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The relaxation of two-well energies with possibly
unequal moduli

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Abstract

The elastic energy of a multiphase solid is a function of its microstructure. Determining the infimum of the energy of such a solid and characterizing the associated optimal microstructures is an important problem that arises in the modeling of the shape memory effect, microstructure evolution and optimal design. Mathematically, the problem is to determine the relaxation under fixed phase fraction of a multiwell energy. This paper addresses two such problems in the geometrically linear setting.

First, in two dimensions, we compute the relaxation under fixed phase fraction for a two-well elastic energy with arbitrary elastic moduli and transformation strains, and provide a characterization of the optimal microstructures and the associated strain.

Second, in three dimensions, we compute the relaxation under fixed phase fraction for a two-well elastic energy when either (1) both elastic moduli are isotropic, or (2) the elastic moduli are well-ordered and the smaller elastic modulus is isotropic. In both cases we impose no restrictions on the transformation strains. We provide a characterization of the optimal microstructures and the associated strain.

We also compute a lower bound that is optimal except possibly in one regime when either (1) both elastic moduli are cubic, or (2) the elastic moduli are well-ordered and the smaller elastic modulus is cubic; for moduli with arbitrary symmetry we obtain a lower bound that is sometimes optimal. In all these cases we impose no restrictions on the transformation strains and whenever the bound is optimal we provide a characterization of the optimal microstructures and the associated strain.

In both two and three dimensions the quasiconvex envelope of the energy can be obtained by minimizing over the phase fraction. We also characterize optimal microstructures under applied stress.

1. Introduction

1.1. Relaxation

The elastic energy of a multiphase solid is a function of its microstructure. Determining the infimum of the energy of such a solid and characterizing the associated optimal microstructures is an important problem that arises in the modeling of the shape memory effect, microstructure evolution and optimal design. Mathematically, the problem is to determine the relaxation under fixed phase fraction of a multiwell energy.

We work in the framework of geometrically linear (infinitesimal) kinematics. Let $\epsilon_i^T \in \mathbb{R}_{\text{sym}}^{n \times n}$ be the stress-free (transformation) stain of the i^{th} phase relative to a reference configuration, $\alpha_i \in \mathcal{L}_{>}^*(\mathbb{R}_{\text{sym}}^{n \times n})$ be its elastic modulus and $w_i \in \mathbb{R}$ be its chemical energy. (We use $\mathcal{L}^*(\cdot)$ to denote self-adjoint linear operators, $\mathcal{L}_{\geq}^*(\cdot)$ to denote positive-semidefinite self-adjoint linear operators and $\mathcal{L}_{>}^*(\cdot)$ to denote positive-definite self-adjoint linear operators on \cdot , respectively.) Then the energy density $W_i: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ of this phase subject to a linearized strain $\epsilon \in \mathbb{R}_{\text{sym}}^{n \times n}$ is given by

$$W_i(\epsilon) = \frac{1}{2} \langle \alpha_i(\epsilon - \epsilon_i^T), (\epsilon - \epsilon_i^T) \rangle + w_i. \quad (1.1)$$

Here, the inner product $\langle \cdot, \cdot \rangle$ is defined as usual by $\forall \epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{n \times n}$, $\langle \epsilon_1, \epsilon_2 \rangle := \text{Tr}(\epsilon_1 \epsilon_2)$. We write the *energy density* $W: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ of the material with N phases as the minimum over N quadratic energy wells,

$$W(\epsilon) := \min_{i=1, \dots, N} W_i(\epsilon). \quad (1.2)$$

Classically one postulates that the state of the solid occupying a region $\Omega \subset \mathbb{R}^n$ is described by displacement fields $u: \Omega \rightarrow \mathbb{R}^n$ that minimize the potential energy,

$$\int_{\Omega} W(\epsilon(u)) \, dx. \quad (1.3)$$

Here $\epsilon(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$. (Henceforth we shall not write the dependence of ϵ on u —and on $x \in \Omega$ through u —explicitly.) Since W has a multi-well structure, the problem of minimizing the total energy might not have any solution; instead minimizing sequences develop oscillations and do not converge in any classical

sense [Dac89]. In other words, we find ourselves in a situation where we can reduce the energy with strain fields that have finer and finer oscillations but can never attain the minimum. We interpret this as the emergence of microstructure [BJ87, CK88]. We refer the reader to [Bha03] for a detailed introduction.

Relaxation (with affine boundary conditions). Once a material forms microstructure, its effective behavior is not described by W but by a *relaxed energy density* $\overline{W}: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ that describes its overall effective energy after the formation of microstructure. The theory of relaxation [Dac82, AF84, Dac89, KP91, DM93] provides a characterization of such an energy:

$$\overline{W}(\bar{\epsilon}) := \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_{\Omega} W(\epsilon) \, dx. \quad (1.4)$$

(We use $\int_{\Omega} \cdot \, dx$ and $\langle \cdot \rangle$ to denote $\frac{1}{\text{volume}(\Omega)} \int_{\Omega} \cdot \, dx$.) This definition is independent of the choice of domain, Ω (c.f., e.g., [Dac89, §4.1.1.1, pg.101] or [Mil01, §31.2, pg.674]).

The relaxed energy density can be thought of as the average energy density of the solid accounting for microstructure and describes the behavior of the solid on macroscopic length scales. The theory justifies this since minimizing $\int_{\Omega} W(\cdot) \, dx$ with specified boundary conditions is equivalent to minimizing the relaxed problem $\int_{\Omega} \overline{W}(\cdot) \, dx$ with the same boundary conditions:

$$\inf_{\epsilon \in \mathcal{E}} \int_{\Omega} W(\epsilon) \, dx = \min_{\epsilon \in \mathcal{E}} \int_{\Omega} \overline{W}(\epsilon) \, dx$$

where \mathcal{E} is the set of all strain fields that satisfy the specified boundary conditions.

Relaxation (with affine boundary conditions) with fixed phase fractions. Now consider the problem of finding the optimal microstructure (arrangement of phases) and the optimal strain field when the phase fractions of the phases and overall strain are given.

A microstructure of N phases can be described by a characteristic function $\chi: \Omega \rightarrow \{0, 1\}^N$ chosen such that for $i = 1, \dots, N$,

$$\chi_i(x) = \begin{cases} 1 & \text{if the point } x \in \Omega \text{ is occupied by the } i^{\text{th}} \text{ phase,} \\ 0 & \text{otherwise.} \end{cases}$$

(Consequently $\sum_{i=1}^N \chi_i = 1$.) The phase fractions $\lambda = (\lambda_1, \dots, \lambda_N) \in [0, 1]^N$ (satisfying $\sum_{i=1}^N \lambda_i = 1$) are given by $\lambda = \langle \chi \rangle$.

Given some microstructure χ and a displacement field u , the potential energy of the crystal is

$$\int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) \, dx. \quad (1.5)$$

We define the *relaxed energy density under fixed phase fraction*, $\overline{W}_{\lambda}: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$, through the variational problem

$$\overline{W}_{\lambda}(\bar{\epsilon}) := \inf_{\langle \chi \rangle = \lambda} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) \, dx. \quad (1.6)$$

Relationship between \overline{W}_λ and \overline{W} . From (1.2) and (1.4),

$$\overline{W}(\bar{\epsilon}) = \inf_{u|_{\partial\Omega}=\bar{\epsilon}\cdot x} \int_{\Omega} \min_{i=1,\dots,N} W_i(\epsilon) \, dx.$$

Note that the minimization over i is to be carried out pointwise. Using the characteristic function χ introduced earlier,

$$\begin{aligned} \overline{W}(\bar{\epsilon}) &= \inf_{u|_{\partial\Omega}=\bar{\epsilon}\cdot x} \int_{\Omega} \min_{\chi} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) \, dx \\ &= \inf_{u|_{\partial\Omega}=\bar{\epsilon}\cdot x} \min_{\chi} \int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) \, dx \\ &= \inf_{\chi} \inf_{u|_{\partial\Omega}=\bar{\epsilon}\cdot x} \int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) \, dx \\ &= \min_{\lambda} \inf_{\langle\chi\rangle=\lambda} \inf_{u|_{\partial\Omega}=\bar{\epsilon}\cdot x} \int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) \, dx \\ &= \min_{\lambda} \overline{W}_\lambda(\bar{\epsilon}). \end{aligned} \tag{1.7}$$

Note that the evaluation of \overline{W} from \overline{W}_λ is a simple finite dimensional minimization problem. Therefore, for the energy density (1.2), the problem of computing \overline{W} is essentially that of computing \overline{W}_λ . Thus the problem we study is the characterization of \overline{W}_λ and the optimal microstructures.

Relaxation with traction boundary conditions. When the specimen is subjected to tractions at the boundary the relevant potential energy is not (1.3) but

$$\int_{\Omega} W(\epsilon) \, dx - \int_{\partial\Omega} t(x) \cdot u(x) \, dS.$$

If it is further supposed that the applied traction corresponds to a uniform stress, i.e., $\exists \bar{\sigma} \in \mathbb{R}_{\text{sym}}^{n \times n}$, $\forall x \in \partial\Omega$, $t(x) = \bar{\sigma} \cdot \hat{n}(x)$, where \hat{n} is the unit outward normal to $\partial\Omega$, this reduces to

$$\int_{\Omega} W(\epsilon) - \langle \bar{\sigma}, \epsilon \rangle \, dx.$$

Analogous to (1.4) we define the *relaxed conjugate energy density*, $\overline{W}^\sigma : \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$, through the variational problem

$$\overline{W}^\sigma(\bar{\sigma}) := \inf_{\substack{\epsilon \\ u|_{\partial\Omega}=\bar{\epsilon}\cdot x}} \int_{\Omega} W(\epsilon) - \langle \bar{\sigma}, \epsilon \rangle \, dx; \tag{1.8}$$

and analogous to (1.6) (c.f., (1.5)) we define the *relaxed conjugate energy density under fixed phase fraction*, $\overline{W}_\lambda^\sigma : \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$, through the variational problem

$$\overline{W}_\lambda^\sigma(\bar{\sigma}) := \inf_{\langle\chi\rangle=\lambda} \inf_{\substack{\epsilon \\ u|_{\partial\Omega}=\bar{\epsilon}\cdot x}} \int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) - \langle \bar{\sigma}, \epsilon \rangle \, dx. \tag{1.9}$$

As before

$$\overline{W}^\sigma(\bar{\sigma}) = \min_{\lambda} \overline{W}_\lambda^\sigma(\bar{\sigma}).$$

Relationship between relaxation with affine boundary conditions and relaxation with traction boundary conditions. $\overline{W}_\lambda^\sigma$ is the negative of the Legendre-Fenchel transform of \overline{W}_λ :

$$\begin{aligned} \overline{W}_\lambda^\sigma(\bar{\sigma}) &= \inf_{\langle \chi \rangle = \lambda} \inf_{\substack{\bar{\epsilon} \\ u|_{\partial\Omega} = \bar{\epsilon} \cdot x}} \int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) - \langle \bar{\sigma}, \epsilon \rangle \, dx \\ &= \min_{\bar{\epsilon}} \left(\inf_{\langle \chi \rangle = \lambda} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_{\Omega} \sum_{i=1}^N \chi_i(x) W_i(\epsilon) \, dx - \langle \bar{\sigma}, \bar{\epsilon} \rangle \right) \\ &= \min_{\bar{\epsilon}} \left(\overline{W}_\lambda(\bar{\epsilon}) - \langle \bar{\sigma}, \bar{\epsilon} \rangle \right) \\ &= - \max_{\bar{\epsilon}} \left(\langle \bar{\sigma}, \bar{\epsilon} \rangle - \overline{W}_\lambda(\bar{\epsilon}) \right). \end{aligned}$$

\overline{W}^σ is similarly related to \overline{W} .

1.2. Previous results

Two phases in two dimensions. Lurie and Cherkaev [LC88] used the translation method to consider the relaxation of a two-phase material with equal isotropic elastic moduli (c.f., also [Ser96]). Allaire and Kohn [AK93a] extended this to two isotropic phases with unequal elastic moduli albeit with equal transformation strains, which latter restriction Lu [Lu93] overcame (c.f., also [Ser00]). Grabovsky [Gra96], also using the translation method, considered two phases with arbitrary elastic moduli albeit with equal transformation strains. Our work completes this by studying a general two-phase material with no restrictions on the elastic moduli or transformation strains.

Two phases in arbitrary dimension. Pipkin [Pip91] and Kohn [Koh91] considered the relaxation of a two-phase material with equal elastic moduli ($\alpha_1 = \alpha_2$). Pipkin's approach was to determine the rank-one lamination envelope of the energy and then show that it coincided with the quasiconvex hull. This approach fails when the elastic moduli are unequal since then rank-one laminates are no longer necessarily optimal (c.f., in two dimensions, [Lu93, Gra96] and §3; and, in three dimensions, §4).

Kohn's approach was to compute a lower bound using Fourier analysis and then show its optimality by constructing microstructures whose energies attain this bound. Fourier analysis is not an useful approach when the elastic moduli of the two phases are unequal. Kohn also used the translation method, and it remains viable even for unequal elastic moduli. Our work here too uses the translation method though the translation we use is different from that used by Kohn.

Allaire and Kohn in a series of papers considered this and related problems for the case of well-ordered materials (i.e., materials for which either $\alpha_1 \leq \alpha_2$ or $\alpha_2 \leq \alpha_1$) [AK93b] and non-well-ordered isotropic materials [AK94]. In these papers the transformation strain of both phases was taken to be equal.

More than two phases. Very little is known when one has more than two phases. In the simple situation where the elastic moduli are equal and the transformation strains are pair-wise strain compatible, \overline{W} is the convexification of the W [Bha03, Result 12.1, pg.215]. The problem remains open, even for equal moduli, when the transformation strains are not strain compatible. For a discussion of difficulties see [Koh91]; for recent progress see [FK93, SW99, FS00, GMH02, CS].

2. Overview

Two dimensions. In §3 we compute the relaxation under fixed phase fraction for a two-well elastic energy in two dimensions for arbitrary elastic moduli and arbitrary transformation strains, and provide a characterization of the optimal microstructures and the associated strain (Theorem 2.1 below).

Three dimensions. In §4 we attempt to compute the relaxation under fixed phase fraction for a two-well elastic energy in three dimensions when either (1) both elastic moduli are cubic¹, or (2) the elastic moduli are well-ordered and the smaller elastic modulus is cubic. In both cases we impose no restrictions on the transformation strains.

We succeed in doing so if either (1) both elastic moduli are isotropic, or (2) the elastic moduli are well-ordered and the smaller elastic modulus is isotropic; otherwise we are partially successful: we obtain a lower bound which is optimal except possibly in one regime. When the lower bound is optimal we provide a characterization of the optimal microstructures and the associated strain. (Theorem 2.2 below.)

For moduli with arbitrary symmetry (still with no restrictions on the transformation strains) we obtain a lower bound for the relaxation under fixed phase fraction. This lower bound is sometimes optimal. For the regimes where the lower bound is known to be optimal we provide a characterization of the optimal microstructures and the associated strain. (Theorem 2.3 below.)

Ancillary results. In both two and three dimensions we can obtain the quasiconvex envelope by minimizing over the phase fraction. We discuss the problem of relaxation under applied stress in §5.1. In [CB] we relate these results to experimental observations on the equilibrium morphology and behavior under external loads of precipitates in Nickel superalloys.

Theorem 2.1 (Two dimensions). *Let $W : \mathbb{R}_{sym}^{2 \times 2} \rightarrow \mathbb{R}$ be given by (1.1) and (1.2) for $N = 2$. Then, $\overline{W}_\lambda : \mathbb{R}_{sym}^{2 \times 2} \rightarrow \mathbb{R}$, defined in (1.6), is given by*

$$\overline{W}_\lambda(\bar{\epsilon}) = \max_{\beta \in [0, \gamma(\alpha_1, \alpha_2)]} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{sym}^{2 \times 2} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \sum_{i=1}^2 \lambda_i W_i(\epsilon_i) + \beta \lambda_1 \lambda_2 \det(\epsilon_2 - \epsilon_1).$$

¹C.f., Definition 4 in §4 for the definition of “cubic moduli”. We use the term “cubic” to include isotropy as a special case.

The interval $[0, \gamma_{(\alpha_1, \alpha_2)}]$ over which β ranges is defined as follows: Let $T \in \mathcal{L}^*(\mathbb{R}_{sym}^{2 \times 2})$ be defined by,

$$\begin{aligned} T\epsilon &:= \epsilon - \text{Tr}(\epsilon)I, \\ I &:= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \end{aligned}$$

and let

$$\gamma_\alpha := \left(\max_{\|\epsilon\|=1} \left\langle \left(\alpha^{-\frac{1}{2}} T \alpha^{-\frac{1}{2}} \right) \epsilon, \epsilon \right\rangle \right)^{-1}, \quad (2.1a)$$

$$\gamma_{(\alpha_1, \alpha_2)} := \min(\gamma_{\alpha_1}, \gamma_{\alpha_2}). \quad (2.1b)$$

Explicitly,

$$\overline{W}_\lambda(\bar{\epsilon}) = \sum_{i=1}^2 \lambda_i W_i(\epsilon_i^*(\beta^*(\bar{\epsilon}), \bar{\epsilon})) + \beta^*(\bar{\epsilon}) \lambda_1 \lambda_2 \det(\epsilon_2^*(\beta^*(\bar{\epsilon}), \bar{\epsilon}) - \epsilon_1^*(\beta^*(\bar{\epsilon}), \bar{\epsilon})),$$

where,

$$\begin{aligned} \epsilon_1^*(\beta^*(\bar{\epsilon}), \bar{\epsilon}) &:= (\lambda_2 \alpha_1 + \lambda_1 \alpha_2 - \beta^*(\bar{\epsilon})T)^{-1} \\ &\quad ((\alpha_2 - \beta^*(\bar{\epsilon})T)\bar{\epsilon} - \lambda_2(\alpha_2 \epsilon_2^T - \alpha_1 \epsilon_1^T)), \\ \epsilon_2^*(\beta^*(\bar{\epsilon}), \bar{\epsilon}) &:= (\lambda_2 \alpha_1 + \lambda_1 \alpha_2 - \beta^*(\bar{\epsilon})T)^{-1} \\ &\quad ((\alpha_1 - \beta^*(\bar{\epsilon})T)\bar{\epsilon} + \lambda_1(\alpha_2 \epsilon_2^T - \alpha_1 \epsilon_1^T)); \\ \beta^*(\bar{\epsilon}) &:= \begin{cases} 0 & \text{if } \phi(\cdot, \bar{\epsilon}) \equiv 0 & (\text{Regime 0}), \\ 0 & \text{if } \phi(0, \bar{\epsilon}) > 0 & (\text{Regime I}), \\ \beta_{II} & \text{if } \phi(0, \bar{\epsilon}) \leq 0 \text{ and } \phi(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon}) \geq 0 & (\text{Regime II}), \\ \gamma_{(\alpha_1, \alpha_2)} & \text{if } \phi(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon}) < 0. & (\text{Regime III}); \end{cases} \end{aligned}$$

$\phi(\cdot, \bar{\epsilon})$ is the mapping

$$[0, \gamma_{(\alpha_1, \alpha_2)}] \ni \beta \mapsto -\det((\lambda_2 \alpha_1 + \lambda_1 \alpha_2 - \beta T)^{-1} (\alpha_2(\epsilon_2^T - \bar{\epsilon}) - \alpha_1(\epsilon_1^T - \bar{\epsilon})))$$

and, in Regime II, $\beta_{II} \in [0, \gamma_{(\alpha_1, \alpha_2)}]$ is the unique root of $\phi(\cdot, \bar{\epsilon})$ when $\phi(0, \bar{\epsilon}) \leq 0$ and $\phi(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon}) \geq 0$.

Further,

1. In Regime 0 every microstructure is optimal. The optimal strain and stress are constant.
2. In Regime I the optimal microstructure is either a rank-one laminate, with either of two possible layering directions, or a microstructure made of these laminates. The optimal strain takes the value ϵ_1^* in phase 1 and ϵ_2^* in phase 2 while the optimal stress is constant.
3. In Regime II the optimal microstructure is unique and is a rank-one laminate. The optimal strain takes the value ϵ_1^* in phase 1 and ϵ_2^* in phase 2.

4. In Regime III, no rank-one laminate is optimal. The class of optimal microstructures is possibly large² and includes at least two rank-two laminates.

In any optimal microstructure, in phase i , $i = 1, 2$, the strain is confined to an affine subspace of dimension $\dim \ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)} T) \leq 2$; the sum of the dimension of the two affine subspaces is also at most 2. In particular, if phase i is harder than the other phase (i.e., if $\gamma_{\alpha_i} > \gamma_{(\alpha_1, \alpha_2)}$) then the strain is ϵ_i^* in that phase.

Theorem 2.2 (Cubic moduli in three dimensions). Let $W: \mathbb{R}_{\text{sym}}^{3 \times 3} \rightarrow \mathbb{R}$ be given by (1.1) and (1.2) for $N = 2$. Moreover, let one of the following conditions hold:

1. Both elastic moduli are cubic (c.f., Definition 4 in §4).
2. The elastic moduli are well ordered³ and the smaller elastic modulus is cubic.

Then a lower bound for $\bar{W}_\lambda: \mathbb{R}_{\text{sym}}^{3 \times 3} \rightarrow \mathbb{R}$, defined in (1.6), is given by

$$\bar{W}_\lambda(\bar{\epsilon}) \geq \max_{\beta \in S_{(\alpha_1, \alpha_2)}} \max_{R \in SO(3)} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \sum_{i=1}^2 \lambda_i W_i(\epsilon_i) - \lambda_1 \lambda_2 \beta \cdot \phi^R(\epsilon_2 - \epsilon_1).$$

Here,

$$S_{(\alpha_1, \alpha_2)} := \begin{cases} S_{\alpha_1} \cap S_{\alpha_2} & \text{if } \alpha_1 \text{ and } \alpha_2 \text{ are cubic,} \\ S_{\alpha_1} & \text{if } \alpha_1 \leq \alpha_2, \\ S_{\alpha_2} & \text{if } \alpha_2 \leq \alpha_1; \end{cases}$$

for a cubic elastic modulus α with lamé modulus ℓ , diagonal shear modulus μ and off-diagonal shear modulus η ,

$$S_\alpha = \left\{ \beta \in \mathbb{R}_+^3 \left| \begin{aligned} &2\beta_1\beta_2\beta_3 - (\ell + 2\min(\mu, \eta))(\beta_1^2 + \beta_2^2 + \beta_3^2) \\ &\quad + 2\ell(\beta_1\beta_2 + \beta_2\beta_3 + \beta_3\beta_1) \\ &\quad - 4\ell\min(\mu, \eta)(\beta_1 + \beta_2 + \beta_3) \\ &\quad + 12\ell(\min(\mu, \eta))^2 + 8(\min(\mu, \eta))^3 \geq 0 \end{aligned} \right. \right\};$$

and $\phi^R: \mathbb{R}_{\text{sym}}^{3 \times 3} \rightarrow \mathbb{R}^3$ is defined by

$$\phi^R(\epsilon) := \phi(R^T \epsilon R), \quad R \in SO(3), \quad (2.2a)$$

$$\phi(\epsilon) := \begin{pmatrix} \epsilon_{23}^2 - \epsilon_{22}\epsilon_{33} \\ \epsilon_{31}^2 - \epsilon_{33}\epsilon_{11} \\ \epsilon_{12}^2 - \epsilon_{11}\epsilon_{22} \end{pmatrix}. \quad (2.2b)$$

To present a more explicit expression let $T \in \mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ be defined by,

$$\begin{aligned} T\epsilon &:= \epsilon - \text{Tr}(\epsilon)I, \\ I &:= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \end{aligned}$$

²In a sense explained in the proof of Theorem 3.16.

³I.e., $\alpha_1 \leq \alpha_2$ or $\alpha_2 \leq \alpha_1$.

let $\gamma_{\alpha_1}, \gamma_{\alpha_2}, \gamma_{(\alpha_1, \alpha_2)}$ be as in (2.1); let $W_\lambda(\beta, \bar{\epsilon}): \mathbb{R}_+^3 \times \mathbb{R}_{\text{sym}}^{3 \times 3} \rightarrow \mathbb{R}$ be defined by

$$W_\lambda(\beta, \bar{\epsilon}) := \max_{R \in SO(3)} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) - \lambda_1 \lambda_2 \beta \cdot \phi^R(\epsilon_2 - \epsilon_1);$$

let $R_\star(\beta, \bar{\epsilon}), \epsilon_1^\star(R_\star(\beta, \bar{\epsilon}), \beta, \bar{\epsilon}), \epsilon_2^\star(R_\star(\beta, \bar{\epsilon}), \beta, \bar{\epsilon})$ attain the extrema above and let $\Delta\epsilon^\star(R, \beta, \bar{\epsilon}) := \epsilon_2^\star(R, \beta, \bar{\epsilon}) - \epsilon_1^\star(R, \beta, \bar{\epsilon})$. We use “ \parallel ” to mean “parallel and not anti-parallel”. For $x \in \mathbb{R}^n$ and $S \subset \mathbb{R}^n$ we say $x \parallel S$ if $\exists y \in S, x \parallel y$. Then,

$$\begin{cases} \overline{W}_\lambda(\bar{\epsilon}) \geqslant \\ \left\{ \begin{array}{ll} W_\lambda(0, \bar{\epsilon}) & \text{if } \Delta\epsilon^\star(\cdot, \cdot, \bar{\epsilon}) \equiv 0 \quad (\text{Regime 0}), \\ W_\lambda(\beta_I, \bar{\epsilon}) & \text{if } \exists \beta \in S_{(\alpha_1, \alpha_2)} \cap (\{0\} \times \mathbb{R}^2 \cup \mathbb{R} \times \{0\} \times \mathbb{R} \cup \mathbb{R}^2 \times \{0\}), \\ & 0 \neq -\phi^{R_\star(\beta_I, \bar{\epsilon})}(\Delta\epsilon^\star(R_\star(\beta_I, \bar{\epsilon}), \beta_I, \bar{\epsilon})) \parallel \{-e_1, -e_2, -e_3\} \quad (\text{Regime I}), \\ W_\lambda(\beta_{II}, \bar{\epsilon}) & \text{otherwise. Here } \beta_{II} \text{ is the unique solution in } S_{(\alpha_1, \alpha_2)} \text{ of} \\ & \phi^{R_\star(\cdot, \bar{\epsilon})}(\Delta\epsilon^\star(R_\star(\cdot, \bar{\epsilon}), \cdot, \bar{\epsilon})) = 0 \quad (\text{Regime II}), \\ W_\lambda(\beta_{III}, \bar{\epsilon}) & \text{if } \exists \beta_{III} \in \left\{ \beta \in \mathbb{R}_+^3 \mid \beta_1 = \gamma_{(\alpha_1, \alpha_2)}, \beta_2 = \beta_3 \in [0, \gamma_{(\alpha_1, \alpha_2)}] \right\} \\ & \cup \left\{ \beta \in \mathbb{R}_+^3 \mid \beta_2 = \gamma_{(\alpha_1, \alpha_2)}, \beta_3 = \beta_1 \in [0, \gamma_{(\alpha_1, \alpha_2)}] \right\} \\ & \cup \left\{ \beta \in \mathbb{R}_+^3 \mid \beta_3 = \gamma_{(\alpha_1, \alpha_2)}, \beta_1 = \beta_2 \in [0, \gamma_{(\alpha_1, \alpha_2)}] \right\}, \\ & 0 \neq -\phi^{R_\star(\beta_{III}, \bar{\epsilon})}(\Delta\epsilon^\star(R_\star(\beta_{III}, \bar{\epsilon}), \beta_{III}, \bar{\epsilon})) \parallel \{e_1, e_2, e_3\} \quad (\text{Regime III}), \\ W_\lambda(\beta_{IV}, \bar{\epsilon}) & \text{if } 0 \neq -\phi^{R_\star(\beta_{IV}, \bar{\epsilon})}(\Delta\epsilon^\star(R_\star(\beta_{IV}, \bar{\epsilon}), \beta_{IV}, \bar{\epsilon})) \parallel \text{Int}(\mathbb{R}_+^3) \\ & \text{where } \beta_{IV} = \gamma_{(\alpha_1, \alpha_2)}(1, 1, 1)^T \quad (\text{Regime IV}). \end{array} \right. \end{cases}$$

In regime II, β_{II} is the unique solution of $\phi^{R_\star(\cdot, \bar{\epsilon})}(\Delta\epsilon^\star(R_\star(\cdot, \bar{\epsilon}), \cdot, \bar{\epsilon})) = 0$ in $S_{(\alpha_1, \alpha_2)}$.

