Ogden-type expression (5.13) with $N = 2$, $c_1 = 1.5$, $\gamma_1 = 1.5$, $c_2 = 0.01$, $\gamma_2 = 5.0$ ($a = 4$, arbitrary units).

The mechanical response in pure shear (5.27) encoded by the Ogden-type energy is shown in Figure 7. The figure shows the force-stretch curves for a plane strain extension experiment starting from the minimal energy configuration associated with a director uniformly aligned with x_3 (this is given by $\lambda = a^{-\frac{1}{6}}$, $\delta = 0$). The prediction of the Neo-Hookean model with $c_1 = 1.0$, $\gamma_1 = 2$ is compared with those of an Ogden-type model with $N = 2$, $c_1 = 1.5$, $\gamma_1 = 1.5$, $c_2 = 0.01$, $\gamma_2 = 5.0$. The second model is able to capture the stiffening response at large imposed stretches, which is typical of rubbers, and which the first model completely misses. As is well known, the plateau at zero applied stress is unrealistic, and it is possible to add anisotropic corrections to ensure that director reorientation need to be triggered by a nonzero minimum stress level (see, e.g., [11, 8]).

6. Appendix

We devote this section to the proof of two lemmas stated in Section 5 and to a remark on Proposition 5.1.

Proof of Lemma 5.2. Since the maximum eigenvalue of M_nBM_n is defined as the maximum value of the scalar product $(M_nBM_nm)\cdot m$ as $|m|=1$, to prove the lemma it is enough to show that

$$(M_nBM_nm)\cdot m \geq \max\left\{\mu_2, \frac{\mu_3}{a}\right\}, \quad \text{for some} \quad |m|=1.$$

If $\frac{\mu_3}{a}\geq\mu_2$, we define

$$m := \frac{v}{|v|}, \qquad \text{where} \quad v := \frac{1}{\sqrt{a}}M_n^{-1}b_3.$$

With this choice of m, we have that

$$(M_nBM_nm)\cdot m = \frac{1}{|v|^2}(BM_nv)\cdot(M_nv) = \frac{1}{a|v|^2}(Bb_3)\cdot b_3 = \frac{1}{|v|^2}\frac{\mu_3}{a}. \tag{6.1}$$

Recall the definition of M_n (5.4). It turns out that $|v|\leq|b_3|=1$, because $a>1$ and

$$v = \left[n\otimes n + \frac{1}{\sqrt{a}}(I-n\otimes n)\right]b_3.$$

Thus, from (6.1), $(M_nBM_nm)\cdot m\geq\mu_3/a$ follows.

If $\mu_2\geq\frac{\mu_3}{a}$, we consider $(\mathrm{Span}\{n\})^\perp$, the orthogonal space to n, and choose m in the set $\mathrm{Span}\{b_2,b_3\}\cap(\mathrm{Span}\{n\})^\perp$, which is nonempty. Thus, the fact that $m\in\mathrm{Span}\{b_2,b_3\}$ implies

$$(Bm)\cdot m\geq\mu_2, \tag{6.2}$$

while $n\in(\mathrm{Span}\{n\})^\perp$ implies that $M_nm=m$. This fact, together with (6.2), gives that

$$(M_nBM_nm)\cdot m = (BM_nm)\cdot(M_nm)\geq\mu_2.$$

□

Proof of Lemma 5.3. Suppose first that $\overline{x}=\overline{y}=\overline{z}$. In this case, we have to prove that $x^\alpha+y^\alpha+z^\alpha\geq 3\overline{x}^\alpha$. To have this, it is enough to use condition (5.7) (ii), which gives $x+y+z\geq3\overline{x}$. Indeed:

$$x^\alpha+y^\alpha+z^\alpha\geq 3^{1-\alpha}(x+y+z)^\alpha\geq3\overline{x}^\alpha,$$

where the first inequality is standard (descending, e. g., from Hölder's inequality). Thus, in the rest part of the proof, we will suppose