Assume, renumbering if necessary, that $\gamma_{\alpha_1} \leqslant \gamma_{\alpha_2}$. Also let

$$D_{IV} := \begin{cases} 2 & \text{if } \mu_1 < \eta_1, \\ 5 & \text{if } \mu_1 = \eta_1, \\ 3 & \text{if } \mu_1 > \eta_1. \end{cases}$$

The lower bound is sharp except possibly in Regime IV when $\mu_1 \neq \eta_1$. Further,

1. In Regime 0 every microstructure is optimal. The optimal strain and stress are constant.
2. In Regime I the optimal microstructure is either a rank-one laminate, with either of two possible layering directions, or a microstructure made of these laminates. The optimal strain is constant in each phase while the optimal stress is (globally) constant.
3. In Regime II the optimal microstructure is unique and is a rank-one laminate. The optimal strain is constant in each phase.

4. In Regime III, no rank-one laminate is optimal. The class of optimal microstructures is possibly large² and includes at least two rank-two laminates. In any optimal microstructure the strain in each phase is confined to an affine subspace of dimension at most D_{IV} ; the sum of the dimension of the two affine subspaces is also at most D_{IV} .⁴ Moreover, if one phase is harder than the other (i.e., if $\gamma_{\alpha_2} > \gamma_{\alpha_1}$) then the strain in the harder phase is constant.
5. In Regime IV the lower bound is possibly non-optimal when $\mu_1 \neq \eta_1$. If the bound is optimal then:
- (a) No rank-one laminate is optimal.
 - (b) If one phase is harder than the other then no rank-two laminate is optimal.
 - (c) If $\mu_1 = \eta_1$ then there exists an optimal rank-three laminate.
 - (d) In any optimal microstructure the strain in each phase is confined to an affine subspace of dimension at most D_{IV} ; the sum of the dimension of the two affine subspaces is also at most D_{IV} . Moreover, if one phase is harder than the other then the strain in the harder phase is constant.

Theorem 2.3 (Arbitrary moduli in three dimensions). Let $W: \mathbb{R}_{sym}^{3 \times 3} \rightarrow \mathbb{R}$ be given by (1.1) and (1.2) for $N = 2$. Then a lower bound for $\overline{W}_\lambda: \mathbb{R}_{sym}^{3 \times 3} \rightarrow \mathbb{R}$, defined in (1.6), is given by

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\beta \in \cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)} \max_{R \in SO(3)} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{sym}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \sum_{i=1}^2 \lambda_i W_i(\epsilon_i) - \lambda_1 \lambda_2 \beta \cdot \phi^R(\epsilon_2 - \epsilon_1).$$

Here, for $R \in SO(3)$

$$B_{(\alpha_1, \alpha_2)}(R) := B_{\alpha_1}(R) \cap B_{\alpha_2}(R),$$

$$B_\alpha(R) := \left\{ \beta \in \mathbb{R}_+^3 \mid \forall \epsilon \in \mathbb{R}_{sym}^{3 \times 3}, \frac{1}{2} \langle \alpha \epsilon, \epsilon \rangle - \beta \cdot \phi^R(\epsilon) \geq 0 \right\};$$

and $\phi^R: \mathbb{R}_{sym}^{3 \times 3} \rightarrow \mathbb{R}^3$ is defined in (2.2).

Let β^*, R_* attain the maximum above. This lower bound is sharp when

1. (Regime 0) $\alpha_2 \epsilon_2^T - \alpha_1 \epsilon_1^T = (\alpha_2 - \alpha_1) \bar{\epsilon}$.
2. (Regime I) $\beta^* \in (\{0\} \times \mathbb{R}^2 \cup \mathbb{R} \times \{0\}) \times \mathbb{R} \cup \mathbb{R}^2 \times \{0\}$ and

$$0 \neq -\phi^{R_*(\beta^*, \bar{\epsilon})}(\Delta \epsilon^*(R_*(\beta^*, \bar{\epsilon}), \beta^*, \bar{\epsilon})) \parallel \{-e_1, -e_2, -e_3\}.$$

3. (Regime II) β^* solves $\phi^{R_*(\cdot, \bar{\epsilon})}(\Delta \epsilon^*(R_*(\cdot, \bar{\epsilon}), \cdot, \bar{\epsilon})) = 0$.

(The notation \parallel is explained in Theorem 2.2.) Further the statements (1), (2) and (3) in Theorem 2.2 hold.

⁴Sharper results are presented in Theorem 4.37.

Strategy. We prove Theorems 2.1, 2.2 and 2.3 by first using the translation method to obtain a lower bound for \overline{W}_λ in §3.2.1 and §4.10, and then constructing microstructures whose effective energy equals this bound in §3.2.1 and §4.10.

(Note that the construction of a microstructure immediately leads to an upper bound for \overline{W}_λ . Various such microstructures, and thus upper bounds—including some bounds now known to be optimal—are explicit or implicit in the metallurgy literature. [Roy93] surveys work in this direction. The challenge is to prove a matching lower bound for \overline{W}_λ .)

Good introductions and overviews of the translation method can be found in [Che00, Chs. 8, 15, 16] and [Mil01, Chs. 4, 24, 25]. For development of the method and applications to a wide range of problems c.f., e.g., Tartar [Tar79a, Tar85, Tar79b]; Lurie and Cherkaev [LC81, LC82a, LC82b, LC86a]; Kohn and Strang [KS82, KS83, KS86a, KS86b, KS86c, SK88]; Cherkaev and Gibiansky [GC84, GC87, CG92]; Murat and Tartar [MT85]; Murat [Mur87]; Avellaneda, Cherkaev, Lurie and Milton [ACLM88]; Milton [Mil90a, Mil90b]; and Firoozye [Fir91].

Laminates. The microstructures we construct are laminates; these have been used in a variety of problems; c.f., e.g., [Tar79b, Tar85, FM86, Tar00], [Che00, Ch. 7], [Mil01, Ch. 9] and references therein. Good introductions and overviews can be found in [Che00, Ch. 7] and [Mil01, Ch. 9]. Rank-one laminates are alternating layers of two phases at fixed phase fraction; rank-two laminates are rank-one laminates where at least one of the layers is itself a rank-one laminate at a smaller scale; and so on. In order to use laminates in our context, one has to think of them as a sequence of microstructures with fixed geometry but smaller and smaller scales.

3. Two-phase solids in two dimensions

In this section, we consider the two-well problem in two dimensions.

3.1. A lower bound on the relaxed energy

3.1.1. A lower bound using the translation method. We use the translation method to derive a lower bound. We state the basic principle in \mathbb{R}^n since we use it for both two and three dimensions. Recall that $f: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ is quasiconvex if

$$f(\bar{\epsilon}) \leq \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_{\Omega} f(\epsilon) \, dx. \quad (3.1)$$

for each $\bar{\epsilon} \in \mathbb{R}_{\text{sym}}^{n \times n}$. Any quasiconvex function can be used to derive a lower bound on the relaxed energy at fixed phase fraction using the translation method:

Proposition 3.1 (Translation lower bound). *Let $W: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ be as in (1.1) and (1.2) for $N = 1, 2$. Let $f: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ be quasiconvex and $\beta \in \mathbb{R}_+$. Then $\overline{W}_\lambda: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ defined in (1.6) satisfies the lower bound*

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\substack{\beta \geq 0 \\ W_i - \beta f: \text{convex}}} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{n \times n} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \sum_{i=1}^2 \lambda_i (W_i - \beta f)(\epsilon_i) + \beta f(\bar{\epsilon}). \quad (3.2)$$

Proof. From (1.6),

$$\overline{W}_\lambda(\bar{\epsilon}) := \inf_{\langle \chi_i \rangle = \lambda_i} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_{\Omega} \sum_{i=1}^2 \chi_i W_i(\epsilon) \, dx.$$

Since f is quasiconvex we have the lower bound,

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \inf_{\langle \chi_i \rangle = \lambda_i} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_{\Omega} \sum_{i=1}^2 \chi_i (W_i(\epsilon) - \beta f(\epsilon)) \, dx + \beta f(\bar{\epsilon})$$

for each $\beta \geq 0$. Choosing β optimally subject to the restriction that the functions $W_i - \beta f$ are convex (the reason for this will become clear in the next step), we have

$$\begin{aligned} \overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\substack{\beta \geq 0 \\ W_i - \beta f: \text{convex}}} \min_{\langle \chi_i \rangle = \lambda_i} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_{\Omega} \sum_{i=1}^2 \chi_i (W_i(\epsilon) - \beta f(\epsilon)) \, dx \\ + \beta f(\bar{\epsilon}). \end{aligned}$$

Since $W_i - \beta f$ is convex, using Jensen's inequality,

$$\begin{aligned} \overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\substack{\beta \geq 0 \\ W_i - \beta f: \text{convex}}} \min_{\langle \chi_i \rangle = \lambda_i} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \sum_{i=1}^2 \lambda_i (W_i - \beta f) \left(\frac{\int_{\Omega} \chi_i \epsilon \, dx}{\int_{\Omega} \chi_i \, dx} \right) \\ + \beta f(\bar{\epsilon}). \end{aligned}$$

Setting $\epsilon_i = \frac{\langle \chi_i \epsilon \rangle}{\langle \chi_i \rangle}$ and noting that $\lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}$, we obtain the desired result. \square

3.1.2. The determinant as translation. The lower bound presented in Proposition 3.1 is valid for any translation $f: \mathbb{R}_{\text{sym}}^{n \times n} \rightarrow \mathbb{R}$ which is quasiconvex. The art of the translation method lies in choosing the right translation. In two dimensions, we pick the translation to be the negative of the determinant: $f \equiv \phi := -\det$, i.e.,

$$\phi(\epsilon) = \epsilon_{12}^2 - \epsilon_{11}\epsilon_{22}.$$

This choice of translation might appear to be arbitrary, but in fact is a posteriori natural.

Quadraticity of ϕ . It is easy to verify that

$$\phi(\epsilon) = \frac{1}{2} \langle T\epsilon, \epsilon \rangle$$

where $T \in \mathcal{L}^*(\mathbb{R}_{\text{sym}}^{2 \times 2})$ is defined by

$$\begin{aligned} T\epsilon &:= \epsilon - \text{Tr}(\epsilon)I, \\ I &:= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

(i.e., $-T\epsilon$ is the adjoint of ϵ). Alternatively,

$$T \equiv -\mathbf{A}_h + \mathbf{A}_d + \mathbf{A}_o, \quad (3.3)$$

where $\mathbf{A}_h, \mathbf{A}_d, \mathbf{A}_o \in \mathcal{L}_{\geq}^*(\mathbb{R}_{\text{sym}}^{2 \times 2})$ are orthogonal projection operators defined by

$$\text{Range}(\mathbf{A}_h) = \text{Span} \{I\}, \quad (3.4a)$$

$$\text{Range}(\mathbf{A}_d) = \text{Span} \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}, \quad (3.4b)$$

$$\text{Range}(\mathbf{A}_o) = \text{Span} \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}. \quad (3.4c)$$

In particular T has eigenvalues -1 and 1 , repeated once and twice respectively. It follows that T is invertible and is neither positive nor negative definite. Note also that $T^2 = I$.

Quasiconvexity of ϕ . ϕ is quasiconvex since it is quadratic and rank-one convex [Dac89, pg.126]: $\forall m, n \in \mathbb{R}^2$, $\phi(m \otimes_s n) \geq 0$. Here $\hat{m} \otimes_s \hat{n} := \frac{1}{2}(\hat{n} \otimes \hat{m} + \hat{m} \otimes \hat{n})$; $\hat{m} \otimes \hat{n}$ is defined by $(\hat{m} \otimes \hat{n})_{ij} = m_i n_j$, $i, j = 1, 2$.

A lower bound on the relaxed energy. With this choice for the translation, and exploiting the fact that W_i and ϕ are quadratic, we may rewrite (3.2) as

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\substack{\beta \geq 0 \\ W_i - \beta\phi: \text{convex}}} W_\lambda(\beta, \bar{\epsilon}) \quad (3.5a)$$

where $W_\lambda: \mathbb{R} \times \mathbb{R}_{\text{sym}}^{2 \times 2} \rightarrow \mathbb{R}$ is defined by

$$W_\lambda(\beta, \bar{\epsilon}) := \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{2 \times 2} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) - \beta \lambda_1 \lambda_2 \phi(\epsilon_2 - \epsilon_1). \quad (3.5b)$$

3.1.3. Determining the amount of permissible translation. Our next step is to characterize the set $\{\beta \geq 0 \mid W_i - \beta\phi: \text{convex}, i = 1, 2\}$.

Lemma 3.2 (Convexity of translated energies). *Let $\alpha, \alpha_1, \alpha_2 \in \mathcal{L}_{>}^*(\mathbb{R}_{\text{sym}}^{2 \times 2})$. Let $\gamma_\alpha, \gamma_{(\alpha_1, \alpha_2)} > 0$ be defined by*

$$\gamma_\alpha := \left(\max_{\|\epsilon\|=1} \left\langle \left(\alpha^{-\frac{1}{2}} T \alpha^{-\frac{1}{2}} \right) \epsilon, \epsilon \right\rangle \right)^{-1},$$

$$\gamma_{(\alpha_1, \alpha_2)} := \min(\gamma_{\alpha_1}, \gamma_{\alpha_2}).$$

Then,

$$[0, \gamma_{(\alpha_1, \alpha_2)}] = \{\beta \geq 0 \mid W_i - \beta\phi: \text{convex}, i = 1, 2\},$$

$$[0, \gamma_{(\alpha_1, \alpha_2)}) = \{\beta \geq 0 \mid W_i - \beta\phi: \text{strictly convex}, i = 1, 2\}.$$

Proof. Let $i = 1, 2$. The convexity of $W_i - \beta\phi$ is equivalent to the positive-semidefiniteness of $\alpha_i - \beta T$, i.e., to the nonnegativity of $\epsilon \mapsto \langle (\alpha_i - \beta T)\epsilon, \epsilon \rangle$. Now,

$$\begin{aligned} \langle (\alpha_i - \beta T)\epsilon, \epsilon \rangle &= \left\langle \alpha_i^{\frac{1}{2}} \left(I - \beta \alpha_i^{-\frac{1}{2}} T \alpha_i^{-\frac{1}{2}} \right) \alpha_i^{\frac{1}{2}} \epsilon, \epsilon \right\rangle \\ &= \|\tilde{\epsilon}\|^2 - \beta \left\langle \alpha_i^{-\frac{1}{2}} T \alpha_i^{-\frac{1}{2}} \tilde{\epsilon}, \tilde{\epsilon} \right\rangle \end{aligned}$$

where $\tilde{\epsilon} = \alpha_i^{\frac{1}{2}} \epsilon$ and $\alpha_i^{\frac{1}{2}}$ is the unique positive-definite self-adjoint square root of α_i . Thus

$$\begin{aligned} \forall \epsilon, \langle (\alpha_i - \beta T)\epsilon, \epsilon \rangle \geq 0 &\iff \forall \epsilon, \|\epsilon\|^2 - \beta \left\langle \left(\alpha_i^{-\frac{1}{2}} T \alpha_i^{-\frac{1}{2}} \right) \epsilon, \epsilon \right\rangle \geq 0 \\ &\iff \forall \epsilon \neq 0, \frac{1}{\beta} \geq \frac{\left\langle \left(\alpha_i^{-\frac{1}{2}} T \alpha_i^{-\frac{1}{2}} \right) \epsilon, \epsilon \right\rangle}{\|\epsilon\|^2} \end{aligned}$$

where we have used the invertibility of $\alpha_i^{\frac{1}{2}}$. (γ_{α_i} is non-negative since T has a positive eigenvalue and all eigenvalues of α_i are positive.) The result follows. \square

Note 3.3. From (3.3),

$$\langle (\alpha - \gamma_{\alpha} T)I, I \rangle = \langle \alpha I, I \rangle + \gamma_{\alpha} \|I\|^2 > 0.$$

This, with Lemma 3.2 gives,

$$1 \leq \dim \ker(\alpha - \gamma_{\alpha} T) \leq \dim \mathbb{R}_{\text{sym}}^{2 \times 2} - 1 = 2. \quad (3.6)$$

Note 3.4. For cubic α , aligning our axis with the principal axis of α , we have,

$$\alpha = 2\kappa \mathbf{A}_{\mathbf{h}} + 2\mu \mathbf{A}_{\mathbf{d}} + 2\eta \mathbf{A}_{\mathbf{o}},$$

where $\kappa(\alpha), \mu(\alpha), \eta(\alpha) > 0$ are, respectively, the bulk, diagonal shear and off-diagonal shear moduli. (Henceforth we shall leave the dependence on α implicit.) Since $T \equiv -\mathbf{A}_{\mathbf{h}} + \mathbf{A}_{\mathbf{d}} + \mathbf{A}_{\mathbf{o}}$,

$$\alpha^{-\frac{1}{2}} T \alpha^{-\frac{1}{2}} = \frac{-1}{2\kappa} \mathbf{A}_{\mathbf{h}} + \frac{1}{2\mu} \mathbf{A}_{\mathbf{d}} + \frac{1}{2\eta} \mathbf{A}_{\mathbf{o}}.$$

Thus

$$\gamma_{\alpha} = \begin{cases} 2 \min(\mu, \eta) & \text{when } \alpha \text{ is cubic,} \\ 2\mu & \text{when } \alpha \text{ is isotropic.} \end{cases}$$

(An isotropic modulus is a cubic modulus for which $\mu = \eta$.) Moreover, as is easy to verify,

$$\ker(\alpha - \gamma_{\alpha} T) = \begin{cases} \text{Span} \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} & \text{if } \alpha \text{ is cubic with } \mu < \eta, \\ \text{Span} \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} & \text{if } \alpha \text{ is cubic with } \eta < \mu, \\ \text{Span} \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} & \text{if } \alpha \text{ is isotropic.} \end{cases}$$

3.1.4. Explicit expressions for the optimal strains and stresses. Let us return to the minimization problem (3.5b) and find the minimizers $\epsilon_1^*(\beta, \bar{\epsilon})$ and $\epsilon_2^*(\beta, \bar{\epsilon})$. By differentiating the argument on the right-hand side of (3.5b),

$$\alpha_1(\epsilon_1^* - \epsilon_1^T) - \alpha_2(\epsilon_2^* - \epsilon_2^T) + \beta T(\epsilon_2^* - \epsilon_1^*) = 0. \quad (3.7)$$

In other words,

$$\Delta\sigma^* = \beta T \Delta\epsilon^* \quad (3.8)$$

where

$$\begin{aligned} \Delta\epsilon^* &:= \epsilon_2^* - \epsilon_1^*, \\ \Delta\sigma^* &:= \sigma_2^* - \sigma_1^*, \\ \sigma_i^* &:= \alpha_i(\epsilon_i^* - \epsilon_i^T), \quad i = 1, 2. \end{aligned}$$

Since $\lambda_1\epsilon_1^* + \lambda_2\epsilon_2^* = \bar{\epsilon}$, (3.7) gives

$$\begin{aligned} (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)\epsilon_1^* &= (\alpha_2 - \beta T)\bar{\epsilon} - \lambda_2\Delta(\alpha\epsilon^T) \\ (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)\epsilon_2^* &= (\alpha_1 - \beta T)\bar{\epsilon} + \lambda_1\Delta(\alpha\epsilon^T) \\ (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)\Delta\epsilon^* &= \Delta(\alpha\epsilon^T) - (\Delta\alpha)\bar{\epsilon}. \end{aligned}$$

where

$$\begin{aligned} \Delta(\alpha\epsilon^T) &:= \alpha_2\epsilon_2^T - \alpha_1\epsilon_1^T, \\ \Delta\alpha &:= \alpha_2 - \alpha_1. \end{aligned}$$

If $\beta \in [0, \gamma_{(\alpha_1, \alpha_2)})$, then from Lemma 3.2 it follows that $\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T$ is positive definite since it is the sum of the two positive definite linear operators $\lambda_2(\alpha_1 - \beta T)$ and $\lambda_1(\alpha_2 - \beta T)$. Consequently, we may invert the relations above to conclude that

$$\epsilon_1^*(\beta, \bar{\epsilon}) = (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)^{-1} ((\alpha_2 - \beta T)\bar{\epsilon} - \lambda_2\Delta(\alpha\epsilon^T)), \quad (3.9a)$$

$$\epsilon_2^*(\beta, \bar{\epsilon}) = (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)^{-1} ((\alpha_1 - \beta T)\bar{\epsilon} + \lambda_1\Delta(\alpha\epsilon^T)), \quad (3.9b)$$

$$\Delta\epsilon^*(\beta, \bar{\epsilon}) = (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)^{-1} (\Delta(\alpha\epsilon^T) - (\Delta\alpha)\bar{\epsilon}), \quad (3.9c)$$

If $\beta = \gamma_{(\alpha_1, \alpha_2)}$, then $\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T$ might only be positive semi-definite. However, the minimization problem (3.5b) is quadratic. So we can have one of two situations: either (1) the minimum is finite and the solutions in (3.9) are defined up to a constant in $\ker(\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)$, or (2) $W_\lambda(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon}) = -\infty$, in which case,

$$\lim_{\beta \rightarrow \gamma_{(\alpha_1, \alpha_2)}} \phi(\Delta\epsilon^*) = \infty. \quad (3.10)$$

For future use we observe that for $\beta \in [0, \gamma_{(\alpha_1, \alpha_2)})$,

$$\frac{\partial \Delta\epsilon^*}{\partial \beta} = (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta T)^{-1} T \Delta\epsilon^*. \quad (3.11)$$

From (3.9) we also calculate, for $\beta \in [0, \gamma_{(\alpha_1, \alpha_2)})$,

$$\begin{aligned}\sigma_1^* &= \left(\overline{\alpha^{-1}} - \beta \alpha_2^{-1} T \alpha_1^{-1} \right)^{-1} \alpha_2^{-1} ((\alpha_2 - \beta T) \bar{\epsilon} - \lambda_2 \Delta(\alpha \epsilon^T)) - \alpha_1 \epsilon_1^T \\ \sigma_2^* &= \left(\overline{\alpha^{-1}} - \beta \alpha_1^{-1} T \alpha_2^{-1} \right)^{-1} \alpha_1^{-1} ((\alpha_1 - \beta T) \bar{\epsilon} + \lambda_1 \Delta(\alpha \epsilon^T)) - \alpha_2 \epsilon_2^T\end{aligned}$$

where $\overline{\alpha^{-1}} := \lambda_1 \alpha_1^{-1} + \lambda_2 \alpha_2^{-1}$.

3.1.5. A lower bound on the relaxed energy. We are now in a position to derive an explicit lower bound. Applying Lemma 3.2 to the lower bound (3.5a), we have

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\beta \in [0, \gamma_{(\alpha_1, \alpha_2)}]} W_\lambda(\beta, \bar{\epsilon}). \quad (3.12)$$

Determining this maximum is easy since we have the following lemma:

Lemma 3.5. $(0, \gamma_{(\alpha_1, \alpha_2)}) \ni \beta \mapsto W_\lambda(\beta, \bar{\epsilon})$ is either constant or strictly concave.

Proof. From (3.5b) and (3.11),

$$\begin{aligned}\frac{\partial}{\partial \beta} W_\lambda(\beta, \bar{\epsilon}) &= -\lambda_1 \lambda_2 \phi(\Delta \epsilon^*(\beta, \bar{\epsilon})). \\ \frac{\partial^2}{\partial \beta^2} W_\lambda(\beta, \bar{\epsilon}) &= -\lambda_1 \lambda_2 \left\langle T \Delta \epsilon^*(\beta, \bar{\epsilon}), \frac{\partial}{\partial \beta} \Delta \epsilon^*(\beta, \bar{\epsilon}) \right\rangle \\ &= -\lambda_1 \lambda_2 \left\langle T \Delta \epsilon^*(\beta, \bar{\epsilon}), (\lambda_2 \alpha_1 + \lambda_1 \alpha_2 - \beta T)^{-1} T \Delta \epsilon^*(\beta, \bar{\epsilon}) \right\rangle \\ &< 0\end{aligned} \quad (3.13)$$

except when $\Delta \epsilon^*(\beta, \bar{\epsilon}) = 0$. Note, from (3.9), that $\Delta \epsilon^*(\beta, \bar{\epsilon}) = 0$ for some $\beta \in (0, \gamma_{(\alpha_1, \alpha_2)})$ implies that $\Delta \epsilon^*(\beta, \bar{\epsilon}) = 0$ for all $\beta \in (0, \gamma_{(\alpha_1, \alpha_2)})$. However when $\Delta \epsilon^*(\beta, \bar{\epsilon}) \equiv 0$, from (3.13), $W_\lambda(\beta, \bar{\epsilon})$ is independent of β . \square

Incidentally, we also observe that:

Lemma 3.6. $\bar{\epsilon} \mapsto W_\lambda(\beta, \bar{\epsilon})$ is strictly convex.

Proof. From (3.5b),

$$\begin{aligned}& \frac{\partial^2}{\partial \bar{\epsilon}^2} W_\lambda(\beta, \bar{\epsilon}) \\ &= \lambda_1 \frac{\partial^2}{\partial \bar{\epsilon}^2} (W_1 - \beta \phi)(\epsilon_1^*(\beta, \bar{\epsilon})) + \lambda_2 \frac{\partial^2}{\partial \bar{\epsilon}^2} (W_2 - \beta \phi)(\epsilon_2^*(\beta, \bar{\epsilon})) + \beta \frac{\partial^2}{\partial \bar{\epsilon}^2} \phi(\bar{\epsilon}) \\ &= \lambda_1 (\alpha_1 - \beta T) + \lambda_2 (\alpha_2 - \beta T) + \beta T \\ &= \lambda_1 \alpha_1 + \lambda_2 \alpha_2 \\ &> 0\end{aligned}$$

\square

We now obtain the desired lower bound.