$$\overline{x}<\overline{z}. \tag{6.3}$$

We introduce the functions

$$w(x,y,z):=x^\alpha+y^\alpha+z^\alpha, \quad v(x,y,z):=xyz, \quad u(x,y,z):=x+y+z,$$

and the minimum problem

$$\min_{x,y,z>0} w(x,y,z) \tag{6.4}$$

with constraints

$$\text{(i)}\ \ v(x,y,z)=\overline{x}\,\overline{y}\,\overline{z}, \quad \text{(ii)}\ \ u(x,y,z)\geq\overline{x}+\overline{y}+\overline{z}, \quad \text{(iii)}\ \ z\geq\overline{z}. \tag{6.5}$$

By standard arguments it can be proved that the minimum exists. Let (x_0, y_0, z_0) be a minimum point. It is not restrictive to suppose that

$$x_0 \leq y_0 \leq z_0.$$

Claim 1. $x_0 < z_0$.
Suppose, by contradiction, that $x_0 = z_0$. In this case, (6.5) (i) and (ii) would give $x_0^3 = \overline{x}\,\overline{y}\,\overline{z}$ and $3x_0 \geq \overline{x} + \overline{y} + \overline{z}$, respectively. Thus, by the standard inequality between arithmetic and geometric mean, we would obtain

$$x_0 \geq \frac{\overline{x} + \overline{y} + \overline{z}}{3} \geq (\overline{x}\,\overline{y}\,\overline{z})^{\frac{1}{3}} = x_0$$

and in turn $\overline{x} = \overline{z}$, against (6.3).

Claim 1 will be used in the proof of the following claim.
Claim 2. $z_0 = \overline{z}$.

Let us see how the thesis descends from Claim 2 and postpone the proof of the claim. Since $z_0 = \overline{z}$, conditions (6.5) (i) and (ii) become

$$x_0 y_0 = \overline{x}\,\overline{y}, \qquad x_0 + y_0 \geq \overline{x} + \overline{y}. \tag{6.6}$$

This two conditions imply the inequality

$$y_0^2 - (\overline{x} + \overline{y})y_0 + \overline{x}\,\overline{y} \geq 0$$

and in turn that

$$\text{either} \qquad y_0 \leq \overline{x} \qquad \text{or} \qquad y_0 \geq \overline{y}. \tag{6.7}$$

As an intermediate step, we want to prove that

$$x_0^\alpha + y_0^\alpha \geq \overline{x}^\alpha + \overline{y}^\alpha. \tag{6.8}$$

If the contrary were true, by considering also the first condition in (6.6) we would obtain the inequality

$$(y_0^\alpha)^2 - (\overline{x}^\alpha + \overline{y}^\alpha)y_0^\alpha + (\overline{x}\,\overline{y})^\alpha < 0$$

which is true if and only if

$$\overline{x} < y_0 < \overline{y},$$

against (6.7). Thus, (6.8) holds and therefore

$$\overline{x}^\alpha + \overline{y}^\alpha + \overline{z}^\alpha = \overline{x}^\alpha + \overline{y}^\alpha + z_0^\alpha \leq x_0^\alpha + y_0^\alpha + z_0^\alpha.$$

This fact, together with the definition of (x_0, y_0, z_0) as a minimum point of (6.4)-(6.5), gives the thesis.
Proof of Claim 2. Suppose, by contradiction, that

$$z_0 > \overline{z}. \tag{6.9}$$

Constraint (6.5) (ii) tells us that $x_0+y_0+z_0 \geq \overline{x}+\overline{y}+\overline{z}$. If $x_0+y_0+z_0 > \overline{x}+\overline{y}+\overline{z}$, this strict inequality, together with conditions (6.5) (i) and (6.9), gives

$$\nabla v(x_0, y_0, z_0) = \mu \nabla w(x_0, y_0, z_0),$$

for some Lagrange multiplier $\mu \neq 0$. A direct computation shows that this last condition implies $x_0 = z_0$, against Claim 1. Therefore, we must have

$$x_0 + y_0 + z_0 = \overline{x} + \overline{y} + \overline{z}. \tag{6.10}$$

Since $x_0 < z_0$ from Claim 1, we have three possibilities which we treat separately in the following cases (a), (b) and (c). We are going to show that every case leads to a contradiction resulting from (6.9).

(a). Here we suppose that

$$x_0 = y_0 < z_0.$$

Let $\varepsilon > 0$ be such that $x(\varepsilon) := y_0 - \varepsilon > 0$ and let $y = y(\varepsilon)$ and $z = z(\varepsilon) \geq y$ satisfy the conditions

$$\begin{cases} x(\varepsilon) + y + z = 2y_0 + z_0, \\ x(\varepsilon)yz = y_0^2 z_0. \end{cases}$$

Setting

$$a_0 = y_0 + z_0, \qquad b_0 = y_0 z_0,$$

it turns out that

$$\begin{aligned} y(\varepsilon) &= \frac{1}{2}\left\{a_0 + \varepsilon - \sqrt{(a_0+\varepsilon)^2 - 4b_0\left(\frac{y_0}{y_0-\varepsilon}\right)}\right\}, \\ z(\varepsilon) &= \frac{1}{2}\left\{a_0 + \varepsilon + \sqrt{(a_0+\varepsilon)^2 - 4b_0\left(\frac{y_0}{y_0-\varepsilon}\right)}\right\}. \end{aligned}$$

It is easy to show that $x(\varepsilon) \leq y(\varepsilon) \leq z(\varepsilon)$ for ε sufficiently small. Moreover, up to a smaller ε, we have that $z(\varepsilon) \geq \overline{z}$, since $z(0) = z_0$ and (6.9) holds. Now, let us introduce the function

$$f(\varepsilon) := x(\varepsilon)^\alpha + y(\varepsilon)^\alpha + z(\varepsilon)^\alpha.$$

Since $(x(0), y(0), z(0)) = (x_0, y_0, z_0)$ and $(x(\varepsilon), y(\varepsilon), z(\varepsilon))$ satisfies the constraints (6.5) of the minimum problem (6.4), it follows that

$$f'(0) = 0 \quad \text{and} \quad f''(0) \geq 0. \tag{6.11}$$

Simple computations show that $f'(0) = 0$ and

$$f''(0) = \frac{2\alpha}{y_0(z_0 - y_0)}\left[y_0^\alpha + \alpha y_0^{\alpha-1}(z_0 - y_0) - z_0^\alpha\right]. \tag{6.12}$$

Now, since $y_0 < z_0$, we have that $y_0^\alpha + \alpha y_0^{\alpha-1}(z_0 - y_0) < z_0^\alpha$, in view of the strict convexity of the function $t \mapsto t^\alpha$ $(\alpha > 1)$. Thus, from (6.12) we obtain that $f''(0) < 0$, against (6.11).

(b). Here we suppose that

$$x_0 < y_0 = z_0.$$

In this case, constraints (6.5) (i) and (6.10) give

$$\begin{cases} x_0 z_0^2 = G^2 \overline{z}, \\ x_0 + 2z_0 = 2A + \overline{z}, \end{cases} \tag{6.13}$$

where

$$A := \frac{\overline{x} + \overline{y}}{2}, \qquad G := \sqrt{\overline{x}\,\overline{y}}.$$

From (6.13) we deduce that z_0 solves the third-order equation

$$P(t) := 2t^3 - (2A + \overline{z})t^2 + G^2 \overline{z} = 0.$$

The function P has a local maximum at $t = 0$ with $P(0) > 0$ and a local minimum at $t = \frac{2A+\overline{z}}{3}$ with $P\left(\frac{2A+\overline{z}}{3}\right) < 0$. Now, from (6.9), from the fact that

$$\overline{z} > \frac{2A + \overline{z}}{3} \tag{6.14}$$

and that z_0 is a zero of P, it is easy to deduce that

$$P(t) < 0 \quad \text{for} \quad \frac{2A+\overline{z}}{3} < t < z_0 \quad \text{and } P(t) \geq 0 \quad \text{for} \quad t \geq z_0. \tag{6.15}$$

On the other hand,

$$P(\overline{z}) = \overline{z}\left[\overline{z}^2 - (\overline{x}+\overline{y})\overline{z} + \overline{x}\,\overline{y}\right],$$

so that $P(\overline{z}) \geq 0$ in view of the fact that $\overline{z} \geq \overline{y}$. Together with (6.14) and (6.15), this implies that $\overline{z} \geq z_0$, against (6.9).