Theorem 3.7 (Lower bound). $\overline{W}_\lambda \geq \overline{W}_\lambda^l$ where $\overline{W}_\lambda^l: \mathbb{R}_{\text{sym}}^{2 \times 2} \rightarrow \mathbb{R}$ is defined by

$$\overline{W}_\lambda^l(\bar{\epsilon}) := \begin{cases} W_\lambda(0, \bar{\epsilon}) & \text{if } \Delta\epsilon^*(\cdot, \bar{\epsilon}) \equiv 0 & (\text{Regime 0}), \\ W_\lambda(0, \bar{\epsilon}) & \text{if } \phi(\Delta\epsilon^*(0, \bar{\epsilon})) > 0 & (\text{Regime I}), \\ W_\lambda(\beta_{\text{II}}, \bar{\epsilon}) & \text{otherwise} & (\text{Regime II}), \\ W_\lambda(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon}) & \text{if } \phi(\Delta\epsilon^*(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon})) < 0. & (\text{Regime III}); \end{cases} \quad (3.14)$$

and, in Regime II, $\beta_{\text{II}} \in [0, \gamma_{(\alpha_1, \alpha_2)}]$ is the unique solution of $\phi(\Delta\epsilon^*(\beta, \bar{\epsilon})) = 0$.

Proof. When $\Delta\epsilon^*(\beta, \bar{\epsilon}) \equiv 0$, from Lemma 3.5, $\beta \mapsto W_\lambda(\beta, \bar{\epsilon})$ is constant and we may set $\beta = 0$ in (3.12).

Otherwise, from Lemma 3.5, $\beta \mapsto W_\lambda(\beta, \bar{\epsilon})$ is strictly concave. Using (3.13), the maximum occurs at

$$\beta = \begin{cases} 0 & \text{when } \phi(\Delta\epsilon^*(0, \bar{\epsilon})) \geq 0, \\ \beta = \gamma_{(\alpha_1, \alpha_2)} & \text{when } \phi(\Delta\epsilon^*(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon})) \leq 0. \end{cases}$$

Since $\beta \mapsto W_\lambda(\beta, \bar{\epsilon})$ is strictly concave, from (3.13) that $\beta \mapsto \phi(\Delta\epsilon^*(\beta, \bar{\epsilon}))$ is strictly increasing. Thus when $\phi(\Delta\epsilon^*(0, \bar{\epsilon})) \leq 0$ and (if necessary, interpreting as a limit) $\phi(\Delta\epsilon^*(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon})) \geq 0$ there exists a unique root $\beta_{\text{II}} \in [0, \gamma_{(\alpha_1, \alpha_2)}]$ such that $\phi(\Delta\epsilon^*(\beta_{\text{II}}, \bar{\epsilon})) = 0$ and the maximum of W_λ occurs at $\beta = \beta_{\text{II}}$. \square

Note 3.8. From (3.10), Regime III does not occur whenever $\phi(\Delta\epsilon^*(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon}))$ does not exist. From §3.1.4 this happens when $\ker(\alpha_1 - \gamma_{(\alpha_1, \alpha_2)}T) \cap \ker(\alpha_2 - \gamma_{(\alpha_1, \alpha_2)}T) \neq \{0\}$. This includes, in particular, the cases (i) $\alpha_1 = \alpha_2$ (c.f., Note 3.9 below) and (ii) both phases being isotropic with equal shear moduli.

Note 3.9 (Equal moduli). We remark on the special case $\alpha_1 = \alpha_2 =: \alpha$ studied by Pipkin [Pip91] and Kohn [Koh91]. In this case, $\gamma_{\alpha_1} = \gamma_{\alpha_2} = \gamma_{(\alpha_1, \alpha_2)}$ so that $\lambda_2\alpha_1 + \lambda_1\alpha_2 - \gamma_{(\alpha_1, \alpha_2)}T = \alpha - \gamma_{(\alpha_1, \alpha_2)}T$ is not invertible. Thus, as mentioned in Note 3.8 above, Regime III does not occur.

From (3.9), $\Delta\epsilon^*(\cdot, \cdot, \bar{\epsilon}) \equiv 0$ implies that $\epsilon_1^\top = \epsilon_2^\top$. Thus Regime 0 does not occur for distinct materials.⁵

Let $\Delta\epsilon^\top := \epsilon_2^\top - \epsilon_1^\top$. From (3.5b) and (3.14) we obtain

$$\overline{W}_\lambda^l(\bar{\epsilon}) = \begin{cases} \lambda_1 W_1(\epsilon_1^*(0, \bar{\epsilon})) + \lambda_2 W_2(\epsilon_2^*(0, \bar{\epsilon})) & \text{if } \phi(\Delta\epsilon^\top) > 0 & (\text{Regime I}), \\ \lambda_1 W_1(\epsilon_1^*(\beta_{\text{II}}, \bar{\epsilon})) + \lambda_2 W_2(\epsilon_2^*(\beta_{\text{II}}, \bar{\epsilon})) & \text{if } \phi(\Delta\epsilon^\top) \leq 0 & (\text{Regime II}). \end{cases} \quad (3.15)$$

Here, from (3.9),

$$\epsilon_1^*(\beta, \bar{\epsilon}) = \bar{\epsilon} - \lambda_2(\alpha - \beta T)^{-1} \alpha \Delta\epsilon^\top, \quad (3.16a)$$

$$\epsilon_2^*(\beta, \bar{\epsilon}) = \bar{\epsilon} + \lambda_1(\alpha - \beta T)^{-1} \alpha \Delta\epsilon^\top; \quad (3.16b)$$

and, in Regime II, β_{II} is the unique solution in $[0, \gamma_{(\alpha_1, \alpha_2)})$ of

$$\phi((\alpha - \beta T)^{-1} \alpha \Delta\epsilon^\top) = 0. \quad (3.17)$$

⁵I.e., when either $\alpha_1 \neq \alpha_2$ or $\epsilon_1^\top \neq \epsilon_2^\top$.

Note that β_{Π} is independent of $\bar{\epsilon}$.

From (3.16)

$$\begin{aligned}\epsilon_1^*(\beta, \bar{\epsilon}) - \epsilon_1^T &= (\bar{\epsilon} - \bar{\epsilon}^T) - \lambda_2 \beta (\alpha - \beta T)^{-1} T \Delta \epsilon^T, \\ \epsilon_2^*(\beta, \bar{\epsilon}) - \epsilon_2^T &= (\bar{\epsilon} - \bar{\epsilon}^T) + \lambda_1 \beta (\alpha - \beta T)^{-1} T \Delta \epsilon^T,\end{aligned}$$

where $\bar{\epsilon}^T := \lambda_1 \epsilon_1^T + \lambda_2 \epsilon_2^T$. Substituting this in (3.15) gives

$$\begin{aligned}\bar{W}_\lambda^l(\bar{\epsilon}) &= \frac{1}{2} \langle \alpha(\bar{\epsilon} - \bar{\epsilon}^T), (\bar{\epsilon} - \bar{\epsilon}^T) \rangle + (\lambda_1 w_1 + \lambda_2 w_2) \\ &+ \begin{cases} 0 & \text{if } \phi(\Delta \epsilon^T) > 0 \quad (\text{Regime I}), \\ \frac{1}{2} \lambda_1 \lambda_2 \beta_{\Pi}^2 \|\alpha^{\frac{1}{2}}(\alpha - \beta_{\Pi} T)^{-1} T \Delta \epsilon^T\|^2 & \text{if } \phi(\Delta \epsilon^T) \leq 0 \quad (\text{Regime II}); \end{cases}\end{aligned}$$

where β_{Π} is the unique solution in $[0, \gamma_{(\alpha_1, \alpha_2)})$ of (3.17).

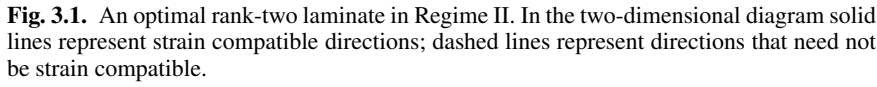
3.2. Optimality of the lower bound and optimal microstructures

In this section we prove that the lower bound presented in Theorem 3.7 is optimal, and characterize the optimal microstructures. This will complete the proof of Theorem 2.1. Our strategy is to construct upper bounds on the relaxed energy \bar{W}_λ by constructing microstructures and using test strain fields whose energy is exactly equal to the lower bound \bar{W}_λ^l . In the process we will also build insight that will allow us to identify properties of *optimal microstructures* that attain the relaxed energy.

3.2.1. Optimality of the lower bound.

Theorem 3.10 (Optimality of the lower bound). $\bar{W}_\lambda = \bar{W}_\lambda^l$.

Before we present the proof of Theorem 3.10, we present the (geometric) picture that underlies it. In the three-dimensional linear space of two-dimensional strains, the set of $\{\epsilon : \phi(\epsilon - \epsilon_2^*) = 0\}$ is the surface of the large dark cone shown in the Figure 3.1(a), the set $\{\epsilon : \phi(\epsilon - \epsilon_2^*) < 0\}$ is inside the large dark cone and the set $\{\epsilon : \phi(\epsilon - \epsilon_2^*) > 0\}$ is outside the large dark cone. From Lemma 3.11 it follows that one can form rank-one laminates between ϵ_2^* and any point that does not lie inside the large dark cone. In Regimes I and II ϵ_1^* does not lie inside the large dark cone, and we may form optimal rank-one laminates between them. In Regime III, ϵ_1^* lies inside the large dark cone and we can not form a rank-one laminate. So we proceed from ϵ_1^* along the ‘degenerate’ direction (which, from §3.1.2, is not hydrostatic, i.e., vertical) till we hit the large dark cone at ϵ^I . Pick ϵ^{II} along this line so that the ϵ_1^* is the average of ϵ^I and ϵ^{II} . Now construct a cone centered at ϵ^{II} , the small grey cone in the figure. ϵ^{III} is the intersection between the line joining ϵ^I and ϵ_2^* and the ellipse defined by the intersection of the two cones. All relations in (3.20) follow.



where ϵ_1^* and ϵ_2^* are given by (3.9) for $\beta = \beta^*$. Now construct a rank-one laminate χ in which phases 1 and 2 have phase fractions λ_1 and λ_2 respectively and the layers have normal \hat{n} or \hat{m} . The condition (3.19) assures us that we can construct a continuous displacement field u (satisfying $u|_{\partial\Omega} = \bar{e} \cdot x$) with strain ϵ_1^* in phase

1 and ϵ_2^* in phase 2. For this microstructure and displacement field,

$$\begin{aligned} W_\chi(u) &= \lambda_1 W_1(\epsilon_1^*) + \lambda_2 W_1(\epsilon_2^*) \\ &= \lambda_1 W_1(\epsilon_1^*) + \lambda_2 W_1(\epsilon_2^*) - \beta \lambda_1 \lambda_2 \phi(\epsilon_2^* - \epsilon_1^*) \\ &= \overline{W}_\lambda^l(\bar{\epsilon}). \end{aligned}$$

The second equality holds above because $\beta = 0$ in Regime 1 and $\phi = 0$ in Regime II. The result follows by combining this with Theorem 3.7 and (3.18).

Regime III: $\phi(\Delta\epsilon^*(\gamma_{(\alpha_1, \alpha_2)}, \bar{\epsilon})) < 0$, and so, from Lemma 3.11, we can not construct a continuous displacement field directly with the optimal strains. However, one of the translated energies loses strict convexity at $\beta = \gamma_{(\alpha_1, \alpha_2)}$ (Lemma 3.2); we can use this to construct optimal rank-two laminates:

Assume, renumbering if necessary, that $\gamma_{(\alpha_1, \alpha_2)} = \gamma_{\alpha_1}$. It follows that there exists $0 \neq \epsilon_n \in \ker(\alpha_1 - \gamma_{(\alpha_1, \alpha_2)}T)$ and that

$$\mathbb{R} \ni z \mapsto (W_1 - \gamma_{(\alpha_1, \alpha_2)}\phi)(\epsilon_1^* + z\epsilon_n)$$

is affine. In Lemma 3.12 below, we show that there exist $\epsilon^I, \epsilon^II, \epsilon^A \in \mathbb{R}_{\text{sym}}^{2 \times 2}$, $\rho \in (0, \lambda_1)$, $\hat{m} \nparallel \hat{n} \in \mathbb{R}^2$ such that

$$(\epsilon^II - \epsilon^I) \parallel \epsilon_n, \quad (3.20a)$$

$$\frac{\lambda_1 - \rho}{\lambda_1(1 - \rho)}\epsilon^II + \frac{\rho\lambda_2}{\lambda_1(1 - \rho)}\epsilon^I = \epsilon_1^*, \quad (3.20b)$$

$$\phi(\epsilon_2^* - \epsilon^I) = 0 \quad (3.20c)$$

(or equivalently, from Lemma 3.11, $\exists \hat{n} \in \mathbb{R}^2$, $\epsilon_2^* - \epsilon^I \parallel \hat{n} \otimes \hat{n}$),

$$\rho\epsilon^I + (1 - \rho)\epsilon_2^* = \epsilon^A, \quad (3.20d)$$

$$\phi(\epsilon^A - \epsilon^II) = 0 \quad (3.20e)$$

(or equivalently, from Lemma 3.11, $\exists \hat{m} \in \mathbb{R}^2$, $\epsilon^A - \epsilon^II \parallel \hat{m} \otimes \hat{m}$),

$$\frac{\lambda_1 - \rho}{1 - \rho}\epsilon^II + \frac{\lambda_2}{1 - \rho}\epsilon^A = \bar{\epsilon}. \quad (3.20f)$$

Note that $\rho \in (0, \lambda_1)$ implies that $(\lambda_1 - \rho)/(1 - \rho) \in (0, \lambda_1)$ so that the left-hand-sides of (3.20b), (3.20d) and (3.20f) are convex combinations. These equations are schematically represented in Figure 3.1(b).

We can now construct our rank-two laminate as follows. First construct a rank-one laminate in which phases 1 and 2 have phase fractions ρ and $1 - \rho$ respectively and the layers have normal \hat{n} . Next construct a rank-two laminate in which this rank-one laminate and phase 1 have phase fractions $(\lambda_2)(1 - \rho)$ and $(\lambda_1 - \rho)(1 - \rho)$ respectively and the layers have normal \hat{m} . The compatibility equations (3.20c) and (3.20e) allows the construction of a continuous displacement field u (up to boundary layers) such that the strains take the value ϵ^I in the interior phase 1, ϵ_2^* in the interior phase 2 and ϵ^II in the exterior phase 1. Moreover from (3.20b) and (3.20f) u can be chosen to satisfy $u|_{\partial\Omega} = \bar{\epsilon} \cdot x$. For this microstructure and

displacement field,

$$\begin{aligned}
W_\chi(u) &= \frac{\lambda_1 - \rho}{1 - \rho} W_1(\epsilon^\Pi) + \frac{\lambda_2}{1 - \rho} (\rho W_1(\epsilon^I) + (1 - \rho) W_2(\epsilon_2^*)) \\
&= \lambda_2 W_2(\epsilon_2^*) + \frac{\lambda_1 - \rho}{1 - \rho} W_1(\epsilon^\Pi) + \frac{\rho \lambda_2}{1 - \rho} W_1(\epsilon^I) \\
&= \lambda_2 W_2(\epsilon_2^*) + \frac{\lambda_1 - \rho}{1 - \rho} (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon^\Pi) + \frac{\rho \lambda_2}{1 - \rho} (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon^I) \\
&\quad + \frac{\lambda_1 - \rho}{1 - \rho} \gamma_{(\alpha_1, \alpha_2)} \phi(\epsilon^\Pi) + \frac{\rho(1 - \lambda_1)}{1 - \rho} \gamma_{(\alpha_1, \alpha_2)} \phi(\epsilon^I)
\end{aligned}$$

Since $W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi$ is affine in the direction ϵ_n , from it follows that

$$\begin{aligned}
&\frac{\lambda_1 - \rho}{1 - \rho} (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon^\Pi) + \frac{\rho \lambda_2}{1 - \rho} (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon^I) \\
&= \lambda_1 (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi) \left(\frac{\lambda_1 - \rho}{\lambda_1(1 - \rho)} \epsilon^\Pi + \frac{\rho \lambda_2}{\lambda_1(1 - \rho)} \epsilon^I \right) \\
&= \lambda_1 (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon_1^*)
\end{aligned}$$

where the second equality uses (3.20b). So,

$$\begin{aligned}
W_\chi(u) &= \lambda_1 (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon_1^*) + \lambda_2 W_2(\epsilon_2^*) \\
&\quad + \gamma_{(\alpha_1, \alpha_2)} \left(\frac{\lambda_1 - \rho}{1 - \rho} \phi(\epsilon^\Pi) + \frac{\rho \lambda_2}{1 - \rho} \phi(\epsilon^I) \right)
\end{aligned}$$

Since ϕ is quadratic, it follows from (3.20) that

$$\begin{aligned}
\frac{\lambda_1 - \rho}{1 - \rho} \phi(\epsilon^\Pi) + \frac{\lambda_2}{1 - \rho} \phi(\epsilon^\Lambda) &= \phi(\bar{\epsilon}), \\
\rho \phi(\epsilon^I) + (1 - \rho) \phi(\epsilon_2^*) &= \phi(\epsilon^\Lambda).
\end{aligned}$$

Putting these together, and once again using the quadraticity of ϕ ,

$$\begin{aligned}
W_\chi(u) &= \lambda_1 (W_1 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon_1^*) + \lambda_2 (W_2 - \gamma_{(\alpha_1, \alpha_2)} \phi)(\epsilon_2^*) + \gamma_{(\alpha_1, \alpha_2)} \phi(\bar{\epsilon}) \\
&= \lambda_1 W_1(\epsilon_1^*) + \lambda_2 W_2(\epsilon_2^*) - \gamma_{(\alpha_1, \alpha_2)} \lambda_1 \lambda_2 \phi(\epsilon_2^* - \epsilon_1^*) \\
&= \overline{W}_\lambda^l(\bar{\epsilon}).
\end{aligned}$$

The result follows by combining this with Theorem 3.7 and (3.18). \square

The proof above used the following Lemmas. The first is well-known (c.f., e.g., [Koh91]) and the proof is omitted.

Lemma 3.11 (Strain and rank-one compatibility). *Let $\epsilon \in \mathbb{R}_{\text{sym}}^{n \times n}$ with eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$. Then, there exist $\hat{m} \nparallel \hat{n} \in \mathbb{R}^n$ such that*

$$\begin{aligned} \epsilon \parallel \hat{m} \otimes_s \hat{n} &\iff \lambda_1 < 0 < \lambda_2 &\iff \phi(\epsilon) > 0, \\ \epsilon \parallel \hat{n} \otimes \hat{n} &\iff \lambda_1 \lambda_2 = 0 &\iff \phi(\epsilon) = 0 \end{aligned}$$

when $n = 2$; and when $n > 2$,

$$\begin{aligned} \epsilon \parallel \hat{m} \otimes_s \hat{n} &\iff \lambda_1 < 0 = \lambda_2, \dots, \lambda_{n-1} = 0 < \lambda_n \\ \epsilon \parallel \hat{n} \otimes \hat{n} &\iff \lambda_2 = \lambda_3 = \dots = \lambda_{n-1} = 0 \text{ and } \lambda_1 \lambda_n = 0. \end{aligned}$$

Lemma 3.12. *Let $\alpha \in \mathcal{L}_>^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ and $0 \neq \epsilon_n \in \ker(\alpha - \gamma_\alpha T)$. Let $\phi(\Delta\epsilon^*) < 0$. Then there exist $\epsilon^I, \epsilon^{II}, \epsilon^A \in \mathbb{R}_{\text{sym}}^{2 \times 2}$, $\rho \in (0, \lambda_1)$, $\hat{m} \nparallel \hat{n} \in \mathbb{R}^2$ such that (3.20) holds.*

Proof. Since $\epsilon_n \in \ker(\alpha - \gamma_\alpha T)$ and α is positive-definite, it follows that

$$\phi(\epsilon_n) = \frac{1}{2} \langle T\epsilon_n, \epsilon_n \rangle = \frac{1}{2\gamma_\alpha} \langle \alpha\epsilon_n, \epsilon_n \rangle > 0. \quad (3.21)$$

Combining this with the fact that $\phi(\Delta\epsilon^*) < 0$ we conclude that the quadratic polynomial $\mathbb{R} \ni z \mapsto \phi(\Delta\epsilon^* + z\epsilon_n)$ has two real roots $z_1 < 0 < z_2$ since

$$\phi(\Delta\epsilon^* + z\epsilon_n) = 0 \iff \phi(\Delta\epsilon^*) + z \langle T\Delta\epsilon^*, \epsilon_n \rangle + z^2 \phi(\epsilon_n) = 0. \quad (3.22)$$

Set

$$\rho := \frac{-z_1 z_2}{z_2 - z_1} \lambda_1, \quad (3.23a)$$

$$\epsilon^I := \epsilon_1^* - z_2 \epsilon_n, \quad (3.23b)$$

$$\epsilon^{II} := \epsilon_1^* - (\rho z_2 + (1 - \rho) z_1) \epsilon_n, \quad (3.23c)$$

$$\epsilon^A := \rho \epsilon^I + (1 - \rho) \epsilon_2^* \quad (3.23c)$$

With these definitions, $\rho \in (0, \lambda_1)$ as required, and (3.20a), (3.20b), (3.20d) and (3.20f) are obvious. Now observe that

$$\begin{aligned} \epsilon_2^* - \epsilon^I &= \epsilon_2^* - \epsilon_1^* + z_2 \epsilon_n \\ &= \Delta\epsilon^* + z_2 \epsilon_n. \end{aligned} \quad (3.24a)$$

$$\begin{aligned} \epsilon^A - \epsilon^{II} &= \rho \epsilon^I + (1 - \rho) \epsilon_2^* - \epsilon_1^* + (\rho z_2 + (1 - \rho) z_1) \epsilon_n \\ &= \rho(\epsilon_1^* - z_2 \epsilon_n) + (1 - \rho) \epsilon_2^* - \epsilon_1^* + (\rho z_2 + (1 - \rho) z_1) \epsilon_n \\ &= (1 - \rho)(\Delta\epsilon^* + z_1 \epsilon_n). \end{aligned} \quad (3.24b)$$

Since z_1 and z_2 are roots of $\phi(\Delta\epsilon^* + z\epsilon_n) = 0$, (3.20c) and (3.20e) follow. It remains to show that $\hat{m} \nparallel \hat{n}$. If the contrary were true, then,

$$(\epsilon^A - \epsilon^{II}) \parallel (\epsilon_2^* - \epsilon^I),$$

and thus, from (3.24),

$$(\Delta\epsilon^* + z_2 \epsilon_n) \parallel (\Delta\epsilon^* + z_1 \epsilon_n)$$

i.e., since $z_1 \neq z_2$, either $\Delta\epsilon^* \parallel \epsilon_n$ or $\Delta\epsilon^* = 0$. It follows from (3.21) that $\phi(\Delta\epsilon^*) \geq 0$ which, however, contradicts the assumption that $\phi(\Delta\epsilon^*) < 0$. \square

Note 3.13. The construction of the rank-two laminate in the proof of Theorem 3.10 uses only rank-one connections, as opposed to symmetrized-rank-one connections (i.e., (3.20c) and (3.20e) enforce equalities instead of the inequality permitted by Lemma 3.11). This notes explains why.

Optimal microstructures satisfy the the Euler-Lagrange equation associated with the variational principle i.e., the equilibrium equation. In particular, at an interface with normal $\hat{n} \in \mathbb{R}^2$ the stress difference $\llbracket \sigma \rrbracket$ is required to satisfy the relation

$$\llbracket \sigma \rrbracket \hat{n} = 0 \quad (3.25a)$$

From (3.8) and (3.24), using $\alpha_1 \epsilon_n = \gamma_{\alpha_1} T \epsilon_n$, in regime III, at any interface the stress difference is related to the strain difference through

$$\llbracket \sigma \rrbracket \parallel T \llbracket \epsilon \rrbracket \quad (3.25b)$$

and the constant of proportionality is non-zero. The strain compatibility condition is

$$\llbracket \epsilon \rrbracket \parallel \hat{m} \otimes_s \hat{n} \quad (3.25c)$$

for some $\hat{m} \in \mathbb{R}^2$. Lemma 3.14 below shows that (3.25) is equivalent to requiring $\llbracket \epsilon \rrbracket \parallel \hat{n} \otimes \hat{n}$ which in turn necessitates $\phi(\llbracket \epsilon \rrbracket) = 0$.

Lemma 3.14. *Let $\hat{m}, \hat{n} \in \mathbb{R}^2$. Then the following are equivalent.*

1. $(T(\hat{m} \otimes_s \hat{n})) \hat{m} = 0$.
2. $(T(\hat{m} \otimes_s \hat{n})) \hat{n} = 0$.
3. $\hat{m} \parallel \hat{n}$.

Proof. The equivalence of the first two statements is trivial. The rest of the lemma follows from the observation that

$$T(\hat{m} \otimes_s \hat{n}) = \hat{m}^\perp \otimes_s \hat{n}^\perp.$$

where, for every $v \in \mathbb{R}^2$, $v^\perp := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} v$. \square

3.2.2. Optimal microstructures. A microstructure χ for which the energy is optimal, i.e., for which

$$\overline{W}_{\langle \chi \rangle}(\bar{\epsilon}) = \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} W_\chi(u)$$

is an *optimal microstructure*. Given a microstructure, any displacement field $u: \Omega \rightarrow \mathbb{R}^n$ (with $u|_{\partial\Omega} = \bar{\epsilon} \cdot x$) whose energy is optimal, i.e., for which

$$W_\chi(u) = \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} W_\chi(u)$$

is an *optimal displacement field* for that microstructure; the associated strain field is an *optimal strain field*.

We have proved (cf. Theorems 3.7 and 3.10) the translated variational principle

$$\overline{W}_\chi(\bar{\epsilon}) = \inf_{\chi, u} \int_\Omega \sum_{i=1}^2 \chi_i (W_i - \beta^* \phi)(\epsilon) \, dx + \beta^* \phi(\bar{\epsilon}) \quad (3.26a)$$

where $\langle \chi \rangle = \lambda$, $u|_{\partial\Omega} = \bar{\epsilon} \cdot x$ and

$$\beta^* := \begin{cases} 0 & \text{in Regimes O and I,} \\ \beta_{\text{II}} & \text{in Regime II,} \\ \gamma_{(\alpha_1, \alpha_2)} & \text{in Regime III.} \end{cases} \quad (3.26b)$$

Theorem 3.15 (Equivalence of optimal microstructures for original and translated variational principles). *A microstructure and strain field is optimal for the original variational principle (1.6) if and only if it is optimal for the translated variational principle (3.26).*

Proof. The variational principles are identical when $\beta^* = 0$, which occurs in Regimes 0 and I, and possibly in Regime II. We consider the case when $\beta^* \neq 0$.

Consider a minimizing sequence (χ^η, u^η) for the original variational statement of $\bar{W}_\lambda(\bar{\epsilon})$ in (1.6). We have

$$\begin{aligned} \bar{W}_\lambda(\bar{\epsilon}) &= \lim_{\eta \rightarrow 0} \int_{\Omega} \sum_{i=1}^2 \chi_i^\eta (W_i - \beta^* \phi)(\epsilon^\eta) \, dx + \beta^* \phi(\bar{\epsilon}) \\ &= \bar{W}_\lambda(\bar{\epsilon}) - \beta^* \left(\lim_{\eta \rightarrow 0} \int_{\Omega} \phi(\epsilon^\eta) \, dx - \phi(\bar{\epsilon}) \right). \end{aligned}$$

Thus

$$\phi(\bar{\epsilon}) = \lim_{\eta \rightarrow 0} \int_{\Omega} \phi(\epsilon^\eta) \, dx,$$

from which the result follows. \square

Theorem 3.16 (Optimal microstructures).

1. *In Regime 0 any microstructure is optimal. The optimal strain and stress are constant.*
2. *In Regime I the optimal microstructure is either a rank-one laminate, with either of two possible layering directions, or a microstructure made up of these laminates. The optimal strain takes the value ϵ_1^* in phase 1 and ϵ_2^* in phase 2 while the optimal stress is constant.*
3. *In Regime II the optimal microstructure is unique and is a rank-one laminate. The optimal strain takes the value ϵ_1^* in phase 1 and ϵ_2^* in phase 2.*
4. *In Regime III, no rank-one laminate is optimal. The class of optimal microstructures is possibly large (in a sense explained in the proof) and includes at least two rank-two laminates.*

In any optimal microstructure, in phase i , $i = 1, 2$, the strain is confined to an affine subspace of dimension $\dim \ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)} T) \leq 2$; the sum of the dimensions of the affine subspaces is also at most 2. In particular, if phase i is harder than the other phase (i.e., if $\gamma_{\alpha_i} > \gamma_{(\alpha_1, \alpha_2)}$) then the strain is ϵ_i^ in that phase.*

Proof. In the proof of Theorem 3.10, we showed that in Regimes 0, I and II,

$$\overline{W}_\lambda(\bar{\epsilon}) = \lambda W_1(\epsilon_1^*) + (1 - \lambda)W_2(\epsilon_2^*).$$

Further, recall that α_1 and α_2 are positive-definite by assumption so that W_1 and W_2 are strictly convex. It follows that in any optimal microstructure the optimal strain field is as in the statement of the theorem.

The other statements pertaining to Regime 0 follow immediately from the proof of Theorem 3.10 and (3.8).

In Regime I, $\phi(\Delta\epsilon^*) < 0$ so that from Lemma 3.11, we find $\hat{m} \nparallel \hat{n} \in \mathbb{R}^2$ such that $\Delta\epsilon^* \parallel \hat{m} \otimes_s \hat{n}$. It follows that the strain and thus the microstructure is either a rank-one laminates (with layering direction either \hat{m} or \hat{n}) or a microstructure of these laminates. Finally since $\beta = 0$ in this regime, it follows from (3.8) that $\Delta\sigma^* = 0$; thus the stress is constant.

In Regime II, $\phi(\Delta\epsilon^*) = 0$ so that from Lemma 3.11, we find unique (upto scaling) $\hat{n} \in \mathbb{R}^2$ such that $\Delta\epsilon^* \parallel \hat{n} \otimes \hat{n}$. It follows that the strain and thus the microstructure is a unique rank-one laminate with layering direction \hat{n} .

We now turn to Regime III. The non-existence of optimal rank-one laminates and the existence of an optimal rank-two laminate follows from Theorem 3.10 (and Lemma 3.12). There exists at least one other optimal rank-two laminate which can be obtained by interchanging the roles of z_1 and z_2 in (3.23) (and (3.24)). If $\dim(\ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)}T)) > 1$ (which is the case, e.g., when α_i is isotropic), $i = 1, 2$, then one can find an uncountably infinite number of directions ϵ_n which one can use in the proof of Theorem 3.10 (and Lemma 3.12) to construct the rank-two laminates; moreover, one can also construct optimal microstructures that are not laminates but ‘Hashin-Strikhman confocal ellipses’ or ‘Vigdergauz microstructures’. The reader is referred to [Lu93, Vig94, GK95a, GK95b, GK95c, Gra96] for a discussion of these microstructures.

That $\dim \ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)}T) \leq 2$ restates (3.6) and $\sum_{i=1}^2 \dim \ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)}T) \leq 2$ follows from Notes 3.3 and 3.8. Finally we turn to characterizing the optimal strains: Since

$$\begin{aligned} \inf_{\chi, u} \int_{\Omega} \sum_{i=1}^2 \chi_i (W_i - \gamma_{(\alpha_1, \alpha_2)}\phi)(\epsilon) \, dx + \gamma_{(\alpha_1, \alpha_2)}\phi(\bar{\epsilon}) \\ = \sum_{i=1}^2 \lambda_i (W_i - \gamma_{(\alpha_1, \alpha_2)}\phi)(\epsilon_i^*) + \gamma_{(\alpha_1, \alpha_2)}\phi(\bar{\epsilon}), \end{aligned}$$

the result about the optimal strains follows from the strict convexity of $W_2 - \gamma_{(\alpha_1, \alpha_2)}\phi$ and the non-strict convexity of $W_1 - \gamma_{(\alpha_1, \alpha_2)}\phi$. \square

4. Two-phase cubic solids in three dimensions

We generalize the preceding approach to the problem in three dimensions when the elastic moduli α_1 and α_2 are either (1) both cubic (c.f., Definition 4 below), or

(2) well ordered (i.e., either $\alpha_1 \leq \alpha_2$ or $\alpha_2 \leq \alpha_1$) and the smaller elastic modulus is cubic.

Our approach succeeds when the elastic moduli are (1) both isotropic, or (2) well ordered and the smaller elastic modulus is isotropic. Otherwise we obtain a lower bound which is optimal except possibly in one regime.

For ease of exposition we will only present results for the case of both elastic moduli being either isotropic or cubic. The extension of the results to the other case is immediate (c.f., (4.11) below) and is thus left as an exercise to the reader.

Overview of §4. After introducing some preliminary definitions in §4.1, we introduce the translation that we shall be using in §4.2 and use it to obtain a (non-explicit) lower bound on the relaxed energy in §4.3. §4.4, 4.5 and 4.6 are concerned with determining the amount of permissible translation. An important intermediate result is presented in §4.7 and explicit expressions for the optimal strains in §4.8. In §4.9 we are finally ready to explicitly compute the lower bound presented in §4.3. In §4.10 we comment on optimality and the optimal microstructures.

4.1. Preliminary definitions.

Definition 1. Let $R \in SO(3)$. The linear operator $\mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3}) \ni L \mapsto L^R \in \mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ is defined by

$$L^R \epsilon := R (L (R^T \epsilon R)) R^T, \quad \forall \epsilon \in \mathbb{R}_{\text{sym}}^{3 \times 3}.$$

It is easy to check that \cdot^R preserves the algebraic structure of $\mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$: $\forall L_1, L_2 \in \mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$,

$$(L_1 L_2)^R = L_1^R L_2^R.$$

In particular, when $L \in \mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ is invertible,

$$(L^{-1})^R = (L^R)^{-1}.$$

Clearly,

$$\ker(L^R) = R \ker(L) R^T. \quad (4.1)$$

Finally, we note that $\forall R_1, R_2 \in SO(3)$,

$$(\cdot^{R_1 R_2}) = (\cdot^{R_1})^{R_2}.$$

Definition 2 (Orthogonal subspaces of $\mathbb{R}_{\text{sym}}^{3 \times 3}$). Let

$$\begin{aligned} \mathcal{H} &:= \text{Span} \{I\}, \\ I &:= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\ \mathcal{D} &:= \text{Span} \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\}, \\ \mathcal{O} &:= \text{Span} \left\{ \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\}. \end{aligned}$$

(These symbols stand for “Hydrostatic”, “Diagonal” and “Off-diagonal” respectively.) Note that $\mathbb{R}_{\text{sym}}^{3 \times 3} = \mathcal{H} \oplus \mathcal{D} \oplus \mathcal{O}$.

We write $\text{Diag} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ to mean $\begin{pmatrix} x_1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & x_3 \end{pmatrix}$.

Definition 3 (Orthogonal projection operators). Analogous to (3.4), the orthogonal projection operators $\mathbf{A}_h, \mathbf{A}_s, \mathbf{A}_d, \mathbf{A}_o \in \mathcal{L}_{\geq}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ are defined by

$$\begin{aligned} \text{Range}(\mathbf{A}_h) &= \mathcal{H}, \\ \mathbf{A}_s &:= \mathbf{A}_d + \mathbf{A}_o, \\ \text{Range}(\mathbf{A}_d) &= \mathcal{D}, \\ \text{Range}(\mathbf{A}_o) &= \mathcal{O}. \end{aligned}$$

Note that

$$\mathbf{A}_h \epsilon = \frac{1}{3} \text{Tr}(\epsilon) I,$$

and

$$\mathbf{A}_h + \mathbf{A}_s = \mathbf{I} \in \mathcal{L}_{>}^*(\mathbb{R}_{\text{sym}}^{3 \times 3}),$$

the identity operator. Moreover, $\forall R \in SO(3)$, $\mathbf{A}_h^R = \mathbf{A}_h$ and $\mathbf{A}_s^R = \mathbf{A}_s$.

Definition 4 (Cubic elastic moduli). $\alpha \in \mathcal{L}_{>}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ is *cubic* if $\exists R_\alpha(\alpha) \in SO(3)$ and $\kappa(\alpha), \mu(\alpha), \eta(\alpha) > 0$ such that

$$\alpha^{R_\alpha} = 3\kappa \mathbf{A}_h + 2\mu \mathbf{A}_d + 2\eta \mathbf{A}_o. \quad (4.2)$$

(Henceforth we shall leave the dependence on α implicit.) Here κ is the bulk modulus, μ the diagonal shear modulus and η the off-diagonal shear modulus.

Definition 5 (Isotropic elastic moduli). $\alpha \in \mathcal{L}_{>}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ is *isotropic* if

$$\forall R \in SO(3), \alpha^R = \alpha. \quad (4.3a)$$

Such an elastic modulus is of the form

$$\alpha = 3\kappa \mathbf{A}_h + 2\mu \mathbf{A}_s \quad (4.3b)$$

where $\kappa(\alpha) > 0$ is the bulk modulus and $\mu(\alpha) > 0$ the shear modulus. (Henceforth we shall leave the dependence on α implicit.) Note that isotropic moduli are cubic moduli for which $\mu = \eta$. Note also that

$$\alpha = \ell \text{Tr}(\cdot) I + 2\mu \mathbf{I} \quad (4.3c)$$

where $\ell = \kappa - \frac{2}{3}\mu > 0$ is the Lamé modulus.

Definition 6. For $\epsilon \in \mathbb{R}_{\text{sym}}^{3 \times 3}$ we define $v_1(\epsilon) \leq v_2(\epsilon) \leq v_3(\epsilon)$ to be the eigenvalues of ϵ . Moreover for a permutation σ on $\{1, 2, 3\}$ let,

$$\begin{aligned} \text{diag}_\sigma(\epsilon) &:= \begin{pmatrix} v_{\sigma(1)}(\epsilon) & 0 & 0 \\ 0 & v_{\sigma(2)}(\epsilon) & 0 \\ 0 & 0 & v_{\sigma(3)}(\epsilon) \end{pmatrix}, \\ \Upsilon_\sigma(\epsilon) &:= \begin{pmatrix} v_{\sigma(2)}(\epsilon) & v_{\sigma(3)}(\epsilon) \\ v_{\sigma(3)}(\epsilon) & v_{\sigma(1)}(\epsilon) \\ v_{\sigma(1)}(\epsilon) & v_{\sigma(2)}(\epsilon) \end{pmatrix} \end{aligned} \quad (4.4)$$

and $R_\sigma(\epsilon) \in SO(3)$ to be a rotation that σ -diagonalizes ϵ , i.e.,

$$\epsilon = R_\sigma^T(\epsilon) \text{diag}_\sigma(\epsilon) R_\sigma(\epsilon).$$

The subscript σ is dropped when σ is the identity map.

4.2. Rotated diagonal subdeterminants as translations.

The determinant is a useful translation in two dimensions because it captures information on strain compatibility: $\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{2 \times 2}$ are strain compatible (i.e., $\exists \hat{m}, \hat{n} \in \mathbb{R}^2$, $\epsilon_2 - \epsilon_1 \parallel \hat{m} \otimes_s \hat{n}$) if and only if $\det(\epsilon_2 - \epsilon_1) \leq 0$; the three-dimensional analogue is that $\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3}$ are strain compatible if and only if of the three eigenvalues of $\epsilon_2 - \epsilon_1$, one is non-negative, another is zero and the third is non-positive (c.f. Lemma 3.11).

Motivated by this we choose a translation of the form $\beta \cdot \phi^R$, where $\beta \in \mathbb{R}_+^3$, $R \in SO(3)$ and $\phi^R: \mathbb{R}_{\text{sym}}^{3 \times 3} \rightarrow \mathbb{R}^3$ is given by

$$\phi^R(\epsilon) := \phi(R^T \epsilon R), \quad (4.5a)$$

$$\phi(\epsilon) := \begin{pmatrix} \epsilon_{23}^2 - \epsilon_{22}\epsilon_{33} \\ \epsilon_{31}^2 - \epsilon_{33}\epsilon_{11} \\ \epsilon_{12}^2 - \epsilon_{11}\epsilon_{22} \end{pmatrix}. \quad (4.5b)$$

For convenience we also define $\phi_j: \mathbb{R}_{\text{sym}}^{3 \times 3} \rightarrow \mathbb{R}$, $j = 1, 2, 3$ by

$$\phi_j(\epsilon) := (\phi(\epsilon))_j; \quad (4.5c)$$

note that these are the diagonal subdeterminants.

Quadraticity of $\beta \cdot \phi^R$. It is easy to verify that

$$\phi_j(\epsilon) = \frac{1}{2} \langle T_j \epsilon, \epsilon \rangle, \quad j = 1, 2, 3, \quad (4.6a)$$

where $T_j \in \mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$, $j = 1, 2, 3$ are defined by

$$T_1 \epsilon := \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\epsilon_{33} & \epsilon_{23} \\ 0 & \epsilon_{23} & -\epsilon_{22} \end{pmatrix}, \quad (4.6b)$$

$$T_2 \epsilon := \begin{pmatrix} -\epsilon_{33} & 0 & \epsilon_{31} \\ 0 & 0 & 0 \\ \epsilon_{31} & 0 & -\epsilon_{11} \end{pmatrix}, \quad (4.6c)$$

$$T_3 \epsilon := \begin{pmatrix} -\epsilon_{22} & \epsilon_{12} & 0 \\ \epsilon_{12} & -\epsilon_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (4.6d)$$

It is clear that T_j , $j = 1, 2, 3$, has eigenvalues $-1, 0$ and 1 repeated once, thrice and twice respectively. It is easy to verify that

$$\ker(\mathbf{A}_s - T_1) = \text{Span} \left\{ I, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\}, \quad (4.7a)$$

$$\ker(\mathbf{A}_s - T_2) = \text{Span} \left\{ I, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right\}, \quad (4.7b)$$

$$\ker(\mathbf{A}_s - T_3) = \text{Span} \left\{ I, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right\}. \quad (4.7c)$$

For $\beta \in \mathbb{R}_+^3$ and $R \in SO(3)$, let $\beta \cdot T^R \in \mathcal{L}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ be defined by

$$\beta \cdot T^R \epsilon := \sum_{j=1}^3 \beta_j T_j^R \epsilon. \quad (4.8a)$$

Then, as is easy to verify,

$$\beta \cdot \phi^R(\epsilon) := \frac{1}{2} \langle (\beta \cdot T^R) \epsilon, \epsilon \rangle. \quad (4.8b)$$

Let $e := (1, 1, 1)^T$. We digress for a useful remark on $e \cdot T^R$ and $e \cdot \phi^R$ which can be easily verified from (4.6).

Note 4.1. $e \cdot T^R$ and $e \cdot \phi^R$ are independent of R . In particular,

$$\begin{aligned} e \cdot T &= \mathbf{I} - \text{Tr}(\cdot) \mathbf{I} \\ &= -2\mathbf{A}_h + \mathbf{A}_s, \end{aligned} \quad (4.9a)$$

$$\begin{aligned} e \cdot \phi(\epsilon) &= (\epsilon_{12}^2 + \epsilon_{23}^2 + \epsilon_{31}^2) - (\epsilon_{11}\epsilon_{22} + \epsilon_{22}\epsilon_{33} + \epsilon_{33}\epsilon_{11}) \\ &= \frac{1}{2} (\text{Tr}(\epsilon^2) - (\text{Tr}(\epsilon))^2) \\ &= -(\nu_1(\epsilon)\nu_2(\epsilon) + \nu_2(\epsilon)\nu_3(\epsilon) + \nu_3(\epsilon)\nu_1(\epsilon)). \end{aligned} \quad (4.9b)$$

Here $\nu_1(\epsilon) \leq \nu_2(\epsilon) \leq \nu_3(\epsilon)$ are the eigenvalues of ϵ .

Quasiconvexity of $\beta \cdot \phi^R$. $\phi_j^R, j = 1, 2, 3$, is quasiconvex since it is quadratic and rank-one convex: $\forall m', n' \in \mathbb{R}^3$,

$$\begin{aligned} \phi_j^R(m' \otimes_s n') &= \phi_j(R^T(m' \otimes_s n')R) \\ &= \phi_j((R^T m') \otimes_s (R^T n')) \\ &= \phi_j(m \otimes_s n) \end{aligned}$$

where $m = R^T m', n = R^T n'$; and, e.g.,

$$\begin{aligned} \phi_1(m \otimes_s n) &= \frac{1}{4}(m_2 n_3 + m_3 n_2)^2 - m_2 n_2 m_3 n_3 \\ &= \frac{1}{4}(m_2 n_3 - m_3 n_2)^2 \\ &\geq 0. \end{aligned}$$

It follows that $\forall \beta \in \mathbb{R}_+^3, \beta \cdot \phi^R$ is quasiconvex. From [Zha03, Thm. 1.2] it follows that $\forall \beta \in \mathbb{R}_+^3, \forall R \in SO(3), \beta \cdot T^R$ has atleast two positive eigenvalues.

$\beta \cdot \phi^R$ is not quasiconvex when $\beta \in \mathbb{R}^3 \setminus \mathbb{R}_+^3$ since for $i \neq j = 1, 2, 3$,

$$\beta \cdot T e_i \otimes_s e_j = \beta_{\{1,2,3\} \setminus \{i,j\}} e_i \otimes_s e_j,$$

where $\{e_1, e_2, e_3\}$ is the standard basis for \mathbb{R}^3 .

4.3. A lower bound on the relaxed energy. I.

For $\alpha \in \mathcal{L}_{>}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ let

$$B_\alpha(R) := \{\beta \in \mathbb{R}_+^3 \mid \alpha - \beta \cdot T^R \geq 0\} \quad (4.10a)$$

$$\begin{aligned} &= \left\{ \beta \in \mathbb{R}_+^3 \mid \forall \epsilon \in \mathbb{R}_{\text{sym}}^{3 \times 3}, \frac{1}{2} \langle \alpha \epsilon, \epsilon \rangle - \beta \cdot \phi(R^T \epsilon R) \geq 0 \right\} \\ &= \left\{ \beta \in \mathbb{R}_+^3 \mid \forall \epsilon \in \mathbb{R}_{\text{sym}}^{3 \times 3}, \frac{1}{2} \langle \alpha R \epsilon R^T, R \epsilon R^T \rangle - \beta \cdot \phi(\epsilon) \geq 0 \right\} \quad (4.10b) \\ &= \left\{ \beta \in \mathbb{R}_+^3 \mid \alpha^{R^T} - \beta \cdot T \geq 0 \right\}. \end{aligned}$$

Note that

$$B_{\alpha_i}(R) = \{\beta \in \mathbb{R}_+^3 \mid W_i - \beta \cdot \phi^R : \text{convex}\}. \quad (4.10c)$$

It is easy to show, e.g., using (4.10), that $B_\alpha(R)$ is compact and convex. Since $\forall \beta \in \mathbb{R}_+^3, \forall R \in SO(3)$, $\beta \cdot T^R$ has at least one (in fact, at least two) positive eigenvalues,

$$\alpha_1 \leq \alpha_2 \implies \forall R \in SO(3), B_{\alpha_1}(R) \subseteq B_{\alpha_2}(R). \quad (4.11)$$

For $\alpha_1, \alpha_2 \in \mathcal{L}_{>}^*(\mathbb{R}_{\text{sym}}^{3 \times 3})$ let

$$B_{(\alpha_1, \alpha_2)}(R) := \cap_{i=1}^2 B_{\alpha_i}(R).$$

Since $\beta \cdot \phi^R$ is quadratic and quasiconvex we immediately obtain the following analogue of (3.5) (c.f., Proposition 3.1 and §3.1.2):

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \max_{R \in SO(3)} \max_{\beta \in B_{(\alpha_1, \alpha_2)}(R)} W_\lambda(R, \beta, \bar{\epsilon}), \quad (4.12a)$$

where

$$W_\lambda(R, \beta, \bar{\epsilon}) := \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) - \lambda_1 \lambda_2 \beta \cdot \phi^R(\epsilon_2 - \epsilon_1). \quad (4.12b)$$

This immediately implies that

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\beta \in \cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)} W_\lambda(\beta, \bar{\epsilon}) \quad (4.13a)$$

where

$$W_\lambda(\beta, \bar{\epsilon}) := \max_{R \in SO(3)} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) - \lambda_1 \lambda_2 \beta \cdot \phi^R(\epsilon_2 - \epsilon_1). \quad (4.13b)$$

We have potentially lost some information in going from (4.12) to (4.13). We show in Corollary 4.9 this is not the case when the elastic moduli are isotropic, and in Theorem 4.32 that this is sometimes not the case when the elastic moduli are cubic. We do not know whether this is true in general.

To evaluate the lower bound (4.13) we need more information about the set $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)$. Thus in the next three sections we investigate, first the set $B_\alpha(R)$ and then the set $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)$ when elastic moduli are isotropic (§4.5) and cubic (§4.6).

4.4. Characterizing the set of allowable translations. I. Preliminaries.

For $\alpha \in \mathcal{L}_{>}^* (\mathbb{R}_{\text{sym}}^{3 \times 3})$ let

$$\begin{aligned} B_{\alpha, \text{I}}(R) &:= \partial B_{\alpha}(R) \cap \partial \mathbb{R}_{+}^3, \\ B_{\alpha, \text{II}}(R) &:= \partial B_{\alpha}(R) \cap \text{Int}(\mathbb{R}_{+}^3). \end{aligned}$$

In other words $B_{\alpha, \text{I}}(R)$ is that part of the boundary of $B_{\alpha}(R)$ that intersects the coordinate planes and $B_{\alpha, \text{II}}(R)$ is that part of the boundary of $B_{\alpha}(R)$ that does not intersect the coordinate planes; $\partial B_{\alpha}(R)$ is the disjoint union of $B_{\alpha, \text{I}}(R)$ and $B_{\alpha, \text{II}}(R)$.

From (4.10a) and (4.10c) it is easy to see that

$$\begin{aligned} \overline{B_{\alpha_i, \text{II}}(R)} &= \{ \beta \in \mathbb{R}_{+}^3 \mid W_i - \beta \cdot \phi^R : \text{convex but not strictly convex} \} \\ &= \{ \beta \in \mathbb{R}_{+}^3 \mid \alpha_i - \beta \cdot T^R \geq 0, \alpha_i - \beta \cdot T^R \not\equiv 0 \}, \end{aligned}$$

$$\begin{aligned} B_{\alpha_i}(R) \setminus \overline{B_{\alpha_i, \text{II}}(R)} &= \{ \beta \in \mathbb{R}_{+}^3 \mid W_i - \beta \cdot \phi^R : \text{strictly convex} \} \\ &= \{ \beta \in \mathbb{R}_{+}^3 \mid \alpha_i - \beta \cdot T^R > 0 \}, \end{aligned}$$

Thus $\alpha_i - \beta \cdot T^R$ is invertible on $B_{\alpha_i}(R) \setminus \overline{B_{\alpha_i, \text{II}}(R)}$ but not on $\overline{B_{\alpha_i, \text{II}}(R)}$.

For $\alpha_1, \alpha_2 \in \mathcal{L}_{>}^* (\mathbb{R}_{\text{sym}}^{3 \times 3})$ let

$$B_{(\alpha_1, \alpha_2), \text{II}}(R) := \partial B_{(\alpha_1, \alpha_2)}(R) \cap \text{Int}(\mathbb{R}_{+}^3).$$

From (4.10a) and (4.10c) it is easy to see that

$$\begin{aligned} B_{(\alpha_1, \alpha_2), \text{II}}(R) &= \cap_{i=1}^2 B_{\alpha_i, \text{II}}(R), \\ B_{(\alpha_1, \alpha_2)}(R) \setminus B_{(\alpha_1, \alpha_2), \text{II}}(R) &= \cap_{i=1}^2 (B_{\alpha_i}(R) \setminus B_{\alpha_i, \text{II}}(R)). \end{aligned}$$

Thus, both $\alpha_1 - \beta \cdot T^R$ and $\alpha_2 - \beta \cdot T^R$ are invertible on $B_{(\alpha_1, \alpha_2)}(R) \setminus \overline{B_{(\alpha_1, \alpha_2), \text{II}}(R)}$ and at least one of them is not invertible on $\overline{B_{(\alpha_1, \alpha_2), \text{II}}(R)}$.