(c). Finally, we suppose that

$$x_0 < y_0 < z_0.$$

In this case, we consider the matrix whose lines are the gradients $\nabla w(x_0, y_0, z_0)$, $\nabla v(x_0, y_0, z_0)$, $\nabla u(x_0, y_0, z_0)$. Considering (6.4), (6.5) (i), (6.9), and (6.10), it turns out that

$$D := \det \begin{bmatrix} \nabla w(x_0, y_0, z_0) \\ \nabla v(x_0, y_0, z_0) \\ \nabla u(x_0, y_0, z_0) \end{bmatrix} = 0. \tag{6.16}$$

Computing such a determinant gives

$$\begin{aligned} D &= \alpha\left[x_0\left(y_0^\alpha - z_0^\alpha\right) - y_0\left(x_0^\alpha - z_0^\alpha\right) + z_0\left(x_0^\alpha - y_0^\alpha\right)\right] \\ &= -\alpha\left[y_0^\alpha(z_0 - x_0) - z_0^\alpha(y_0 - x_0) - x_0^\alpha(z_0 - y_0)\right]. \end{aligned} \tag{6.17}$$

Setting $\lambda := \frac{y_0 - x_0}{z_0 - x_0} \in (0,1)$, so that

$$y_0 = \lambda z_0 + (1-\lambda)x_0, \tag{6.18}$$

from (6.17) we obtain that

$$D = -\alpha(z_0 - x_0)\left[y_0^\alpha - \lambda z_0^\alpha - (1-\lambda)x_0^\alpha\right].$$

This last equality, together with (6.18) and the strict convexity of the function $t \mapsto t^\alpha$ $(\alpha > 1)$, implies that $D > 0$, against (6.16). □

With the following remark we want to show that in the case where the two largest eigenvalues of $B \in Psym(3)$ are equal it is possible to find the analytical expression of the eigenvalues of $L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}}$ and prove Proposition 5.1 in a more direct way.

Remark 6.1. Let $B \in Psym(3)$ and suppose that $\lambda_1^2 < \lambda_2^2 = \lambda_3^2$ (the case $\lambda_1^2 = \lambda_2^2 = \lambda_3^2$ is trivial), where λ_1^2, λ_2^2, λ_3^2 are the ordered eigenvalues of B. Let b_1, b_2, b_3 be the corresponding orthonormal eigenvectors. For $a > 1$ and a unit vector $n \in \mathbb{R}^3$, consider $L_n = L_n(a)$ defined as in (5.21) and suppose that

$$n = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} \quad \text{in the orthonormal basis } \{b_1, b_2, b_3\}.$$

Then, up to the multiplicative constant $a^{\frac{1}{3}}$, we have that the spectrum of $L_n^{-\frac{1}{2}} B L_n^{-\frac{1}{2}}$ is

$$\left\{\lambda_2^2, \frac{g(n_1^2) + \sqrt{g^2(n_1^2) - 4\frac{\lambda_1^2\lambda_2^2}{a}}}{2}, \frac{g(n_1^2) - \sqrt{g^2(n_1^2) - 4\frac{\lambda_1^2\lambda_2^2}{a}}}{2}\right\}, \tag{6.19}$$

where

$$g(t) := (\lambda_2^2 - \lambda_1^2)\left(1 - \frac{1}{a}\right)t + \lambda_1^2 + \frac{\lambda_2^2}{a}, \qquad \text{for every} \quad 0 \leq t \leq 1. \tag{6.20}$$

Moreover, we have that

$$\min_{|n|=1}\left(L_n^{-\frac{1}{2}}BL_n^{-\frac{1}{2}}\right)^{\frac{\gamma}{2}} = a^{\frac{\gamma}{6}}\left[\left(\lambda_1^2\right)^{\frac{\gamma}{2}} + \left(1+a^{-\frac{\gamma}{2}}\right)\left(\lambda_2^2\right)^{\frac{\gamma}{2}}\right],$$

and the minimum is attained for $n \in (\mathrm{Span}\{b_1\})^{\perp}$.