Lemma 4.2. For $\alpha, \alpha_1, \alpha_2 \in \mathcal{L}_{>}^* (\mathbb{R}_{\text{sym}}^{3 \times 3})$ let $\gamma_{\alpha}, \gamma_{(\alpha_1, \alpha_2)} > 0$ be defined by

$$\gamma_{\alpha} := \left(\max_{\|\epsilon\|=1} \left\langle \left(\alpha^{-\frac{1}{2}} (e \cdot T) \alpha^{-\frac{1}{2}} \right) \epsilon, \epsilon \right\rangle \right)^{-1}, \quad (4.14a)$$

$$\gamma_{(\alpha_1, \alpha_2)} := \min(\gamma_{\alpha_1}, \gamma_{\alpha_2}). \quad (4.14b)$$

Then,

$$\begin{aligned} \gamma_{\alpha} e &\in \partial \left(\cap_{R \in SO(3)} B_{\alpha}(R) \right), \partial \left(\cap_{R \in SO(3)} B_{\alpha, \text{II}}(R) \right), \\ \gamma_{(\alpha_1, \alpha_2)} e &\in \partial \left(\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R) \right), \partial \left(\cap_{R \in SO(3)} B_{\star, \text{II}}(R) \right). \end{aligned}$$

In particular, $\forall R \in SO(3)$,

$$\begin{aligned} \gamma_{\alpha} e &\in B_{\alpha}(R), B_{\alpha, \text{II}}(R), \\ \gamma_{(\alpha_1, \alpha_2)} e &\in B_{(\alpha_1, \alpha_2)}(R), B_{\star, \text{II}}(R). \end{aligned}$$

Proof. Since, from Note 4.1, $e \cdot T^R$ is independent of R , it follows that for sufficiently small $\gamma' > 0$,

$$\forall R \in SO(3), \gamma' e \cdot T \in B_\alpha(R).$$

Since $\forall R \in SO(3)$, $B_\alpha(R)$ is closed it follows that $\exists \gamma_\alpha > 0$ such that

$$\forall R \in SO(3), \gamma_\alpha e \cdot T \in B_{\alpha, \text{II}^+}(R).$$

That γ_α and $\gamma_{(\alpha_1, \alpha_2)}$ are given by (4.14) follows from a proof similar to the proof of Lemma 3.2. The results follow. \square

Note 4.3. From (4.9a),

$$\langle (\alpha - \gamma_\alpha(e \cdot T))I, I \rangle = \langle \alpha I, I \rangle + 2\gamma_\alpha \|I\|^2 > 0.$$

This, with Lemma 4.2 gives,

$$1 \leq \dim \ker(\alpha - \gamma_\alpha T) \leq \dim \mathbb{R}_{\text{sym}}^{3 \times 3} - 1 = 5. \quad (4.15)$$

We end this section by observing that as a consequence of (4.1),

$$\ker(\alpha - \beta \cdot T^R) = R \ker(\alpha^{R^T} - \beta \cdot T) R^T. \quad (4.16)$$

4.5. Characterizing the set of allowable translations. II. Isotropic elastic moduli.

4.5.1. The set $B_\alpha(R)$. In this section we first show that for an isotropic elastic modulus α , $B_\alpha(R)$ is independent of R (Lemma 4.4). Then we explicitly characterize B_α (Lemma 4.5), the normal cone to B_{α, II^+} (Lemma 4.7) and $\ker(\alpha - \beta \cdot T^R)$ on a subset of B_{α, II^+} (Lemma 4.8).

Lemma 4.4. *When α is isotropic, $B_\alpha(R)$ is independent of R .*

Proof. By the definition of isotropy,

$$\forall R \in SO(3), \langle \alpha R \epsilon R^T, R \epsilon R^T \rangle = \langle \alpha \epsilon, \epsilon \rangle.$$

This, with (4.10b), immediately implies that for isotropic α , $B_\alpha(R)$ is independent of R and has the characterization

$$\begin{aligned} B_\alpha &= \{ \beta \in \mathbb{R}_+^3 \mid \alpha - \beta \cdot T \geq 0 \} \\ &= \left\{ \beta \in \mathbb{R}_+^3 \mid \forall \epsilon \in \mathbb{R}_{\text{sym}}^{3 \times 3}, \frac{1}{2} \langle \alpha \epsilon, \epsilon \rangle - \beta \cdot \phi(\epsilon) \geq 0 \right\} \end{aligned} \quad (4.17)$$

\square

Lemma 4.5 (Characterization of the set of allowable translations. I). *Let α be isotropic. Then,*

$$\begin{aligned} B_\alpha &= S(\kappa, \mu) \\ &:= \left\{ \beta \in [0, 2\mu]^3 \mid 2\beta'_1\beta'_2\beta'_3 - ((\beta'_1)^2 + (\beta'_2)^2 + (\beta'_3)^2) + 1 \geq 0 \right\}, \end{aligned} \quad (4.18a)$$

$$\begin{aligned} B_{\alpha, \iota} &= S_{\iota^*}(\kappa, \mu) \\ &:= \left\{ \beta \in [0, 2\mu]^3 \cap \partial\mathbb{R}_+^3 \mid 2\beta'_1\beta'_2\beta'_3 - ((\beta'_1)^2 + (\beta'_2)^2 + (\beta'_3)^2) + 1 \geq 0 \right\}, \\ B_{\alpha, \Pi^+} &= S_{\Pi^*}(\kappa, \mu) \\ &:= \left\{ \beta \in (0, 2\mu]^3 \mid 2\beta'_1\beta'_2\beta'_3 - ((\beta'_1)^2 + (\beta'_2)^2 + (\beta'_3)^2) + 1 = 0 \right\}. \end{aligned} \quad (4.18b)$$

Here, for $i = 1, 2, 3$,

$$\beta'_i := \frac{\ell + \beta_i}{\ell + 2\mu}. \quad (4.19)$$

Proof. From (4.17),

$$B_\alpha = \left\{ \beta \in \mathbb{R}_+^3 \mid \forall \epsilon \in \mathbb{R}_{\text{sym}}^{3 \times 3}, \langle \alpha \epsilon, \epsilon \rangle - 2\beta \cdot \phi(\epsilon) \geq 0 \right\}.$$

A calculation reveals that

$$\begin{aligned} \langle \alpha \epsilon, \epsilon \rangle - 2\beta \cdot \phi(\epsilon) &= (\ell + 2\mu)(\epsilon_{11}^2 + \epsilon_{22}^2 + \epsilon_{33}^2) \\ &\quad + 2(\ell + \beta_3)\epsilon_{11}\epsilon_{22} + 2(\ell + \beta_1)\epsilon_{22}\epsilon_{33} + 2(\ell + \beta_2)\epsilon_{33}\epsilon_{11} \\ &\quad + 2(2\mu - \beta_3)\epsilon_{12}^2 + 2(2\mu - \beta_1)\epsilon_{23}^2 + 2(2\mu - \beta_2)\epsilon_{31}^2. \end{aligned}$$

This function is non-negative precisely when $\beta_1, \beta_2, \beta_3 \leq 2\mu$ (i.e., $\beta' \in [\frac{\ell}{\ell+2\mu}, 1]^3$) and the Hessian

$$H := 2 \begin{pmatrix} \ell+2\mu & \ell+\beta_3 & \ell+\beta_2 \\ \ell+\beta_3 & \ell+2\mu & \ell+\beta_1 \\ \ell+\beta_2 & \ell+\beta_1 & \ell+2\mu \end{pmatrix}$$

of $(\ell + 2\mu)(\epsilon_{11}^2 + \epsilon_{22}^2 + \epsilon_{33}^2) + 2(\ell + \beta_3)\epsilon_{11}\epsilon_{22} + 2(\ell + \beta_1)\epsilon_{22}\epsilon_{33} + 2(\ell + \beta_2)\epsilon_{33}\epsilon_{11}$ is positive-semidefinite. Set

$$H' := \frac{1}{2(\ell + 2\mu)} H = \begin{pmatrix} 1 & \beta'_3 & \beta'_2 \\ \beta'_3 & 1 & \beta'_1 \\ \beta'_2 & \beta'_1 & 1 \end{pmatrix},$$

and verify through calculations that its invariants are

$$\begin{aligned} \text{Tr } H' &= 3, \\ \frac{1}{2} ((\text{Tr}(H'))^2 - \text{Tr}((H')^2)) &= 3 - ((\beta'_1)^2 + (\beta'_2)^2 + (\beta'_3)^2), \\ \det H' &= 2\beta'_1\beta'_2\beta'_3 - ((\beta'_1)^2 + (\beta'_2)^2 + (\beta'_3)^2) + 1. \end{aligned}$$

The result follows. \square

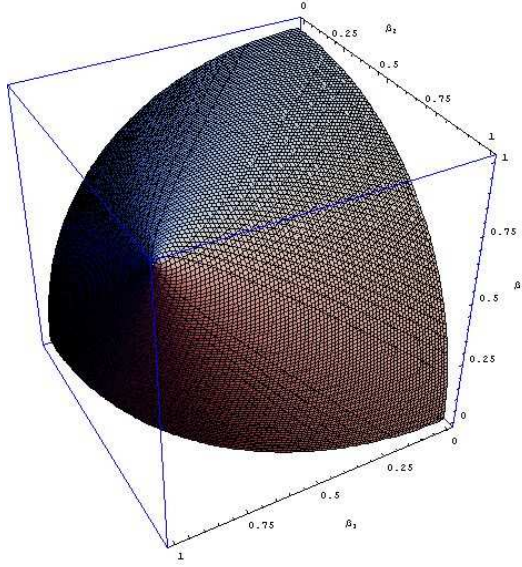


Fig. 4.1. The set $S_{II+}(\frac{4}{3}, \frac{1}{2})$.

Note 4.6. The surface $S_{II+}(\frac{4}{3}, \frac{1}{2})$ is illustrated in Figure 4.1. We highlight certain features of S so that its geometry could be better understood.

1. $S(\kappa, \mu)$, $S_{I+}(\kappa, \mu)$ and $\bar{S}_{II+}(\kappa, \mu)$ intersect the coordinate axes at 2μ .
2. $S_{I+}(\kappa, \mu)$ consists of three segments of ellipses: When $\beta_3 = 0$, (4.18b) reduces to $-(\ell + 2\mu)(\beta_1^2 + \beta_2^2) + 2\ell\beta_1\beta_2 - 4\ell\mu(\beta_1 + \beta_2) + 12\ell\mu^2 + 8\mu^3 = 0$, which is the equation of an ellipse. The same is true when $\beta_3 = \beta_1 = 0$ and $\beta_1 = \beta_2 = 0$.
3. The intersection of $S(\kappa, \mu)$ and $\bar{S}_{II+}(\kappa, \mu)$ with the plane $\beta_3 = 2\mu$ is the straight line segment $\beta_1 = \beta_2 \in [0, 2\mu]$; similar statements are true when $\beta_2 = 2\mu$ and $\beta_3 = 2\mu$. Thus the intersection of $S(\kappa, \mu)$ with $\text{Span}\{e\}$ is $\{2\mu e\}$. Thus, when α is isotropic, (c.f., (4.14)),

$$\gamma_\alpha = 2\mu.$$

Subregions of S_{I+} and S_{II+} . It is useful to divide S_I and $S_{II+}(\kappa, \mu)$ into subregions. The definitions below are motivated partially by Note 4.6 and partially by results to follow. Note that some of these subregions are independent of κ .

$$S_I(\kappa, \mu) := S_{I+}(\kappa, \mu) \setminus S_{I\&III}(\mu), \quad (4.20a)$$

$$S_{I\&III}(\mu) := \cup_{i=1}^3 S_{I\&III}^{(i)}(\mu); \quad (4.20a)$$

$$S_{I\&III}^{(1)}(\mu) := \{(2\mu, 0, 0)^T\}, \quad (4.20b)$$

$$S_{I\&III}^{(2)}(\mu) := \{(0, 2\mu, 0)^T\}, \quad (4.20c)$$

$$S_{I\&III}^{(3)}(\mu) := \{(0, 0, 2\mu)^T\}; \quad (4.20d)$$

$$S_{\Pi^+}^{(1)}(\kappa, \mu) := S_{\Pi^+}(\kappa, \mu) \cap \{\beta \in \mathbb{R}_+^3 \mid \beta_2, \beta_3 > \beta_1\}, \quad (4.21a)$$

$$S_{\Pi^+}^{(2)}(\kappa, \mu) := S_{\Pi^+}(\kappa, \mu) \cap \{\beta \in \mathbb{R}_+^3 \mid \beta_3, \beta_1 > \beta_2\}, \quad (4.21b)$$

$$S_{\Pi^+}^{(3)}(\kappa, \mu) := S_{\Pi^+}(\kappa, \mu) \cap \{\beta \in \mathbb{R}_+^3 \mid \beta_1, \beta_2 > \beta_3\}; \quad (4.21c)$$

$$S_{\text{III}}(\mu) := \cup_{i=1}^3 S_{\text{III}}^{(i)}(\mu); \quad (4.22a)$$

$$S_{\text{III}}^{(1)}(\mu) := \{\beta \in \mathbb{R}_+^3 \mid \beta_2 = \beta_3 \in (0, 2\mu), \beta_1 = 2\mu\}, \quad (4.22b)$$

$$S_{\text{III}}^{(2)}(\mu) := \{\beta \in \mathbb{R}_+^3 \mid \beta_3 = \beta_1 \in (0, 2\mu), \beta_2 = 2\mu\}, \quad (4.22c)$$

$$S_{\text{III}}^{(3)}(\mu) := \{\beta \in \mathbb{R}_+^3 \mid \beta_1 = \beta_2 \in (0, 2\mu), \beta_3 = 2\mu\}; \quad (4.22d)$$

$$S_{\text{III}\&\text{IV}}(\mu) := \{2\mu e\}. \quad (4.23)$$

Note that $S_{\Pi^+}(\kappa, \mu)$ is the union of the disjoint sets $S_{\Pi^+}^{(1)}(\kappa, \mu)$, $S_{\Pi^+}^{(2)}(\kappa, \mu)$, $S_{\Pi^+}^{(3)}(\kappa, \mu)$, $S_{\text{III}}(\mu)$ and $S_{\text{III}\&\text{IV}}(\mu)$. For conciseness we shall write, e.g., $(S_{\text{I}\&\text{III}}^{(1)} \cup S_{\text{III}}^{(1)})(\mu)$ to mean $S_{\text{I}\&\text{III}}^{(1)}(\mu) \cup S_{\text{III}}^{(1)}(\mu)$.

The surface $S_{\Pi^+}(\kappa, \mu) \setminus S_{\text{III}\&\text{IV}}(\mu)$ is smooth. From (4.18b), $N(\beta)$, the outward normal to $S(\kappa, \mu)$ at $\beta \in S_{\Pi^+}(\kappa, \mu) \setminus S_{\text{III}\&\text{IV}}(\mu)$ is given by

$$\begin{aligned} N(\beta) &\parallel -\frac{\partial}{\partial \beta} (2\beta'_1\beta'_2\beta'_3 - ((\beta'_1)^2 + (\beta'_2)^2 + (\beta'_3)^2) + 1) \\ &\parallel \frac{\partial}{\partial \beta'} (2\beta'_1\beta'_2\beta'_3 - ((\beta'_1)^2 + (\beta'_2)^2 + (\beta'_3)^2) + 1) \\ &\parallel \begin{pmatrix} \beta'_1 - \beta'_2\beta'_3 \\ \beta'_2 - \beta'_3\beta'_1 \\ \beta'_3 - \beta'_1\beta'_2 \end{pmatrix}. \end{aligned} \quad (4.24)$$

(We use “ \parallel ” to mean “parallel and not anti-parallel”.) The next Lemma fills in some important details.

Lemma 4.7 (Outward normal cone to S_{Π^+}). *Let α be isotropic. Let $N(\beta)$ belong to the outward normal cone to $S(\kappa, \mu)$ at $\beta \in S_{\Pi^+}(\kappa, \mu)$. Then*

$$\text{sign}(N) \in \begin{cases} \mathbb{R}_+^3 & \text{on } S_{\text{III}\&\text{IV}}(\mu), \\ \left\{ \begin{pmatrix} + \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ + \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ + \end{pmatrix} \right\} & \text{on } S_{\text{III}}(\mu), \\ \left\{ \begin{pmatrix} - \\ + \\ + \end{pmatrix}, \begin{pmatrix} + \\ - \\ + \end{pmatrix}, \begin{pmatrix} + \\ + \\ - \end{pmatrix} \right\} & \text{elsewhere on } S_{\Pi^+}(\kappa, \mu). \end{cases}$$

More precisely (4.25) and (4.26) below hold.

Proof. We prove the last case by showing that,

$$\text{sign}(N) = \begin{cases} (-, +, +)^T & \text{on } S_{\Pi^+}^{(1)}(\kappa, \mu), \\ (+, -, +)^T & \text{on } S_{\Pi^+}^{(2)}(\kappa, \mu), \\ (+, +, -)^T & \text{on } S_{\Pi^+}^{(3)}(\kappa, \mu). \end{cases} \quad (4.25)$$

Let $\beta \in S_{\Pi^+}^{(1)}(\kappa, \mu)$. From (4.19),

$$\beta_2, \beta_3 > \beta_1 \iff \beta'_2, \beta'_3 > \beta'_1.$$

Clearly,

$$\begin{aligned} \beta'_2 - \beta'_3 \beta'_1 &\geq \beta'_2 - \beta'_1 > 0, \\ \beta'_3 - \beta'_1 \beta'_2 &\geq \beta'_3 - \beta'_1 > 0; \end{aligned}$$

so, from (4.24), it remains to show that $\beta'_1 - \beta'_2 \beta'_3 < 0$. It is a calculation to verify that (4.18b), which defines $S_{\Pi^+}(\kappa, \mu)$, may be rewritten as

$$\frac{(\beta'_2 + \beta'_3)^2}{2(1 + \beta'_1)} + \frac{(\beta'_2 - \beta'_3)^2}{2(1 - \beta'_1)} = 1.$$

Thus, the intersection of $S_{\Pi^+}(\kappa, \mu)$ with a plane of constant β'_1 is an ellipse with minor and major axes equal to $\sqrt{2(1 + \beta'_1)}$ and $\sqrt{2(1 - \beta'_1)}$ and oriented in the $(1, 1)$ and $(1, -1)$ directions respectively. This is shown in Figure 4.2. This ellipse intersects the hyperbola $\beta'_2 \beta'_3 = \beta'_1$ at $(\beta'_2, \beta'_3) = (1, \beta'_1)$ and $(\beta'_2, \beta'_3) = (\beta'_1, 1)$, and the portion of the ellipse consistent with our assumption $\beta'_1 \leq \beta'_2, \beta'_3$ satisfies $\beta'_1 - \beta'_2 \beta'_3 < 0$. The cases $\beta \in S_{\Pi^+}^{(2)}(\kappa, \mu)$ and $\beta \in S_{\Pi^+}^{(3)}(\kappa, \mu)$ are analogous.

The second case follows immediately from (4.19), (4.22) and (4.24). Indeed,

$$\text{sign}(N) = \begin{cases} (+, 0, 0)^T & \text{on } S_{\Pi}^{(1)}(\mu), \\ (0, +, 0)^T & \text{on } S_{\Pi}^{(2)}(\mu), \\ (0, 0, +)^T & \text{on } S_{\Pi}^{(3)}(\mu). \end{cases} \quad (4.26)$$

Thus,

$$\lim_{S_{\Pi}^{(i)}(\mu) \ni \beta' \rightarrow e} N(\beta) = e_i, \quad i = 1, 2, 3.$$

The first case follows from this and the fact that the normal cone to any surface is convex. \square

We end this section by characterizing $\ker(\alpha - \beta \cdot T^R)$.

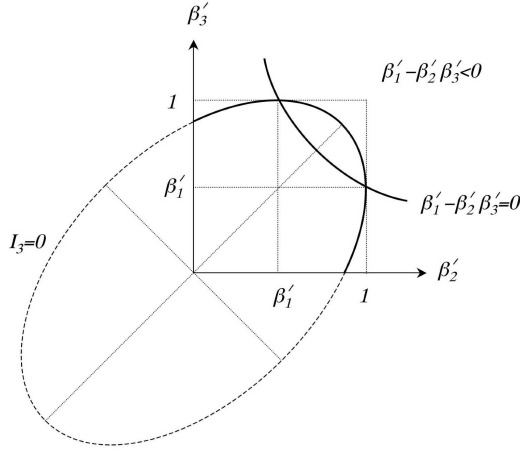


Fig. 4.2. A section of the set $B_{i,II+}$ through the plane $\beta'_1 = \text{constant}$.

Lemma 4.8 (Kernel of the translated elastic modulus). *Let α be isotropic. Then,*

$$\ker(\alpha - \beta \cdot T^R) = R \ker(\alpha - \beta \cdot T) R^T,$$

$$\ker(\alpha - \beta \cdot T) = \begin{cases} \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\} & \text{on } (S_{I\&III}^{(1)} \cup S_{III}^{(1)})(\mu), \\ \text{Span} \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right\} & \text{on } (S_{I\&III}^{(2)} \cup S_{III}^{(2)})(\mu), \\ \text{Span} \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right\} & \text{on } (S_{I\&III}^{(3)} \cup S_{III}^{(3)})(\mu), \\ \mathcal{D} \oplus \mathcal{O} & \text{on } S_{III\&IV}(\mu). \end{cases}$$

Proof. The first statement follows from (4.16) and the isotropy of α .

When $\beta \in (S_{\text{I&III}}^{(1)} \cup S_{\text{III}}^{(1)})(\mu)$, from (4.22) and (4.20), $\beta_1 = 2\mu$ and $\beta_2 = \beta_3 \in [0, 2\mu)$. Thus from (4.3) and (4.6),

$$\begin{aligned}
& (\alpha - \beta \cdot T)\epsilon \\
&= \alpha\epsilon - (2\mu T_1 + \beta_2 T_2 + \beta_2 T_3)\epsilon \\
&= \kappa(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) \\
&\quad + 2\mu \begin{pmatrix} \epsilon_{11} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} & \epsilon_{12} & \epsilon_{31} \\ \epsilon_{12} & \epsilon_{22} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{23} & \epsilon_{33} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} \end{pmatrix} \\
&\quad - 2\mu \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\epsilon_{33} & \epsilon_{23} \\ 0 & \epsilon_{23} & -\epsilon_{22} \end{pmatrix} - \beta_2 \begin{pmatrix} -\epsilon_{33} & 0 & \epsilon_{31} \\ 0 & 0 & 0 \\ \epsilon_{31} & 0 & -\epsilon_{11} \end{pmatrix} - \beta_2 \begin{pmatrix} -\epsilon_{22} & \epsilon_{12} & 0 \\ \epsilon_{12} & -\epsilon_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) & (2\mu - \beta_2)\epsilon_{12} & (2\mu - \beta_2)\epsilon_{31} \\ +2\mu\epsilon_{11} + \beta_2\epsilon_{22} + \beta_2\epsilon_{33} & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) & 0 \\ (2\mu - \beta_2)\epsilon_{12} & +\beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\mu\epsilon_{33} & \\ (2\mu - \beta_2)\epsilon_{31} & 0 & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) \\ & & +\beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\mu\epsilon_{33} \end{pmatrix} \quad (4.27)
\end{aligned}$$

Thus $(\alpha - \beta \cdot T)\epsilon = 0$ if and only if $\epsilon_{31} = \epsilon_{12} = 0$ and

$$\begin{aligned}
& (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) + 2\mu\epsilon_{11} + \beta_2\epsilon_{22} + \beta_2\epsilon_{33} = 0, \\
& (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) + \beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\mu\epsilon_{33} = 0.
\end{aligned}$$

When $\beta_2 \neq 2\mu$ these four equations are independent: $\dim(\ker(\alpha - \beta \cdot T)) = 2$. It is easy to verify that

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \in \ker(\alpha - \beta \cdot T).$$

This proves the first statement; the proofs of the second and third statements are almost identical.

The fourth statement immediately follows by setting $\beta_2 = \beta_3 = 2\mu$ in (4.27). Alternatively, from (4.3) and Note 4.1,

$$\begin{aligned}
(\alpha - 2\mu e \cdot T)\epsilon &= (\ell \operatorname{Tr}(\epsilon)I + 2\mu\epsilon) - 2\mu(\epsilon - \operatorname{Tr}(\epsilon)I) \\
&= (\ell + 2\mu) \operatorname{Tr}(\epsilon)I.
\end{aligned}$$

It follows that,

$$\epsilon \in \ker(\alpha - 2\mu e \cdot T) \iff \operatorname{Tr}(\epsilon) = 0.$$

This completes the proof. \square

4.5.2. The set $B_{(\alpha_1, \alpha_2)}(R)$. Finally we explicitly characterize $B_{(\alpha_1, \alpha_2)}(R)$ (Corollary 4.9) and the normal cone to $B_{(\alpha_1, \alpha_2), \Pi^+}$ (Corollary 4.10).

Using (4.11) if necessary, we immediately have the following corollary to Lemmas 4.4 and 4.5:

Corollary 4.9 (Characterization of the set of allowable translations. II). *Let α_1 and α_2 be isotropic. Then $B_{(\alpha_1, \alpha_2)}(R)$ is independent of R . Moreover*

$$B_{(\alpha_1, \alpha_2)} = S(\kappa_1, \mu_1) \cap S(\kappa_2, \mu_2)$$

and (c.f., (4.14)),

$$\gamma_{(\alpha_1, \alpha_2)} = 2 \min(\mu_1, \mu_2).$$

Lemma 4.7 can also be extended:

Corollary 4.10. *Let α_1 and α_2 be isotropic. Let $N \in \mathbb{R}_+^3$ belong to the outward normal cone to $B_{(\alpha_1, \alpha_2), \Pi^+}$. Then*

$$\text{sign}(N) \in \begin{cases} \mathbb{R}_+^3 & \text{on } S_{\text{III}\&\text{IV}}(\min(\mu_1, \mu_2)), \\ \left\{ \begin{pmatrix} + \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ + \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ + \end{pmatrix} \right\} & \text{on } (S_{\text{I}\&\text{III}} \cup S_{\text{III}})(\min(\mu_1, \mu_2)), \\ \left\{ \begin{pmatrix} - \\ + \\ + \end{pmatrix}, \begin{pmatrix} + \\ + \\ - \end{pmatrix}, \begin{pmatrix} + \\ - \\ + \end{pmatrix} \right\} & \text{elsewhere.} \end{cases}$$

Proof. The first two cases are easy, once it is observed that, from the geometry of $S(\kappa, \mu)$,

$$(S_{\text{III}} \cup S_{\text{III}\&\text{IV}})(\min(\mu_1, \mu_2)) \subsetneq S_{\Pi^+}(\kappa_1, \mu_1) \cap S_{\Pi^+}(\kappa_2, \mu_2).$$

We turn to the third case. In addition to the corners of $S_{\Pi^+}(\kappa_1, \mu_1)$ and $S_{\Pi^+}(\kappa_2, \mu_2)$, $S_{\Pi^+}(\kappa_1, \mu_1) \cap S_{\Pi^+}(\kappa_2, \mu_2)$ can have corners where $S_{\Pi^+}(\kappa_1, \mu_1)$ and $S_{\Pi^+}(\kappa_2, \mu_2)$ intersect.

Consider the case $\beta \in S_{\Pi^+}^{(1)}(\kappa_1, \mu_1) \cap S_{\Pi^+}^{(1)}(\kappa_2, \mu_2)$. From (4.25) the sign of the normals at β to both $S_{\Pi^+}^{(1)}(\kappa_1, \mu_1)$ and $S_{\Pi^+}^{(1)}(\kappa_2, \mu_2)$ is $(-, +, +)^T$. It follows that $\text{sign}(N) = (-, +, +)^T$. The cases $\beta \in S_{\Pi^+}^{(2)}(\kappa_1, \mu_1) \cap S_{\Pi^+}^{(2)}(\kappa_2, \mu_2)$ and $\beta \in S_{\Pi^+}^{(3)}(\kappa_1, \mu_1) \cap S_{\Pi^+}^{(3)}(\kappa_2, \mu_2)$ are analogous. (From (4.21) it is clear that there are no other cases.) \square

4.6. Characterizing the set of allowable translations. III. Cubic elastic moduli.

In this section we extend the results of the previous section (§4.5) to cubic moduli. Since the case $\mu = \eta$ has already been considered there we shall prove the results in this section only for $\mu \neq \eta$.