In order to prove this, let us use the same position used for the proof of Proposition 5.1: $\mu_i := \lambda_i^2$, $i = 1, 2, 3$, $\alpha = \frac{\gamma}{2}$, and

$$M_n := a^{-\frac{1}{6}}L_n^{-\frac{1}{2}} = \left(\frac{1}{\sqrt{a}} - 1\right) n\otimes n + I.$$

With this notation, we are going to check that the spectrum of M_nBM_n is (6.19) and that

$$\min_{|n|=1}\mathrm{tr}(M_nBM_n)^{\alpha} = \mu_1^{\alpha} + \left(1 + \frac{1}{a^{\alpha}}\right)\mu_2^{\alpha} \tag{6.21}$$

with the minimum attained for $n \in (\mathrm{Span}\{b_1\})^{\perp}$.

We note that, as $\mu_1 < \mu_2 = \mu_3$, we can write B in the following way:

$$B = \mu_1(b_1\otimes b_1) + \mu_2(I - b_1\otimes b_1) = \mu_2 C, \tag{6.22}$$

where

$$\rho := \frac{\mu_1}{\mu_2} < 1, \qquad C := \rho\, b_1\otimes b_1 + (I - b_1\otimes b_1).$$

We are going to find the eigenvalues of M_nCM_n. Note that M_n^{-1} is an invertible matrix and that there exist $\lambda \in \mathbb{R}$ and $v \in \mathbb{R}^3 \setminus \{0\}$ such that $M_nCM_nv = \lambda v$ if and only if $CM_n^2\left(M_n^{-1}v\right) = \lambda\left(M_n^{-1}v\right)$. Therefore, we look for the eigenvalues of the matrix

$$\begin{aligned} CM_n^2 &= [(\rho-1)b_1\otimes b_1 + I]\left[\left(\frac{1}{a} - 1\right) n\otimes n + I\right] \\ &= (\rho-1)\left(\frac{1}{a} - 1\right)(b_1\cdot n)b_1\otimes n + (\rho-1)b_1\otimes b_1 + \left(\frac{1}{a} - 1\right) n\otimes n + I, \end{aligned} \tag{6.23}$$

since in this case there are shorter formulas to handle. Recall that we have fixed the orthonormal basis $\{b_1, b_2, b_3\}$ where

$$b_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \text{and} \quad n = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix}.$$

Using these expressions we can compute the coefficients of the matrix CM_n^2 and obtain

$$CM_n^2 = \begin{bmatrix} \rho\left[\left(\dfrac{1}{a} - 1\right)n_1^2 + 1\right] & \rho\left(\frac{1}{a} - 1\right)n_1n_2 & \rho\left(\frac{1}{a} - 1\right)n_1n_3 \\ \left(\dfrac{1}{a} - 1\right)n_1n_2 & \left(\frac{1}{a} - 1\right)n_2^2 + 1 & \left(\frac{1}{a} - 1\right)n_2n_3 \\ \left(\dfrac{1}{a} - 1\right)n_1n_3 & \left(\frac{1}{a} - 1\right)n_2n_3 & \left(\frac{1}{a} - 1\right)n_3^2 + 1 \end{bmatrix}$$