4.6.1. The set $\cap_{R \in SO(3)} B_\alpha(R)$. After some preliminary results, in Lemma 4.13 we at least partially characterize $\cap_{R \in SO(3)} B_\alpha(R)$. This result derives its importance from Lemma 4.14 which shows that $\forall R \in SO(3)$, $\alpha^R - \beta \cdot T$ is not invertible on a certain subset of $\cap_{R \in SO(3)} B_\alpha(R)$. We end by characterizing $\ker(\alpha^{R_\alpha} - \beta \cdot T)$ on this subset (Lemma 4.16) and characterizing $\ker(\alpha - \gamma_\alpha e \cdot T)$ (Lemma 4.17).

Lemma 4.11. *Let α be cubic. Then*

$$S(\kappa, \min(\mu, \eta)) \subseteq \cap_{R \in SO(3)} B_\alpha(R) \subseteq S(\kappa, \max(\mu, \eta))$$

Proof. From (4.2),

$$3\kappa \mathbf{A}_h + 2 \min(\mu, \eta) \mathbf{A}_s \leq \alpha^{R_\alpha} \leq 3\kappa \mathbf{A}_h + 2 \max(\mu, \eta) \mathbf{A}_s$$

and thus, by using (4.3), $\forall R \in SO(3)$,

$$3\kappa \mathbf{A}_h + 2 \min(\mu, \eta) \mathbf{A}_s \leq \alpha^R \leq 3\kappa \mathbf{A}_h + 2 \max(\mu, \eta) \mathbf{A}_s.$$

From (4.11) and Lemmas 4.4 and 4.5,

$$S(\kappa, \min(\mu, \eta)) \subseteq B_\alpha(R) \subseteq S(\kappa, \max(\mu, \eta)),$$

from which the result follows. \square

When α is cubic, $B_{\alpha^{R_\alpha}}$ and $B_{\alpha^{R_\alpha}, \Pi^+}$ have simple explicit characterizations:

Lemma 4.12. *When α is cubic,*

$$B_{\alpha^{R_\alpha}} = \begin{cases} S(\kappa, \mu) & \text{if } \eta \geq \mu, \\ S(\kappa, \mu) \cap [0, 2\eta]^3 & \text{if } \mu \geq \eta; \end{cases}$$

$$B_{\alpha^{R_\alpha}, \Pi^+} = \begin{cases} S_{\Pi^+}(\kappa, \mu) & \text{if } \eta \geq \mu, \\ S_{\Pi^+}(\kappa, \mu) \cap (0, 2\eta]^3 & \text{if } \mu \geq \eta. \end{cases}$$

The proof of Lemma 4.12 is almost identical to that of Lemma 4.5. Lemmas 4.11 and 4.12 immediately lead to the following at least partial characterization of $\cap_{R \in SO(3)} B_\alpha(R)$ when α is cubic:

Lemma 4.13. *Let α be cubic. Then, when $\eta \geq \mu$,*

$$\cap_{R \in SO(3)} B_\alpha(R) = S(\kappa, \mu); \quad (4.28a)$$

and, when $\mu \geq \eta$,

$$S(\kappa, \eta) \subseteq \cap_{R \in SO(3)} B_\alpha(R) \subseteq S(\kappa, \mu) \cap [0, 2\eta]^3. \quad (4.28b)$$

In particular,

$$S(\kappa, \min(\mu, \eta)) \subseteq \cap_{R \in SO(3)} B_\alpha(R), \quad (4.28c)$$

$$(S_{I \& III} \cup S_{III} \cup S_{III \& IV})(\min(\mu, \eta)) \subsetneq \partial(\cap_{R \in SO(3)} B_\alpha(R)). \quad (4.28d)$$

Proof. When $\eta > \mu$, (4.28a) follows immediately from the observation that

$$S(\kappa, \mu) \subseteq \cap_{R \in SO(3)} B_\alpha(R) \subseteq B_\alpha(R_\alpha^T) = S(\kappa, \mu).$$

(The first inclusion follows from Lemmas 4.11 and the last equality from Lemma 4.12.)

When $\mu > \eta$, again from Lemmas 4.11 and 4.12,

$$S(\kappa, \eta) \subseteq \cap_{R \in SO(3)} B_\alpha(R) \subseteq B_\alpha(R_\alpha^T) = S(\kappa, \mu) \cap [0, 2\eta]^3.$$

In both cases (4.28c) and 4.28d follow immediately from (4.28a) and 4.28b. \square

Thus, for cubic α , (c.f., (4.14)),

$$\gamma_\alpha = 2 \min(\mu, \eta). \quad (4.29)$$

Lemma 4.14. *Let α be cubic. For any $R \in SO(3)$, $\alpha - \beta \cdot T^R$ is not invertible when $\beta \in (S_{I\&III} \cup S_{III})(\min(\mu, \eta))$.*

Lemma 4.17 shows that the result is true also for $\beta \in S_{III\&IV}(\min(\mu, \eta))$.

Proof. We begin by observing that α^{R_α} can be written as the sum of non-negative operators as

$$\alpha^{R_\alpha} = \begin{cases} 3\kappa \mathbf{A}_h + 2\mu \mathbf{A}_s + 2(\eta - \mu) \mathbf{A}_o & \text{if } \eta > \mu, \\ 3\kappa \mathbf{A}_h + 2\eta \mathbf{A}_s + 2(\mu - \eta) \mathbf{A}_d & \text{if } \mu > \eta. \end{cases}$$

Let $R' \in SO(3)$ and $R := R_\alpha^{-1} R'$. Then

$$\begin{aligned} \alpha^{R'} &= \alpha^{R_\alpha R} \\ &= \begin{cases} 3\kappa \mathbf{A}_h + 2\mu \mathbf{A}_s + 2(\eta - \mu) \mathbf{A}_o^R & \text{if } \eta > \mu, \\ 3\kappa \mathbf{A}_h + 2\eta \mathbf{A}_s + 2(\mu - \eta) \mathbf{A}_d^R & \text{if } \mu > \eta. \end{cases} \end{aligned}$$

From (4.1) it suffices to show that $\forall R' \in SO(3)$, $\alpha^{R'} - \beta \cdot T$ is not invertible when $\beta \in (S_{I\&III} \cup S_{III})(\min(\mu, \eta))$. Consider first the case

$$\beta \in (S_{I\&III}^{(1)} \cup S_{III}^{(1)} \cup S_{III\&IV})(\min(\mu, \eta)).$$

Then from (4.22), (4.23) and (4.20), $\beta = (2 \min(\mu, \eta), \beta_2, \beta_2)^T$ and $\beta_2 \in [0, 2 \min(\mu, \eta)]$.

We consider the cases $\mu > \eta$ and $\eta > \mu$ separately.

$\mu > \eta$: Using Note 4.1,

$$\begin{aligned} \alpha^{R'} - \beta \cdot T &= \alpha^{R'} - \beta_2 e \cdot T - (2\eta - \beta_2) T_1 \\ &= (3\kappa + 2\beta_2) \mathbf{A}_h + (2\eta - \beta_2)(\mathbf{A}_s - T_1) + 2(\mu - \eta) \mathbf{A}_d^R. \end{aligned} \quad (4.30)$$

Since, from (4.7),

$$\ker((3\kappa + 2\beta_2) \mathbf{A}_h + (2\eta - \beta_2)(\mathbf{A}_s - T_1)) = \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\}, \quad (4.31)$$

$\alpha^{R'} - \beta \cdot T$ is invertible only if

$$\begin{aligned} \ker(\mathbf{A}_d^R) &\subseteq \left(\text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\} \right)^\perp \\ &= \text{Span} \left\{ I, \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right\} \end{aligned}$$

Since $\dim \ker(\mathbf{A}_d^R) = \dim \ker(\mathbf{A}_d) = 4$ the inclusion above is in fact an equality. I.e., $\alpha^{R'} - \beta \cdot T$ is invertible only if $\forall x \in \mathbb{R}^3$,

$$\mathbf{A}_d \left(R^T \begin{pmatrix} 2x_1 & x_2 & x_3 \\ x_2 & -x_1 & 0 \\ x_3 & 0 & -x_1 \end{pmatrix} R \right) = 0.$$

I.e., $\forall x \in \mathbb{R}^3$,

$$\begin{aligned} (3R_{11}^2 - 1)x_1 + 2R_{11}R_{21}x_2 + 2R_{11}R_{31}x_3 &= 0, \\ (3R_{12}^2 - 1)x_1 + 2R_{12}R_{32}x_2 + 2R_{12}R_{32}x_3 &= 0, \\ (3R_{13}^2 - 1)x_1 + 2R_{13}R_{23}x_2 + 2R_{13}R_{33}x_3 &= 0. \end{aligned}$$

This implies that $R = 0$ (e.g., pick $x = e_1, e_2, e_3$), which is a contradiction.

$\eta > \mu$: Similar to the case $\mu > \eta$,

$$\alpha^{R'} - \beta \cdot T = (3\kappa + 2\beta_2)\mathbf{A}_h + (2\mu - \beta_2)(\mathbf{A}_s - T_1) + 2(\eta - \mu)\mathbf{A}_o^R \quad (4.32)$$

and $\alpha^{R'} - \beta \cdot T$ is invertible only if

$$\ker(\mathbf{A}_o^R) \subseteq \left(\text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\} \right)^\perp.$$

Now,

$$\ker(\mathbf{A}_o^R) = R \ker(\mathbf{A}_o) R^T = \left\{ R \begin{pmatrix} x_1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & x_3 \end{pmatrix} R^T \mid x \in \mathbb{R}^3 \right\}$$

Thus $\alpha^{R'} - \beta \cdot T$ is invertible only if $\forall x \in \mathbb{R}^3$,

$$\begin{aligned} \left\langle R \begin{pmatrix} x_1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & x_3 \end{pmatrix} R^T, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\rangle &= 0, \\ \left\langle R \begin{pmatrix} x_1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & x_3 \end{pmatrix} R^T, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\rangle &= 0. \end{aligned}$$

I.e., $\forall x \in \mathbb{R}^3$,

$$\begin{aligned} R_{21}R_{31}x_1 + R_{22}R_{32}x_2 + R_{23}R_{33}x_3 &= 0, \\ (R_{21}^2 - R_{31}^2)x_1 + (R_{22}^2 - R_{32}^2)x_2 + (R_{23}^2 - R_{33}^2)x_3 &= 0. \end{aligned}$$

This implies that $R = 0$ (e.g., pick $x = e_1, e_2, e_3$), which is a contradiction.

Similar results hold for $\beta \in (S_{\text{I&III}}^{(2)} \cup S_{\text{III}}^{(2)})(\min(\mu, \eta))$ and $\beta \in (S_{\text{I&III}}^{(3)} \cup S_{\text{III}}^{(3)})(\min(\mu, \eta))$. \square

Corollary 4.15. *Let α be cubic and $\beta \in (S_{\text{I&III}} \cup S_{\text{III}})(\min(\mu, \eta))$. Then, for any $R \in SO(3)$,*

$$\dim \ker(\alpha - \beta \cdot T^R) = \begin{cases} 2 & \text{if } \alpha \text{ is isotropic,} \\ 1 & \text{otherwise} \end{cases}$$

Proof. When α is isotropic the result is immediate from Lemma 4.8; we turn to the case when α is not isotropic.

From the proof of Lemma 4.14 (c.f., (4.30), (4.31) and (4.32)),

$$1 \leq \dim \ker(\alpha - \beta \cdot T^R) \leq 2. \quad (4.33)$$

Let $\beta \in (S_{\text{I&III}}^{(1)} \cup S_{\text{III}}^{(1)})(\min(\mu, \eta))$. We consider the cases $\mu > \eta$ and $\eta > \mu$ separately.

$\mu > \eta$: From the proof of Lemma 4.14 (c.f., (4.30) and (4.31)),

$$\begin{aligned} \dim \ker(\alpha - \beta \cdot T^R) &= 2 \\ \iff \ker(\mathbf{A}_d^R) &= \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\} \\ \implies \forall x, y \in \mathbb{R}, \quad \mathbf{A}_d \left(R^T \begin{pmatrix} 0 & 0 & 0 \\ 0 & x & y \\ 0 & y & -x \end{pmatrix} R \right) &= 0 \\ \iff \forall x, y \in \mathbb{R}, \quad \begin{cases} (R_{21}^2 - R_{31}^2)x + 2R_{21}R_{31}y \\ = (R_{22}^2 - R_{32}^2)x + 2R_{22}R_{32}y \\ = (R_{23}^2 - R_{33}^2)x + 2R_{23}R_{33}y. \end{cases} \end{aligned}$$

This implies

$$R_{21}^2 - R_{31}^2 = R_{22}^2 - R_{32}^2 = R_{23}^2 - R_{33}^2 =: k_1 \text{ (say)}, \quad (4.34a)$$

$$R_{21}R_{31} = R_{22}R_{32} = R_{23}R_{33}. \quad (4.34b)$$

(4.34a) implies

$$1 = R_{21}^2 + R_{22}^2 + R_{23}^2 = R_{31}^2 + R_{32}^2 + R_{33}^2 + 3k_1 = 1 + 3k_1,$$

and thus $k_1 = 0$, giving, $R_{21}^2 = R_{31}^2$, $R_{22}^2 = R_{32}^2$ and $R_{23}^2 = R_{33}^2$. This, with (4.34b) implies

$$R_{21}^2 = R_{31}^2 = R_{22}^2 = R_{32}^2 = R_{23}^2 = R_{33}^2 = k_2^2 \text{ (say).}$$

Thus $R \in SO(3)$ is of the form

$$\begin{pmatrix} \pm k_2 & \pm k_2 & \pm k_2 \\ \pm k_2 & \pm k_2 & \pm k_2 \end{pmatrix}$$

which is a contradiction since the second row of the matrix above cannot be orthogonal to the third row (for any choice of signs). Thus $\dim \ker(\alpha - \beta \cdot T^R) \neq 2$. The result follows from (4.33).

$\eta > \mu$: From the proof of Lemma 4.14 (c.f., (4.31) and (4.32)),

$$\begin{aligned}
& \dim \ker(\alpha - \beta \cdot T^R) = 2 \\
\iff & \ker(\mathbf{A}_\mathbf{o}^R) = \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\} \\
\implies & \forall x, y \in \mathbb{R}, \quad \mathbf{A}_\mathbf{o} \left(R^T \begin{pmatrix} 0 & 0 & 0 \\ 0 & x & y \\ 0 & y & -x \end{pmatrix} R \right) = 0 \\
\iff & \forall x, y \in \mathbb{R}, \quad \begin{cases} (R_{21}R_{22} - R_{31}R_{32})x + (R_{22}R_{31} + R_{21}R_{32})y = 0, \\ (R_{21}R_{23} - R_{31}R_{33})x + (R_{23}R_{31} + R_{21}R_{33})y = 0, \\ (R_{22}R_{23} - R_{32}R_{33})x + (R_{23}R_{32} + R_{22}R_{33})y = 0. \end{cases} \\
\implies & \begin{cases} R_{21}R_{22} - R_{31}R_{32} = 0, & R_{22}R_{31} + R_{21}R_{32} = 0, \\ R_{21}R_{23} - R_{31}R_{33} = 0, & R_{23}R_{31} + R_{21}R_{33} = 0, \\ R_{22}R_{23} - R_{32}R_{33} = 0, & R_{23}R_{32} + R_{22}R_{33} = 0. \end{cases}
\end{aligned}$$

Squaring and adding these three pairs of equations gives,

$$\begin{aligned}
& (R_{21}^2 + R_{31}^2)(R_{22}^2 + R_{32}^2) = 0, \\
& (R_{21}^2 + R_{31}^2)(R_{23}^2 + R_{33}^2) = 0, \\
& (R_{22}^2 + R_{32}^2)(R_{23}^2 + R_{33}^2) = 0.
\end{aligned}$$

I.e., at least two of $R_{21}^2 + R_{31}^2$, $R_{22}^2 + R_{32}^2$ and $R_{23}^2 + R_{33}^2$ must vanish. It is easy to see that no such $R \in SO(3)$ exists. Thus $\dim \ker(\alpha - \beta \cdot T^R) \neq 2$. The result follows from (4.33).

Similar results hold for $\beta \in (S_{\text{I&III}}^{(2)} \cup S_{\text{III}}^{(2)})(\min(\mu, \eta))$ and $\beta \in (S_{\text{I&III}}^{(3)} \cup S_{\text{III}}^{(3)})(\min(\mu, \eta))$. \square

We end this section by characterizing, in Lemma 4.16, $\ker(\alpha^{R_\alpha} - \beta \cdot T)$ for $\beta \in (S_{\text{I&III}} \cup S_{\text{III}})(\min(\mu, \eta))$ and characterizing, in Lemma 4.17, $\ker(\alpha - \beta \cdot T^R)$ for $\beta \in S_{\text{III&IV}}(\min(\mu, \eta))$:

Lemma 4.16. *Let α be cubic. When $\eta > \mu$,*

$$\ker(\alpha^{R_\alpha} - \beta \cdot T) = \begin{cases} \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\} & \text{on } (S_{\text{I&III}}^{(1)} \cup S_{\text{III}}^{(1)})(\mu), \\ \text{Span} \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\} & \text{on } (S_{\text{I&III}}^{(2)} \cup S_{\text{III}}^{(2)})(\mu), \\ \text{Span} \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right\} & \text{on } (S_{\text{I&III}}^{(3)} \cup S_{\text{III}}^{(3)})(\mu), \\ \mathcal{D} & \text{on } S_{\text{III&IV}}(\mu); \end{cases}$$

and when $\mu > \eta$,

$$\ker(\alpha^{R_\alpha} - \beta \cdot T) = \begin{cases} \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\} & \text{on } (S_{I\&III}^{(1)} \cup S_{III}^{(1)})(\eta), \\ \text{Span} \left\{ \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right\} & \text{on } (S_{I\&III}^{(2)} \cup S_{III}^{(2)})(\eta), \\ \text{Span} \left\{ \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right\} & \text{on } (S_{I\&III}^{(3)} \cup S_{III}^{(3)})(\eta), \\ \mathcal{O} & \text{on } S_{III\&IV}(\eta). \end{cases}$$

The case $\mu = \eta$ was considered in Lemma 4.8.

Proof. We consider the cases $\eta > \mu$ and $\mu > \eta$ separately.

$\eta > \mu$: When $\beta \in (S_{I\&III}^{(1)} \cup S_{III}^{(1)})(\mu)$, from (4.22) and (4.20), $\beta_1 = 2\mu$ and $\beta_2 = \beta_3 \in [0, 2\mu)$. From (4.2) and (4.6),

$$\begin{aligned} & (\alpha^{R_\alpha} - \beta \cdot T)\epsilon \\ &= \alpha^{R_\alpha}\epsilon - (2\mu T_1 + \beta_2 T_2 + \beta_2 T_3)\epsilon \\ &= \kappa(\epsilon_{11} + \epsilon_{22} + \epsilon_{33})I \\ &+ 2\mu \begin{pmatrix} \epsilon_{11} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} & 0 & 0 \\ 0 & \epsilon_{22} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} & 0 \\ 0 & 0 & \epsilon_{33} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} \end{pmatrix} + 2\eta \begin{pmatrix} 0 & \epsilon_{12} & \epsilon_{31} \\ \epsilon_{12} & 0 & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{23} & 0 \end{pmatrix} \\ &- 2\mu \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\epsilon_{33} & \epsilon_{23} \\ 0 & \epsilon_{23} & -\epsilon_{22} \end{pmatrix} - \beta_2 \begin{pmatrix} -\epsilon_{33} & 0 & \epsilon_{31} \\ 0 & 0 & 0 \\ \epsilon_{31} & 0 & -\epsilon_{11} \end{pmatrix} - \beta_2 \begin{pmatrix} -\epsilon_{22} & \epsilon_{12} & 0 \\ \epsilon_{12} & -\epsilon_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) & (2\eta - \beta_2)\epsilon_{12} & (2\eta - \beta_2)\epsilon_{31} \\ +2\mu\epsilon_{11} + \beta_2\epsilon_{22} + \beta_2\epsilon_{33} & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) & 2(\eta - \mu)\epsilon_{23} \\ (2\eta - \beta_2)\epsilon_{12} & +\beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\mu\epsilon_{33} & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) \\ (2\eta - \beta_2)\epsilon_{31} & 2(\eta - \mu)\epsilon_{23} & +\beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\mu\epsilon_{33} \end{pmatrix} \quad (4.35) \end{aligned}$$

Thus $(\alpha - \beta \cdot T)\epsilon = 0$ if and only if $\epsilon_{23} = \epsilon_{31} = \epsilon_{12} = 0$ and

$$\begin{aligned} & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) + 2\mu\epsilon_{11} + \beta_2\epsilon_{22} + \beta_2\epsilon_{33} = 0, \\ & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) + \beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\mu\epsilon_{33} = 0. \end{aligned}$$

When $\beta_2 \neq 2\mu$ the last two equations are independent: $\dim(\ker(\alpha - \beta \cdot T)) = 1$.

It is easy to verify that

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \in \ker(\alpha - \beta \cdot T).$$

This proves the first case; the proofs of the second and third cases are almost identical.

The fourth case immediately follows by setting $\beta_2 = \beta_3 = 2\mu$ in (4.35). Alternatively, from (4.2) and Note 4.1,

$$\alpha^{R_\alpha} - 2\mu e \cdot T = (3\kappa + 4\mu)\mathbf{A}_h + 2(\eta - \mu)\mathbf{A}_o$$

It follows that,

$$\epsilon \in \ker(\alpha^{R_\alpha} - 2\mu e \cdot T) \iff \mathbf{A}_h \epsilon = \mathbf{A}_o \epsilon = 0.$$

$\mu > \eta$: When $\beta \in (S_{\text{I&II}}^{(1)} \cup S_{\text{III}}^{(1)})(\eta)$, from (4.22) and (4.20), $\beta_1 = 2\eta$ and $\beta_2 = \beta_3 \in [0, 2\eta)$. From (4.2) and (4.6),

$$\begin{aligned} & (\alpha^{R_\alpha} - \beta \cdot T)\epsilon \\ &= \alpha^{R_\alpha} \epsilon - (2\eta T_1 + \beta_2 T_2 + \beta_2 T_3)\epsilon \\ &= \kappa(\epsilon_{11} + \epsilon_{22} + \epsilon_{33})I \\ & \quad + 2\mu \begin{pmatrix} \epsilon_{11} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} & 0 & 0 \\ 0 & \epsilon_{22} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} & 0 \\ 0 & 0 & \epsilon_{33} - \frac{\epsilon_{11} + \epsilon_{22} + \epsilon_{33}}{3} \end{pmatrix} + 2\eta \begin{pmatrix} 0 & \epsilon_{12} & \epsilon_{31} \\ \epsilon_{12} & 0 & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{23} & 0 \end{pmatrix} \\ & \quad - 2\eta \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\epsilon_{33} & \epsilon_{23} \\ 0 & \epsilon_{23} & -\epsilon_{22} \end{pmatrix} - \beta_2 \begin{pmatrix} -\epsilon_{33} & 0 & \epsilon_{31} \\ 0 & 0 & 0 \\ \epsilon_{31} & 0 & -\epsilon_{11} \end{pmatrix} - \beta_2 \begin{pmatrix} -\epsilon_{22} & \epsilon_{12} & 0 \\ \epsilon_{12} & -\epsilon_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) & (2\eta - \beta_2)\epsilon_{12} & (2\eta - \beta_2)\epsilon_{31} \\ +2\mu\epsilon_{11} + \beta_2\epsilon_{22} + \beta_2\epsilon_{33} & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) & 0 \\ (2\eta - \beta_2)\epsilon_{12} & +\beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\eta\epsilon_{33} & 0 \\ (2\eta - \beta_2)\epsilon_{31} & 0 & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) \\ & & +\beta_2\epsilon_{11} + 2\eta\epsilon_{22} + 2\mu\epsilon_{33} \end{pmatrix} \quad (4.36) \end{aligned}$$

Thus $(\alpha - \beta \cdot T)\epsilon = 0$ if and only if $\epsilon_{31} = \epsilon_{12} = 0$ and

$$\begin{aligned} & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) + 2\mu\epsilon_{11} + \beta_2\epsilon_{22} + \beta_2\epsilon_{33} = 0, \\ & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) + \beta_2\epsilon_{11} + 2\mu\epsilon_{22} + 2\eta\epsilon_{33} = 0, \\ & (\kappa - \frac{2}{3}\mu)(\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) + \beta_2\epsilon_{11} + 2\eta\epsilon_{22} + 2\mu\epsilon_{33} = 0. \end{aligned}$$

When β_2, μ and η are distinct, the last three equations are independent: $\dim(\ker(\alpha - \beta \cdot T)) = 1$. From (4.36) it is clear that

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \in \ker(\alpha - \beta \cdot T).$$

This proves the first case; the proofs of the second and third cases are almost identical.

The fourth case immediately follows by setting $\beta_2 = \beta_3 = 2\eta$ in (4.35). Alternatively, from (4.2) and Note 4.1,

$$\alpha^{R_\alpha} - 2\eta e \cdot T = (3\kappa + 4\mu)\mathbf{A}_h + 2(\mu - \eta)\mathbf{A}_o$$

It follows that,

$$\epsilon \in \ker(\alpha^{R_\alpha} - 2\mu e \cdot T) \iff \Lambda_h \epsilon = \Lambda_d \epsilon = 0.$$

□

Lemma 4.17. *Let α be cubic. For any $R \in SO(3)$, $\alpha - \beta \cdot T^R$ is not invertible when $\beta \in S_{III \& IV}(\min(\mu, \eta))$, i.e., when $\beta = 2 \min(\mu, \eta)e$. Moreover,*

$$\ker(\alpha - 2 \min(\mu, \eta)e \cdot T) = \begin{cases} R_\alpha^T \mathcal{D} R_\alpha & \text{if } \eta > \mu, \\ \mathcal{D} \oplus \mathcal{O} & \text{if } \mu = \eta, \\ R_\alpha^T \mathcal{O} R_\alpha & \text{if } \mu > \eta. \end{cases}$$

Proof. We observe first that

$$\begin{aligned} \ker(\alpha - \beta \cdot T^R) &= \ker(\alpha^{R_\alpha R_\alpha^T} - \beta \cdot T^{RR_\alpha R_\alpha^T}) \\ &= R_\alpha^T \ker(\alpha^{R_\alpha} - \beta \cdot T^{RR_\alpha}) R_\alpha \end{aligned}$$

where we have used (4.1). In particular, when $\beta = 2 \min(\mu, \eta)e$, from Note 4.1,

$$\ker(\alpha - 2 \min(\mu, \eta)e \cdot T^R) = R_\alpha^T \ker(\alpha^{R_\alpha} - 2 \min(\mu, \eta)e \cdot T) R_\alpha.$$

The result follows by combining this with Lemmas 4.8 and 4.16. □

4.6.2. The set $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)$. Finally, in Corollary 4.18, we partially characterize $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)$ and, in Corollary 4.19, the normal cone to $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2), II^+}$.