It is already clear that 1 is an eigenvalue of CM_n^2. Indeed, using expression (6.23), it turns out that $CM_n^2v = v$ for every vector v in the orthogonal space to $\mathrm{Span}\{b_1, n\}$. In order to find the other eigenvalues of CM_n^2, we use the standard procedure and look for the solutions w of the equation $\det\left(CM_n^2 - wI\right) = 0$. A direct computation gives

$$\det\left(CM_n^2 - wI\right) = \left\{\rho\left[\left(\frac{1}{a}-1\right)n_1^2 + 1\right] - w\right\}\left[w^2 - (\delta+1)w + \delta\right] - \rho\left(\frac{1}{a}-1\right)^2 n_1^2\left(n_2^2+n_3^2\right)(1-w), \quad (6.24)$$

where

$$\delta := \left(\frac{1}{a}-1\right)\left(n_2^2+n_3^2\right)+1.$$

Now, since $\left[w^2-(\delta+1)w+\delta\right] = (w-1)(w-\delta)$, we use the fact that $1-n_2^2-n_3^2 = n_1^2$ and rewrite (6.24) as

$$\det\left(CM_n^2 - wI\right) = (w-1)P(w), \quad (6.25)$$

where

$$P(w) = -w^2 + \frac{1}{\mu_2}g(n_1^2)w - \frac{\mu_1}{\mu_2 a},$$

and g is defined in (6.20). The zeros of P are

$$\frac{g(n_1^2) \pm \sqrt{g^2(n_1^2) - 4\frac{\mu_1\mu_2}{a}}}{2\mu_2}$$

and

$$\Delta(t) := g^2(t) - 4\frac{\mu_1\mu_2}{a} = (\mu_2-\mu_1)^2\left(1-\frac{1}{a}\right)^2 t^2 + 2(\mu_2-\mu_1)\left(1-\frac{1}{a}\right)\left(\mu_1+\frac{\mu_2}{a}\right)t + \left(\mu_1 - \frac{\mu_2}{a}\right)^2 \geq 0 \quad \text{for every } 0 \leq t \leq 1. \quad (6.26)$$

Thus, looking at (6.25), we have that the spectrum of CM_n^2 is

$$\left\{1, \frac{g(n_1^2)+\sqrt{\Delta(n_1^2)}}{2\mu_2}, \frac{g(n_1^2)-\sqrt{\Delta(n_1^2)}}{2\mu_2}\right\}.$$

Recalling (6.22), multiplying these eigenvalues by μ_2 gives the spectrum of BM_n^2, which is the same of M_nBM_n.

In order to prove (6.21), let us introduce the function

$$f(t) := \mu_2^\alpha + \left[\frac{g(t)+\sqrt{\Delta(t)}}{2}\right]^\alpha + \left[\frac{g(t)-\sqrt{\Delta(t)}}{2}\right]^\alpha,$$

and observe that $f(n_1^2) = \operatorname{tr}(M_nBM_n)^\alpha$. Now, we differentiate f in $(0,1)$:

$$f'(t) = \frac{\alpha g'(t)}{\sqrt{\Delta(t)}}\left[\left(\frac{g(t)+\sqrt{\Delta(t)}}{2}\right)^\alpha - \left(\frac{g(t)-\sqrt{\Delta(t)}}{2}\right)^\alpha\right] \quad \text{for every } 0<t<1.$$

This tells us that

$$f'(t) > 0 \quad \text{for every} \quad 0<t<1,$$

since $g'(t) = (\mu_2-\mu_1)\left(1-\frac{1}{a}\right) > 0$ and $\Delta(t)>0$ for every $t>0$ (see (6.26)). Thus,

$$f(0) \leq f(t) \quad \text{for every} \quad 0<t\leq 1,$$

and therefore

$$f(0) = \mu_2^\alpha + \mu_1^\alpha + \left(\frac{\mu_2}{a}\right)^\alpha = \min_{|n|=1} f(n_1^2) = \min_{|n|=1} \operatorname{tr}(M_n B M_n)^\alpha. \tag{6.27}$$

Finally, observe that

$$f(0) = \operatorname{tr}(M_n B M_n)^\alpha, \quad \text{where} \quad n = \begin{bmatrix} 0 \\ n_2 \\ n_3 \end{bmatrix} \in (\operatorname{Span}\{b_1\})^\perp. \tag{6.28}$$

Considering (6.27) and (6.28), the proof of (6.21) is completed.

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