Using (4.11) if necessary, we immediately have the following corollary to Lemma 4.13:

Corollary 4.18. *Let α_1 and α_2 be cubic. Then*

$$\begin{aligned} \cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R) &\supseteq S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2)), \quad (4.37) \\ \partial(\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)) &\supseteq (S_{I \& III} \cup S_{III} \cup S_{III \& IV})(\min(\mu_1, \eta_1, \mu_2, \eta_2)) \end{aligned}$$

and

$$\gamma_{(\alpha_1, \alpha_2)} = 2 \min(\mu_1, \eta_1, \mu_2, \eta_2)$$

Lemma 4.7 can also be extended:

Corollary 4.19. *Let α_1 and α_2 be cubic. Let $N \in \mathbb{R}_+^3$ belong to the outward normal cone to $B_{(\alpha_1, \alpha_2), II^+}$. Then*

$$\text{sign}(N) \in \begin{cases} \mathbb{R}_+^3 & \text{on } S_{III \& IV}(\min(\mu_1, \eta_1, \mu_2, \eta_2)), \\ \left\{ \begin{pmatrix} + \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ + \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ + \end{pmatrix} \right\} & \text{on } (S_{I \& III} \cup S_{III})(\min(\mu_1, \eta_1, \mu_2, \eta_2)), \\ \left\{ \begin{pmatrix} - \\ + \\ + \end{pmatrix}, \begin{pmatrix} + \\ - \\ + \end{pmatrix}, \begin{pmatrix} + \\ + \\ - \end{pmatrix} \right\} & \text{elsewhere.} \end{cases}$$

4.7. An optimal rotation diagonalizes the optimal strain jump.

Now that we have attained our goal of characterizing—to a degree sufficient for our purposes—the set $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)$ (c.f., (4.13a)) we turn to the maximization over $SO(3)$ in (4.13b). The main result of this section is:

Theorem 4.20 (An optimal rotation diagonalizes the optimal strain jump). *There exist $R_*(\beta, \bar{\epsilon}) \in SO(3)$ and $\epsilon_1^*(R_*, \beta, \bar{\epsilon})$, $\epsilon_2^*(R_*, \beta, \bar{\epsilon}) \in \mathbb{R}_{sym}^{3 \times 3}$ that extremize (4.13b) such that $R_*^T \Delta \epsilon^* R_*$ is diagonal.*

(From Note 4.1 this is trivially true when $\beta \parallel e$.) Our proof of theorem 4.20 uses doubly stochastic matrices and is presented at the end of this section.

Doubly stochastic matrices. Doubly stochastic matrices are square matrices, all of whose entries are non-negative and each of whose rows and columns add up to one. Ω_n , the set of all doubly stochastic matrices in $\mathbb{R}^{n \times n}$, is a $(n-1)^2$ -dimensional convex set. The set of extreme points of Ω_n is \mathbb{P}_n , the set of permutation matrices in $\mathbb{R}^{n \times n}$ ([Bir46] or, e.g., [MI79, pg.19,34]). In particular, the set of extreme points of Ω_3 is

$$\mathbb{P}_3 := \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \right\}.$$

Note that the first three of these belong to $SO(3)$ and the next three to $O(3) \setminus SO(3)$.

The following lemma is elementary:

Lemma 4.21. *Let $v, w \in \mathbb{R}^n$. Then*

1. $\exists D_* \in \mathbb{P}_n$ that maximizes $\Omega_n \ni D \mapsto Dv \cdot w \in \mathbb{R}$.
2. *The ordering of the components of D_*v is the same as the ordering of the components of w . I.e., if σ is a permutation of $\{1, 2, \dots, n\}$ such that $w_{\sigma(i)} \leq w_{\sigma(i+1)}$, $i = 1, 2, \dots, n-1$, then $(D_*v)_{\sigma(i)} \leq (D_*v)_{\sigma(i+1)}$, $i = 1, 2, \dots, n-1$.*
3. *The maximizer is unique precisely when all the components of v are distinct and all the components of w are distinct.*

We define $S: SO(3) \rightarrow \Omega_3$ by

$$SO(3) \ni \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \xrightarrow{S} \begin{pmatrix} R_{11}^2 & R_{12}^2 & R_{13}^2 \\ R_{21}^2 & R_{22}^2 & R_{23}^2 \\ R_{31}^2 & R_{32}^2 & R_{33}^2 \end{pmatrix} \in \Omega_3. \quad (4.38)$$

Some of the following properties of S will be used in the sequel.

Lemma 4.22.

1. $\forall P \in \mathbb{P}_3$, $\phi(P^T \epsilon P) = P^T \phi(\epsilon)$.
2. $\forall P \in \mathbb{P}_3 \setminus SO(3)$ there exists $R(P) \in SO(3)$ such that

$$\phi(P^T \epsilon P) = \phi(R(P)^T \epsilon R(P)).$$

3. For $R(P)$ defined as in (2), $S(R(P)) = P$. Thus $P_3 \subset \text{Range}(S)$.
4. The fixed points of S are precisely $\mathbb{P}_3 \cap SO(3)$ (and thus $\mathbb{P}_3 \cap SO(3) \subset \text{Range}(S)$); S can be extended to a map from $O(3)$ to Ω_3 , in which case its fixed points are precisely \mathbb{P}_3 .
5. S is not onto.

Proof. The first statement is easily verified.

(2): Each $P \in \mathbb{P}_3$ is a matrix precisely three of whose components is 1. For each $P \in \mathbb{P} \setminus SO(3)$ replacing one or three 1s by -1 generates a matrix $R(P) \in SO(3)$. It is easily verified that for every such choice of $R(P)$, $\Phi(P^T \epsilon P) = \Phi(R(P)^T \epsilon R(P))$.

(4): This follows from the fact that the only fixed points of $\mathbb{R} \ni x \mapsto x^2 \in \mathbb{R}$ are 0 and 1.

(5): Assume on the contrary that $\exists R \in SO(3)$ such that

$$S(R) = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \in \Omega_3.$$

Then, from (4.38), for some choice of signs

$$R = \frac{1}{\sqrt{3}} \begin{pmatrix} \pm 1 & \pm 1 & \pm 1 \\ \pm 1 & \pm 1 & \pm 1 \\ \pm 1 & \pm 1 & \pm 1 \end{pmatrix}.$$

However the rows and columns of this R cannot be orthogonal: $R \notin SO(3)$, which is a contradiction. \square

Lemma 4.23. Let $\epsilon \in \mathbb{R}_{\text{sym}}^{3 \times 3}$ and $R \in SO(3)$. There exists $D \in \Omega_3$ such that $\beta \cdot \phi^R(\epsilon) = -D\beta \cdot \Upsilon(\epsilon)$.

Proof. Let $R' := R(\epsilon)R$. Then

$$R^T \epsilon R = (R(\epsilon)R)^T \text{diag}(\epsilon) R(\epsilon)R = (R')^T \text{diag}(\epsilon) R'.$$

An easy exercise reveals that

$$\begin{aligned} & \phi^R(\epsilon) \\ &= - \begin{pmatrix} (R'_{22}R'_{33} - R'_{32}R'_{23})^2 & (R'_{23}R'_{31} - R'_{33}R'_{21})^2 & (R'_{21}R'_{32} - R'_{31}R'_{22})^2 \\ (R'_{32}R'_{13} - R'_{12}R'_{33})^2 & (R'_{33}R'_{11} - R'_{13}R'_{31})^2 & (R'_{31}R'_{12} - R'_{11}R'_{32})^2 \\ (R'_{12}R'_{23} - R'_{22}R'_{13})^2 & (R'_{13}R'_{21} - R'_{23}R'_{11})^2 & (R'_{11}R'_{22} - R'_{21}R'_{12})^2 \end{pmatrix} \\ & \qquad \qquad \qquad \Upsilon(\epsilon) \end{aligned} \quad (4.39)$$

Using the fact that the rows and columns of R' are orthonormal,

$$\begin{aligned} \beta \cdot \phi^R(\epsilon) &= -\beta \cdot \begin{pmatrix} (R'_{11})^2 & (R'_{12})^2 & (R'_{13})^2 \\ (R'_{21})^2 & (R'_{22})^2 & (R'_{23})^2 \\ (R'_{31})^2 & (R'_{13})^2 & (R'_{11})^2 \end{pmatrix} \Upsilon(\epsilon) \\ &= -\beta \cdot S(R') \Upsilon(\epsilon) \\ &= -(S(R')^T \beta \cdot \Upsilon(\epsilon)) \\ &= -D\beta \cdot \Upsilon(\epsilon). \end{aligned} \quad (4.40)$$

where $D := (S(R(\epsilon)R))^T$. \square

We are now ready to prove Theorem 4.20:

Proof (of Theorem 4.20).

The existence of $R_*(\beta, \bar{\epsilon}) \in SO(3)$ and $\epsilon_1^*(R_*, \beta, \bar{\epsilon}), \epsilon_2^*(R_*, \beta, \bar{\epsilon}) \in \mathbb{R}_{\text{sym}}^{3 \times 3}$ that extremize (4.13b) follows from the continuity of $SO(3) \times \mathbb{R}_{\text{sym}}^{3 \times 3} \ni (R, \bar{\epsilon}) \mapsto W_\lambda(R, \beta, \bar{\epsilon})$, the convexity for each $R \in SO(3)$ of $W_i - \beta \cdot \phi^R$, and the compactness of $SO(3)$. It remains to show that $R_*^T \Delta \epsilon^* R_*$ is diagonal. From (4.13b) and (4.40),

$$W_\lambda(\beta, \bar{\epsilon}) = \max_{R \in SO(3)} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) + \lambda_1 \lambda_2 S^T(R(\epsilon_2 - \epsilon_1)R)\beta \cdot \gamma(\epsilon_2 - \epsilon_1).$$

Thus

$$W_\lambda(\beta, \bar{\epsilon}) \leq \max_{D \in \text{Range}(S)} \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) + \lambda_1 \lambda_2 D\beta \cdot \gamma(\epsilon_2 - \epsilon_1), \quad (4.41)$$

where the inequality arises since we are replacing $S^T(R(\epsilon_2 - \epsilon_1)R)$ with an arbitrary $D \in \Omega_3$. From Lemma 4.21(1), there exists $D_* \in \mathbb{P}_3$ that maximizes the function

$$\Omega_3 \ni D \mapsto \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) + \lambda_1 \lambda_2 D\beta \cdot \gamma(\epsilon_2 - \epsilon_1).$$

Since, from lemma 4.22(4), $\mathbb{P}_3 \subset \text{Range}(S)$, this implies the existence of $R_* \in SO(3)$ such that $S(R(\Delta \epsilon^*)R_*) = D_*$. Thus the inequality in (4.41) is actually an equality. Further

$$\begin{aligned} S(R(\Delta \epsilon^*)R_*) \in \mathbb{P}_3 &\implies R(\Delta \epsilon^*)R_* \text{ is a signed permutation matrix} \\ &\implies (R(\Delta \epsilon^*)R_*)^T \text{diag}(\Delta \epsilon^*)(R(\Delta \epsilon^*)R_*) \text{ is diagonal} \\ &\implies R_*^T \Delta \epsilon^* R_* \text{ is diagonal} \end{aligned}$$

which completes the proof. \square

Note that, since $R_*^T \Delta \epsilon^* R_*$ is diagonal, for some permutation σ (c.f., (4.5) and (4.4)),

$$\phi^{R_*}(\Delta \epsilon^*) = \phi(R_*^T \Delta \epsilon^* R_*) = -\gamma_\sigma(\Delta \epsilon^*). \quad (4.42)$$

4.8. Explicit expressions for the optimal strains and stresses.

We return to the minimization problem (4.12b) and find the minimizers $\epsilon_1^*(R, \beta, \bar{\epsilon})$ and $\epsilon_2^*(R, \beta, \bar{\epsilon})$.

The expressions in this section can be obtained from those in §3.1.4 by the formal substitution of $\beta \cdot T^R$ for βT , $\beta \in B_{(\alpha_1, \alpha_2)}(R) \setminus \overline{B_{(\alpha_1, \alpha_2), \text{II}^+}(R)}$ for $\beta \in [0, \gamma_{(\alpha_1, \alpha_2)})$ and $\beta \in \overline{B_{(\alpha_1, \alpha_2), \text{II}^+}(R)}$ for $\beta = \gamma_{(\alpha_1, \alpha_2)}$.

By differentiating the argument on the right-hand side of (4.12b),

$$\alpha_1(\epsilon_1^* - \epsilon_1^\top) - \alpha_2(\epsilon_2^* - \epsilon_2^\top) + (\beta \cdot T^R)(\epsilon_2^* - \epsilon_1^*) = 0 \quad (4.43)$$

In other words,

$$\Delta\sigma^* = (\beta \cdot T^R)\Delta\epsilon^* \quad (4.44)$$

where

$$\begin{aligned} \Delta\epsilon^* &:= \epsilon_2^* - \epsilon_1^*, \\ \Delta\sigma^* &:= \sigma_2^* - \sigma_1^*, \\ \sigma_i^* &:= \alpha_i(\epsilon_i^* - \epsilon_i^T), \quad i = 1, 2. \end{aligned}$$

Since $\lambda_1\epsilon_1^* + \lambda_2\epsilon_2^* = \bar{\epsilon}$, (4.43) gives

$$\begin{aligned} (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)\epsilon_1^* &= (\alpha_2 - \beta \cdot T^R)\bar{\epsilon} - \lambda_2\Delta(\alpha\epsilon^T), \\ (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)\epsilon_2^* &= (\alpha_1 - \beta \cdot T^R)\bar{\epsilon} + \lambda_1\Delta(\alpha\epsilon^T), \\ (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)\Delta\epsilon^* &= \Delta(\alpha\epsilon^T) - (\Delta\alpha)\bar{\epsilon}. \end{aligned}$$

where

$$\begin{aligned} \Delta(\alpha\epsilon^T) &:= \alpha_2\epsilon_2^T - \alpha_1\epsilon_1^T, \\ \Delta\alpha &:= \alpha_2 - \alpha_1. \end{aligned}$$

If $\beta \in B_{(\alpha_1, \alpha_2)}(R) \setminus \overline{B_{(\alpha_1, \alpha_2), \text{II}^+}(R)}$, then from §4.4 it follows that $\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R = \lambda_2(\alpha_1 - \beta \cdot T^R) + \lambda_1(\alpha_2 - \beta \cdot T^R)$ is positive definite since it is the sum of two positive definite linear operators. Consequently, we may invert the relations above to conclude that

$$\begin{aligned} \epsilon_1^*(R, \beta, \bar{\epsilon}) &= (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)^{-1} \\ &\quad ((\alpha_2 - \beta \cdot T^R)\bar{\epsilon} - \lambda_2\Delta(\alpha\epsilon^T)), \end{aligned} \quad (4.45a)$$

$$\begin{aligned} \epsilon_2^*(R, \beta, \bar{\epsilon}) &= (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)^{-1} \\ &\quad ((\alpha_1 - \beta \cdot T^R)\bar{\epsilon} + \lambda_1\Delta(\alpha\epsilon^T)), \end{aligned} \quad (4.45b)$$

$$\begin{aligned} \Delta\epsilon^*(R, \beta, \bar{\epsilon}) &= (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)^{-1} \\ &\quad (\Delta(\alpha\epsilon^T) - (\Delta\alpha)\bar{\epsilon}). \end{aligned} \quad (4.45c)$$

If $\beta \in \overline{B_{(\alpha_1, \alpha_2), \text{II}^+}(R)}$, then $\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R$ might only be positive semi-definite. However, the minimization problem (4.12b) is quadratic. So we can have one of two situations: either (1) the minimum is finite and the solutions in (4.45) make sense up to a constant in $\ker(\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)$, or (2) $W_\lambda(R, \beta, \bar{\epsilon}) = -\infty$, in which case,

$$\lim_{\beta' \rightarrow \beta} \beta' \cdot \phi^R(\Delta\epsilon^*) = \infty. \quad (4.46)$$

For future use we observe that for $\beta \in B_{(\alpha_1, \alpha_2)}(R) \setminus \overline{B_{(\alpha_1, \alpha_2), \text{II}^+}(R)}$,

$$\frac{\partial \Delta\epsilon^*}{\partial \beta_i} = (\lambda_2\alpha_1 + \lambda_1\alpha_2 - \beta \cdot T^R)^{-1} T_i^R \Delta\epsilon^*. \quad (4.47)$$

From (4.45) we also calculate, for $\beta \in B_{(\alpha_1, \alpha_2)}(R) \setminus \overline{B_{(\alpha_1, \alpha_2), \Pi^+}(R)}$,

$$\begin{aligned}\sigma_1^* &= \left(\overline{\alpha^{-1}} - \alpha_2^{-1} \beta \cdot T^R \alpha_1^{-1} \right)^{-1} \alpha_2^{-1} \left((\alpha_2 - \beta \cdot T^R) \bar{\epsilon} - \lambda_2 \Delta(\alpha \epsilon^T) \right) - \alpha_1 \epsilon_1^T \\ \sigma_2^* &= \left(\overline{\alpha^{-1}} - \alpha_1^{-1} \beta \cdot T^R \alpha_2^{-1} \right)^{-1} \alpha_1^{-1} \left((\alpha_1 - \beta \cdot T^R) \bar{\epsilon} + \lambda_1 \Delta(\alpha \epsilon^T) \right) - \alpha_2 \epsilon_2^T\end{aligned}$$

where $\overline{\alpha^{-1}} := \lambda_1 \alpha_1^{-1} + \lambda_2 \alpha_2^{-1}$.

4.9. A lower bound on the relaxed energy. II.

We are now in a position to derive an explicit lower bound. Recall (4.13a):

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \max_{\beta \in \cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)} W_\lambda(\beta, \bar{\epsilon})$$

where $W_\lambda(\beta, \bar{\epsilon})$ is given by (4.13b). Determining $\max_{\beta \in \cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)} W_\lambda(\beta, \bar{\epsilon})$ is easy since we have the following lemma.

Lemma 4.24. *For $\beta \in \text{Int}(\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R))$, $\beta \mapsto W_\lambda(\beta, \bar{\epsilon})$ is either constant or strictly concave.*

Proof. From (4.13b),

$$\begin{aligned}\nabla_\beta W_\lambda(\beta, \bar{\epsilon}) &= -\lambda_1 \lambda_2 \phi^{R_\star}(\Delta \epsilon^*(R_\star, \beta, \bar{\epsilon})). \\ \frac{\partial^2}{\partial \beta_j \partial \beta_k} W_\lambda(\beta, \bar{\epsilon}) &= -\lambda_1 \lambda_2 \left\langle T_j^{R_\star} \Delta \epsilon^*(R_\star, \beta, \bar{\epsilon}), \frac{\partial}{\partial \beta_k} \Delta \epsilon^*(R_\star, \beta, \bar{\epsilon}) \right\rangle \\ &= -\lambda_1 \lambda_2 \left\langle T_j^{R_\star} \Delta \epsilon^*(R_\star, \beta, \bar{\epsilon}), (\lambda_2 \alpha_1 + \lambda_1 \alpha_2 - \beta \cdot T^{R_\star})^{-1} T_k^{R_\star} \Delta \epsilon^*(R_\star, \beta, \bar{\epsilon}) \right\rangle \\ &< 0\end{aligned}\tag{4.48}$$

except when $\Delta \epsilon^*(R_\star, \beta, \bar{\epsilon}) = 0$. Note, from (4.45), that $\Delta \epsilon^*(R, \beta, \bar{\epsilon}) = 0$ for some $(R, \beta) \in SO(3) \times B$ implies that $\Delta \epsilon^*(R, \beta, \bar{\epsilon}) = 0$ for all $(R, \beta) \in SO(3) \times B$. However when $\Delta \epsilon^*(\cdot, \cdot, \bar{\epsilon}) \equiv 0$, from (4.48), $W_\lambda(\beta, \bar{\epsilon})$ is independent of β . \square

Incidentally, we also observe that:

Lemma 4.25. $\bar{\epsilon} \mapsto W_\lambda(\beta, \bar{\epsilon})$ is strictly convex.

Proof. From (4.13b),

$$\begin{aligned}
& \frac{\partial^2}{\partial \bar{\epsilon}^2} W_\lambda(\beta, \bar{\epsilon}) \\
&= \lambda_1 \frac{\partial^2}{\partial \bar{\epsilon}^2} (W_1 - \beta \cdot \phi^{R_\star(\beta, \bar{\epsilon})})(\epsilon_1^\star(R_\star, \beta, \bar{\epsilon})) \\
&\quad + \lambda_2 \frac{\partial^2}{\partial \bar{\epsilon}^2} (W_2 - \beta \cdot \phi^{R_\star(\beta, \bar{\epsilon})})(\epsilon_2^\star(R_\star, \beta, \bar{\epsilon})) + \frac{\partial^2}{\partial \bar{\epsilon}^2} \beta \cdot \phi^{R_\star(\beta, \bar{\epsilon})}(\bar{\epsilon}) \\
&= \lambda_1 (\alpha_1 - \beta \cdot T^{R_\star(\beta, \bar{\epsilon})}) + \lambda_2 (\alpha_2 - \beta \cdot T^{R_\star(\beta, \bar{\epsilon})}) + \beta \cdot T^{R_\star(\beta, \bar{\epsilon})} \\
&= \lambda_1 \alpha_1 + \lambda_2 \alpha_2 \\
&> 0
\end{aligned}$$

□

We now obtain the desired lower bound when the elastic moduli are cubic. Recall that we use “ \parallel ” to mean “parallel and not anti-parallel”. For $x \in \mathbb{R}^n$ and $S \subset \mathbb{R}^n$ we say $x \parallel S$ if $\exists y \in S$, $x \parallel y$.

Theorem 4.26 (Lower bound). *Let α_1 and α_2 be cubic. Then*

$$\overline{W}_\lambda(\bar{\epsilon}) \geq \overline{W}_\lambda^l(\bar{\epsilon})$$

where

$$\overline{W}_\lambda^l(\bar{\epsilon}) = \left\{ \begin{array}{ll} W_\lambda(0, \bar{\epsilon}) & \text{if } \Delta \epsilon^\star(\cdot, \cdot, \bar{\epsilon}) \equiv 0 \quad (\text{Regime 0}), \\ W_\lambda(\beta_l, \bar{\epsilon}) & \text{if } \exists \beta_l \in (S_l \cup S_{l\&m})(\kappa_1, \min(\mu_1, \eta_1)) \\ & \quad \cap (S_l \cup S_{l\&m})(\kappa_2, \min(\mu_2, \eta_2)), \\ & \quad 0 \neq -\phi^{R_\star(\beta_l, \bar{\epsilon})}(\Delta \epsilon^\star(R_\star(\beta_l, \bar{\epsilon}), \beta_l, \bar{\epsilon})) \parallel \{-e_1, -e_2, -e_3\} \\ & \quad \quad \quad (\text{Regime I}), \\ W_\lambda(\beta_n, \bar{\epsilon}) & \text{otherwise} \quad (\text{Regime II}), \\ W_\lambda(\beta_m, \bar{\epsilon}) & \text{if } \exists \beta_m \in (S_{l\&m} \cup S_m \cup S_{m\&IV})(\min(\mu_1, \eta_1, \mu_2, \eta_2)), \\ & \quad 0 \neq -\phi^{R_\star(\beta_m, \bar{\epsilon})}(\Delta \epsilon^\star(R_\star(\beta_m, \bar{\epsilon}), \beta_m, \bar{\epsilon})) \parallel \{e_1, e_2, e_3\} \\ & \quad \quad \quad (\text{Regime III}), \\ W_\lambda(\beta_{IV}, \bar{\epsilon}) & \text{if } \exists \beta_{IV} \in S_{m\&IV}(\min(\mu_1, \eta_1, \mu_2, \eta_2)), \\ & \quad 0 \neq -\phi^{R_\star(\beta_{IV}, \bar{\epsilon})}(\Delta \epsilon^\star(R_\star(\beta_{IV}, \bar{\epsilon}), \beta_{IV}, \bar{\epsilon})) \parallel \text{Int}(\mathbb{R}_+^3) \\ & \quad \quad \quad (\text{Regime IV}). \end{array} \right. \quad (4.49)$$

Here, in regime II, β_n is the unique solution of $\phi^{R_\star(\cdot, \bar{\epsilon})}(\Delta \epsilon^\star(R_\star(\cdot, \bar{\epsilon}), \cdot, \bar{\epsilon})) = 0$ in $S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2))$. Note that it is possible that $\beta_n \in (S_{l\&m} \cup S_m \cup S_{m\&IV})(\min(\mu_1, \eta_1, \mu_2, \eta_2))$.

Proof. Since α_1 and α_2 are cubic, from (4.37) we obtain a lower bound for $\overline{W}_\lambda(\bar{\epsilon})$ by replacing $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)$ by $S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2))$ in (4.13a).

When $\Delta\epsilon^*(\beta, \bar{\epsilon}) \equiv 0$, from Lemma 4.24, $\beta \mapsto W_\lambda(\beta, \bar{\epsilon})$ is constant and we may set $\beta = 0$ in (4.13a); this is Regime 0. Otherwise, from Lemma 4.24 $\beta \mapsto W_\lambda(\beta, \bar{\epsilon})$ is strictly concave.

Suppose there exists $\beta_{\text{II}} \in S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2))$ such that $\nabla_\beta W_\lambda(\beta, \bar{\epsilon})|_{\beta=\beta_{\text{II}}} = 0$. Then, by the strict concavity of $\beta \mapsto W_\lambda(\beta, \bar{\epsilon})$, β_{II} maximizes $W_\lambda(\beta, \bar{\epsilon})$ in $S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2))$ and is the unique solution of $\phi^{R_\star(\cdot, \bar{\epsilon})}(\Delta\epsilon^*(R_\star(\cdot, \bar{\epsilon}), \cdot, \bar{\epsilon})) = 0$. This is Regime II.

Otherwise the maximum is attained on $\partial(S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2)))$ at β^* (say). Using (4.48), (4.42) and (4.4), we have

$$\begin{aligned} N(\beta^*) &= \nabla_\beta W_\lambda(\beta, \bar{\epsilon})|_{\beta=\beta^*} \\ &= -\lambda_1 \lambda_2 \phi^{R_\star}(\Delta\epsilon^*(R_\star, \beta^*, \bar{\epsilon})) \\ &= \lambda_1 \lambda_2 \mathcal{Y}_\sigma(\Delta\epsilon^*(R_\star, \beta^*, \bar{\epsilon})) \\ &= \lambda_1 \lambda_2 \begin{pmatrix} v_{\sigma(2)}(\Delta\epsilon^*) & v_{\sigma(3)}(\Delta\epsilon^*) \\ v_{\sigma(3)}(\Delta\epsilon^*) & v_{\sigma(1)}(\Delta\epsilon^*) \\ v_{\sigma(1)}(\Delta\epsilon^*) & v_{\sigma(2)}(\Delta\epsilon^*) \end{pmatrix}. \end{aligned} \quad (4.50)$$

In particular we observe that the components of N are the pairwise product of three numbers. Three cases arise:

1. $\beta^* \in S_1(\kappa_1, \min(\mu_1, \eta_1)) \cap S_1(\kappa_2, \min(\mu_2, \eta_2))$. In this case it is immediate that

$$N(\beta^*) \parallel \{-e_1, -e_2, -e_3\}.$$

Note that this is true even at the edges and the corner of $\partial\mathbb{R}_+^3$ since if one component of N is zero then two components on N must be zero. This is Regime I.

2. $\beta^* \in S_{\text{I&II}}(\min(\mu_1, \eta_1)) \cup S_{\text{I&III}}(\min(\mu_2, \eta_2))$. Since the components of N are pairwise product of three numbers, it not possible that precisely one be (strictly) negative and precisely two be (strictly) positive. Thus, from Corollary 4.19, we conclude that either

$$N(\beta^*) \parallel \{-e_1, -e_2, -e_3\},$$

which is Regime I; or, in fact $\beta^* \in S_{\text{I&III}}(\min(\mu_1, \eta_1, \mu_2, \eta_2))$ and

$$N(\beta^*) \parallel \{e_1, e_2, e_3\},$$

which is Regime III.

3. $\beta^* \notin (S_{\text{I}} \cup S_{\text{I&III}})(\kappa_1, \min(\mu_1, \eta_1)) \cap (S_{\text{I}} \cup S_{\text{I&III}})(\kappa_2, \min(\mu_2, \eta_2))$. Again, since the components of N are pairwise product of three numbers, it not possible that precisely one be (strictly) negative and precisely two be (strictly) positive. Thus, from Corollary 4.19, we conclude that in fact $\beta^* \in (S_{\text{III}} \cup S_{\text{III&IV}})(\min(\mu_1, \eta_1, \mu_2, \eta_2))$ and

$$N(\beta^*) \parallel \begin{cases} \{e_1, e_2, e_3\} & \text{if } \beta^* \in S_{\text{III}}(\min(\mu_1, \eta_1, \mu_2, \eta_2)) \\ \mathbb{R}_+^3 & \text{if } \beta^* \in S_{\text{III&IV}}(\min(\mu_1, \eta_1, \mu_2, \eta_2)). \end{cases}$$

Two sub-cases arise:

- (a) $\beta^* \in (S_{\text{III}} \cup S_{\text{III\&IV}})(\min(\mu_1, \eta_1, \mu_2, \eta_2))$ and $N(\beta^*) \parallel \{e_1, e_2, e_3\}$. This is Regime III.
 (b) $\beta^* \in S_{\text{III\&IV}}(\min(\mu_1, \eta_1, \mu_2, \eta_2))$ and $N(\beta^*) \parallel \text{Int}(\mathbb{R}_+^3)$. This is Regime IV.
 \square

Note 4.27. In particular the proof above shows that,

$$\left(\begin{array}{c} v_{\sigma(2)}(\Delta\epsilon^*) \ v_{\sigma(3)}(\Delta\epsilon^*) \\ v_{\sigma(3)}(\Delta\epsilon^*) \ v_{\sigma(1)}(\Delta\epsilon^*) \\ v_{\sigma(1)}(\Delta\epsilon^*) \ v_{\sigma(2)}(\Delta\epsilon^*) \end{array} \right) \parallel \left\{ \begin{array}{ll} \{-e_1, -e_2, -e_3\} & \text{in Regime I} \\ & (\beta^* \in (S_I \cup S_{\text{I\&III}})(\kappa_1, \min(\mu_1, \eta_1)) \\ & \quad \cap (S_I \cup S_{\text{I\&III}})(\kappa_2, \min(\mu_2, \eta_2))), \\ 0 & \text{in Regime II} \\ & (\beta^* \in S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2))), \\ \{e_1, e_2, e_3\} & \text{in Regime III} \\ & (\beta^* \in (S_{\text{I\&III}} \cup S_{\text{III}} \cup S_{\text{III\&IV}})(\min(\mu_1, \eta_1, \mu_2, \eta_2))), \\ \text{Int}(\mathbb{R}_+^3) & \text{in Regime IV} \\ & (\beta^* \in S_{\text{III\&IV}}(\min(\mu_1, \eta_1, \mu_2, \eta_2))). \end{array} \right. \quad (4.51)$$

The following corollary follows immediately from (4.51).

Corollary 4.28 (Eigenvalues of the optimal strain jump).

1. *In Regime I:* $v_2(\Delta\epsilon^*) = 0$, $v_1(\Delta\epsilon^*)v_3(\Delta\epsilon^*) < 0$.
2. *In Regime II:* $v_2(\Delta\epsilon^*) = 0$, $v_1(\Delta\epsilon^*)v_3(\Delta\epsilon^*) = 0$.
3. *In Regime III:* $v_2(\Delta\epsilon^*) = 0$, $v_1(\Delta\epsilon^*)v_3(\Delta\epsilon^*) > 0$.
4. *In Regime IV:* $v_1(\Delta\epsilon^*)v_3(\Delta\epsilon^*) > 0$. Thus all eigenvalues of $\Delta\epsilon^*$ have the same sign, i.e., $\Delta\epsilon^*$ is either negative- or positive-definite.

The following corollary also follows from the proof of Theorem 4.26.

Corollary 4.29.

1. *In Regime 0,*

$$\overline{W}_\lambda^l(\bar{\epsilon}) = \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{\text{sym}}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2).$$

2. *In Regime I,*

$$\beta_l \cdot \phi^{R*}(\Delta\epsilon^*) = 0. \quad (4.52)$$

3. *In Regime II,*

$$\phi^{R*}(\Delta\epsilon^*) = 0.$$

4. In Regime III,

$$R_\star^T \Delta \epsilon^\star R_\star = \begin{cases} \begin{pmatrix} 0 & 0 & 0 \\ 0 & v_{\sigma(2)}(\Delta \epsilon^\star) & 0 \\ 0 & 0 & v_{\sigma(3)}(\Delta \epsilon^\star) \end{pmatrix} \\ \text{when } \beta_{III} \in (S_{I\&III}^{(1)} \cup S_{III}^{(1)} \cup S_{III\&IV})(\min(\mu_1, \eta_1, \mu_2, \eta_2)), \\ \\ \begin{pmatrix} v_{\sigma(1)}(\Delta \epsilon^\star) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & v_{\sigma(3)}(\Delta \epsilon^\star) \end{pmatrix} \\ \text{when } \beta_{III} \in (S_{I\&III}^{(2)} \cup S_{III}^{(2)} \cup S_{III\&IV})(\min(\mu_1, \eta_1, \mu_2, \eta_2)), \\ \\ \begin{pmatrix} v_{\sigma(1)}(\Delta \epsilon^\star) & 0 & 0 \\ 0 & v_{\sigma(2)}(\Delta \epsilon^\star) & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \text{when } \beta_{III} \in (S_{I\&III}^{(3)} \cup S_{III}^{(3)} \cup S_{III\&IV})(\min(\mu_1, \eta_1, \mu_2, \eta_2)). \end{cases} \quad (4.53)$$

5. In Regime III when $\beta_{III} \in S_{III\&IV}$ and in Regime IV, from Note 4.1,

$$\overline{W}_\lambda^l(\bar{\epsilon}) = \min_{\substack{\epsilon_1, \epsilon_2 \in \mathbb{R}_{sym}^{3 \times 3} \\ \lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}}} \lambda_1 W_1(\epsilon_1) + \lambda_2 W_2(\epsilon_2) - 2\lambda_1 \lambda_2 \min(\mu_1, \eta_1, \mu_2, \eta_2) e \cdot \phi(\epsilon_2 - \epsilon_1).$$

Note 4.30. From (4.46), Regimes III and IV do not occur whenever

$$\phi_j^{R_\star(\beta_{II+}, \bar{\epsilon})}(\Delta \epsilon^\star(R_\star(\beta_{II+}, \bar{\epsilon}), \beta_{II+}, \bar{\epsilon}))$$

does not exist. From §4.8 this happens when

$$\ker(\alpha_1 - \beta_{II+} \cdot T^{R_\star(\beta_{II+}, \bar{\epsilon})}) \cap \ker(\alpha_2 - \beta_{II+} \cdot T^{R_\star(\beta_{II+}, \bar{\epsilon})}) \neq \{0\}.$$

This includes, in particular, the cases (i) $\alpha_1 = \alpha_2$ (c.f., Note 4.31 below) and (ii) both phases being cubic with the smaller shear moduli being equal.

Note 4.31 (Equal moduli). We remark on the special case $\alpha_1 = \alpha_2 \equiv \alpha$ studied by Pipkin [Pip91] and Kohn [Koh91]. In this case, $\lambda_2 \alpha_1 + \lambda_1 \alpha_2 - \beta \cdot T^{R_\star} = \alpha - \beta \cdot T^{R_\star}$ is not invertible when $\beta \in \overline{S_{II+}(\kappa, \mu)}$. Thus, as mentioned in Note 4.30 above, Regime III does not occur.

From (4.45), $\Delta \epsilon^\star(\cdot, \cdot, \bar{\epsilon}) \equiv 0$ implies that $\epsilon_1^\top = \epsilon_2^\top$. Thus Regime 0 does not occur for distinct materials.⁵

From (4.13b), (4.49) and (4.52) we obtain

$$\overline{W}_\lambda(\bar{\epsilon}) = \begin{cases} \lambda_1 W_1(\epsilon_1^\star(R_\star(\beta_I, \bar{\epsilon}), \beta_I, \bar{\epsilon})) + \lambda_2 W_2(\epsilon_2^\star(R_\star(\beta_I, \bar{\epsilon}), \beta_I, \bar{\epsilon})) & \text{in Regime I,} \\ \lambda_1 W_1(\epsilon_1^\star(R_\star(\beta_{II}, \bar{\epsilon}), \beta_{II}, \bar{\epsilon})) + \lambda_2 W_2(\epsilon_2^\star(R_\star(\beta_{II}, \bar{\epsilon}), \beta_{II}, \bar{\epsilon})) & \text{in Regime II.} \end{cases}$$

⁵I.e., when either $\alpha_1 \neq \alpha_2$ or $\epsilon_1^\top \neq \epsilon_2^\top$.

Here, from (4.45),

$$\epsilon_1^*(R, \beta, \bar{\epsilon}) = \bar{\epsilon} - \lambda_2(\alpha - \beta \cdot T^R)^{-1} \alpha \Delta \epsilon^\tau, \quad (4.54a)$$

$$\epsilon_2^*(R, \beta, \bar{\epsilon}) = \bar{\epsilon} + \lambda_1(\alpha - \beta \cdot T^R)^{-1} \alpha \Delta \epsilon^\tau, \quad (4.54b)$$

$$\Delta \epsilon^*(R, \beta, \bar{\epsilon}) = (\alpha - \beta \cdot T^R)^{-1} \alpha \Delta \epsilon^\tau. \quad (4.54c)$$

From (4.54c) $\Delta \epsilon^*$ is independent of $\bar{\epsilon}$. From the proof of Theorem 4.20 it follows that R_* is also independent of $\bar{\epsilon}$.

From (4.49) and (4.54) Regime I occurs when

$$\begin{aligned} \exists \beta_I \in S(\kappa_1, \min(\mu_1, \eta_1)) \cap S(\kappa_2, \min(\mu_2, \eta_2)) \cap \partial \mathbb{R}_+^3, \\ 0 \neq \phi^{R_*(\beta_I)} \left((\alpha - \beta_I \cdot T^{R_*(\beta_I)})^{-1} \alpha \Delta \epsilon^\tau \right) \parallel \{e_1, e_2, e_3\}; \end{aligned} \quad (4.55)$$

and Regime II when

$$\exists! \beta_{II} \in S(\kappa, \min(\mu, \eta)), \phi \left((\alpha - \beta \cdot T^{R_*(\beta_{II})})^{-1} \alpha (\Delta \epsilon^\tau) \right) = 0 \quad (4.56)$$

($\kappa := \kappa_1 = \kappa_2$, $\mu := \mu_1 = \mu_2$ and $\eta := \eta_1 = \eta_2$). Note that β_{II} is independent of $\bar{\epsilon}$.

From (4.54),

$$\begin{aligned} \epsilon_1^*(R, \beta, \bar{\epsilon}) - \epsilon_1^\tau &= (\bar{\epsilon} - \bar{\epsilon}^\tau) - \lambda_2(\alpha - \beta \cdot T^R)^{-1} \beta \cdot T^R \Delta \epsilon^\tau, \\ \epsilon_2^*(R, \beta, \bar{\epsilon}) - \epsilon_2^\tau &= (\bar{\epsilon} - \bar{\epsilon}^\tau) + \lambda_1(\alpha - \beta \cdot T^R)^{-1} \beta \cdot T^R \Delta \epsilon^\tau, \end{aligned}$$

where $\bar{\epsilon}^\tau := \lambda_1 \epsilon_1^\tau + \lambda_2 \epsilon_2^\tau$. Thus

$$\begin{aligned} \overline{W}_\lambda^l(\bar{\epsilon}) &= \frac{1}{2} \langle \alpha(\bar{\epsilon} - \bar{\epsilon}^\tau), (\bar{\epsilon} - \bar{\epsilon}^\tau) \rangle + (\lambda_1 w_1 + \lambda_2 w_2) \\ &+ \begin{cases} \frac{1}{2} \lambda_1 \lambda_2 \|\alpha^{\frac{1}{2}} (\alpha - \beta_I \cdot T^{R_*(\beta_I)})^{-1} \beta_I \cdot T \Delta \epsilon^\tau\|^2 & \text{if (4.55) holds} \\ & \text{(Regime I),} \\ \frac{1}{2} \lambda_1 \lambda_2 \|\alpha^{\frac{1}{2}} (\alpha - \beta_{II} \cdot T^{R_*(\beta_{II})})^{-1} \beta_{II} \cdot T \Delta \epsilon^\tau\|^2 & \text{otherwise, i.e., if (4.56) holds} \\ & \text{(Regime II).} \end{cases} \end{aligned}$$

4.10. Optimality of the lower bound and optimal microstructures

In this section we prove that the lower bound presented in Theorem 4.26 is optimal in Regimes 0 to III when the elastic moduli are cubic, and in Regime IV when the elastic moduli are isotropic. Further we characterize the optimal microstructures. This will complete the proof of Theorem 2.2. Our strategy is the same as in §3.2.

The proof of Theorem 2.3 is almost identical to that of Theorem 2.2 and is thus omitted.

4.10.1. Optimality of the lower bound. We have the following results:

Theorem 4.32 (Optimality of the lower bound). *Let α_1 and α_2 be cubic. Assume, renumbering if necessary, that $\gamma_{\alpha_1} \leq \gamma_{\alpha_2}$. Then $\bar{W}_\lambda(\bar{\epsilon}) = \bar{W}_\lambda^l(\bar{\epsilon})$ in Regimes 0 to III, and in Regime IV when $\mu_1 = \eta_1$.*

Proof. For regimes 0, I and II, the proof is almost identical to the proof of Theorem 3.10 with the following changes: In Regime 0 we use (4.45) instead of (3.9); in Regimes I and II we use Corollary 4.28 in addition to Lemma 3.11.

In Regimes III and IV, from Corollary 4.28 and Lemma 3.11 we cannot construct a continuous displacement field with the optimal strains. However one of the translated energies loses strict convexity in these Regimes (c.f., §4.4 and Lemma 4.14); we can use this to construct optimal rank-two and rank-three laminates. Assume, renumbering if necessary, that $\gamma_{\alpha_1} \leq \gamma_{\alpha_2}$. Then $\alpha_1 - \beta^* \cdot T^{R^*}$ is degenerate in Regimes III and IV.

Regime III: Let $P_j: \mathbb{R}_{\text{sym}}^{3 \times 3} \rightarrow \mathbb{R}_{\text{sym}}^{2 \times 2}$, $j = 1, 2, 3$, be the projections and $I_j: \mathbb{R}_{\text{sym}}^{2 \times 2} \rightarrow \mathbb{R}_{\text{sym}}^{3 \times 3}$, $j = 1, 2, 3$, be the imbeddings defined by

$$\begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{12} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{13} & \epsilon_{23} & \epsilon_{33} \end{pmatrix} \xrightarrow{P_1} \begin{pmatrix} \epsilon_{22} & \epsilon_{23} \\ \epsilon_{23} & \epsilon_{33} \end{pmatrix} \xrightarrow{I_1} \begin{pmatrix} 0 & 0 & 0 \\ 0 & \epsilon_{22} & \epsilon_{23} \\ 0 & \epsilon_{23} & \epsilon_{33} \end{pmatrix}, \quad (4.57a)$$

$$\begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{12} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{13} & \epsilon_{23} & \epsilon_{33} \end{pmatrix} \xrightarrow{P_2} \begin{pmatrix} \epsilon_{11} & \epsilon_{13} \\ \epsilon_{13} & \epsilon_{33} \end{pmatrix} \xrightarrow{I_2} \begin{pmatrix} \epsilon_{11} & 0 & \epsilon_{13} \\ 0 & 0 & 0 \\ \epsilon_{13} & 0 & \epsilon_{33} \end{pmatrix}, \quad (4.57b)$$

$$\begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{12} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{13} & \epsilon_{23} & \epsilon_{33} \end{pmatrix} \xrightarrow{P_3} \begin{pmatrix} \epsilon_{11} & \epsilon_{12} \\ \epsilon_{12} & \epsilon_{22} \end{pmatrix} \xrightarrow{I_3} \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & 0 \\ \epsilon_{12} & \epsilon_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (4.57c)$$

Note that these mappings preserve rank-one-ness and symmetrized rank-one-ness. Let $J \in \{1, 2, 3\}$ such that $\beta_{\text{III}} \in (S_{\text{I\&III}}^{(J)} \cup S_{\text{III}}^{(J)} \cup S_{\text{III\&IV}})(\min(\mu_1, \eta_1))$. From (4.53),

$$P_J(R_\star^T \Delta \epsilon^* R_\star) = \begin{cases} \begin{pmatrix} v_{\sigma(2)}(\Delta \epsilon^*) & 0 \\ 0 & v_{\sigma(3)}(\Delta \epsilon^*) \end{pmatrix} & \text{if } J = 1, \\ \begin{pmatrix} v_{\sigma(1)}(\Delta \epsilon^*) & 0 \\ 0 & v_{\sigma(3)}(\Delta \epsilon^*) \end{pmatrix} & \text{if } J = 2, \\ \begin{pmatrix} v_{\sigma(1)}(\Delta \epsilon^*) & 0 \\ 0 & v_{\sigma(2)}(\Delta \epsilon^*) \end{pmatrix} & \text{if } J = 3; \end{cases} \quad (4.58)$$

and from Corollary 4.28(3),

$$\det(P_J(R_\star^T \Delta \epsilon^* R_\star)) > 0. \quad (4.59)$$

From (4.58), (4.59) and the proof of Theorem 3.10, for every choice

$$\epsilon_n \in P_J(R_\star^T \ker(\alpha_1 - \beta_{\text{III}} \cdot T^{R^*}) R_\star),$$

there exist two rank-two laminates (χ_1, χ_2) in \mathbb{R}^2 of the form described in the proof of Theorem 3.10. Likewise there exists two displacement fields u in \mathbb{R}^2 with corresponding strains in $\mathbb{R}_{\text{sym}}^{2 \times 2}$ (schematically represented in Figure 3.1(b) with ϵ_1^*

and ϵ_2^* replaced by $P_J(R_\star^T \epsilon_1^* R_\star)$ and $P_J(R_\star^T \epsilon_2^* R_\star)$, respectively). These rank-two laminates, the displacement fields and the corresponding strain fields can each be imbedded in \mathbb{R}^3 , \mathbb{R}^3 and $\mathbb{R}_{\text{sym}}^{3 \times 3}$, respectively, using the imbeddings

$$\begin{aligned} (\chi_1, \chi_2)(x_1, x_2, x_3) &\leftarrow \begin{cases} (\chi_1, \chi_2)(x_2, x_3) & \text{if } J = 1, \\ (\chi_1, \chi_2)(x_1, x_3) & \text{if } J = 2, \\ (\chi_1, \chi_2)(x_1, x_2) & \text{if } J = 3; \end{cases} \\ u(x_1, x_2, x_3) &\leftarrow \begin{cases} ((\epsilon_1^*)_{11}, (\epsilon_1^*)_{12}, (\epsilon_1^*)_{13})^T \cdot x + u(x_2, x_3) & \text{if } J = 1, \\ ((\epsilon_1^*)_{21}, (\epsilon_1^*)_{22}, (\epsilon_1^*)_{23})^T \cdot x + u(x_1, x_2) & \text{if } J = 2, \\ ((\epsilon_1^*)_{31}, (\epsilon_1^*)_{32}, (\epsilon_1^*)_{33})^T \cdot x + u(x_1, x_2) & \text{if } J = 3; \end{cases} \\ \epsilon &\mapsto R_\star^T \epsilon_1^* R_\star - I_J P_J(R_\star^T \epsilon_1^* R_\star) + I_J \epsilon \end{aligned}$$

respectively. The resulting microstructure and displacement field shows that the lower bound (4.49) is optimal in Regime III. Examples 4.33 and 4.34 below illustrate this construction.

Regime IV when $\mu_1 = \eta_1$: Since $\mu_1 = \eta_1$, α_1 is isotropic. Recall that

$$\Delta \epsilon^* = R(\Delta \epsilon^*) \text{Diag} \begin{pmatrix} v_{\sigma(1)}(\Delta \epsilon^*) \\ v_{\sigma(2)}(\Delta \epsilon^*) \\ v_{\sigma(3)}(\Delta \epsilon^*) \end{pmatrix} R^T(\Delta \epsilon^*).$$

Let

$$\begin{aligned} \epsilon^I &:= \text{Diag} \begin{pmatrix} v_{\sigma(1)}(\Delta \epsilon^*) + v_{\sigma(2)}(\Delta \epsilon^*) + v_{\sigma(3)}(\Delta \epsilon^*) \\ 0 \\ 0 \end{pmatrix}, \\ \epsilon^{II} &:= \text{Diag} \begin{pmatrix} \lambda_1 v_{\sigma(1)}(\Delta \epsilon^*) \\ \lambda_2 v_{\sigma(1)}(\Delta \epsilon^*) + v_{\sigma(2)}(\Delta \epsilon^*) + v_{\sigma(3)}(\Delta \epsilon^*) \\ 0 \end{pmatrix}, \\ \epsilon^{III} &:= \text{Diag} \begin{pmatrix} \lambda_1 v_{\sigma(1)}(\Delta \epsilon^*) \\ \lambda_1 v_{\sigma(2)}(\Delta \epsilon^*) \\ \lambda_2 v_{\sigma(1)}(\Delta \epsilon^*) + \lambda_2 v_{\sigma(2)}(\Delta \epsilon^*) + v_{\sigma(3)}(\Delta \epsilon^*) \end{pmatrix}. \end{aligned}$$

Note that

$$\epsilon^I, \epsilon^{II}, \epsilon^{III} \in \text{Diag} \begin{pmatrix} v_{\sigma(1)}(\Delta \epsilon^*) \\ v_{\sigma(2)}(\Delta \epsilon^*) \\ v_{\sigma(3)}(\Delta \epsilon^*) \end{pmatrix} + \text{Span} \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}, \quad (4.60)$$

and, from Lemma 4.8,

$$R(\Delta \epsilon^*) \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\} R^T(\Delta \epsilon^*) \subsetneq \ker(\alpha_1 - 2\mu_1 \cdot T^{R_\star}).$$

Let

$$\begin{aligned}\rho^I &:= \frac{\lambda_1 v_{\sigma(1)}(\Delta\epsilon^*)}{v_{\sigma(1)}(\Delta\epsilon^*) + v_{\sigma(2)}(\Delta\epsilon^*) + v_{\sigma(3)}(\Delta\epsilon^*)}, \\ \rho^{II} &:= \frac{\lambda_1 v_{\sigma(2)}(\Delta\epsilon^*)}{\lambda_2 v_{\sigma(1)}(\Delta\epsilon^*) + v_{\sigma(2)}(\Delta\epsilon^*) + v_{\sigma(3)}(\Delta\epsilon^*)}, \\ \rho^{III} &:= \frac{\lambda_1 v_{\sigma(3)}(\Delta\epsilon^*)}{\lambda_2 v_{\sigma(1)}(\Delta\epsilon^*) + \lambda_2 v_{\sigma(2)}(\Delta\epsilon^*) + v_{\sigma(3)}(\Delta\epsilon^*)}.\end{aligned}$$

Clearly $\rho^I, \rho^{II}, \rho^{III} \in (0, 1)$. It is easy to verify that

$$\epsilon^I \parallel e_1 \otimes e_1, \quad (4.61a)$$

$$\epsilon^{II} - \rho^I \epsilon^I \parallel e_2 \otimes e_2, \quad (4.61b)$$

$$\epsilon^{III} - ((1 - \rho^{II})\rho^I \epsilon^I + \rho^{II} \epsilon^{II}) \parallel e_3 \otimes e_3. \quad (4.61c)$$

Further,

$$(1 - \rho^{III})((1 - \rho^{II})\rho^I \epsilon^I + \rho^{II} \epsilon^{II}) + \rho^{III} \epsilon^{III} = \lambda_1 \text{Diag} \begin{pmatrix} v_{\sigma(1)}(\Delta\epsilon^*) \\ v_{\sigma(2)}(\Delta\epsilon^*) \\ v_{\sigma(3)}(\Delta\epsilon^*) \end{pmatrix}. \quad (4.62)$$

We can now construct our rank-three laminate as follows. First construct a rank-one laminate in which phases 2 and 1 have phase fractions $1 - \rho^I$ and ρ^I respectively and the layers have normal $R(\Delta\epsilon^*)e_1$. Next construct a rank-two laminate in which this rank-one laminate and phase 1 have phase fractions $1 - \rho^{II}$ and ρ^{II} respectively and the layers have normal $R(\Delta\epsilon^*)e_2$. Finally construct a rank-three laminate in which this rank-two laminate and phase 1 have phase fractions $1 - \rho^{III}$ and ρ^{III} respectively and the layers have normal $R(\Delta\epsilon^*)e_3$.

The compatibility equations (4.61) allow the construction of a continuous displacement field u (up to boundary layers) such that the strains take the value $\epsilon_1^* - R(\Delta\epsilon^*)\epsilon^I R^T(\Delta\epsilon^*)$ in the interior phase 1, $\epsilon_1^* - R(\Delta\epsilon^*)\epsilon^{II} R^T(\Delta\epsilon^*)$ in the middle phase 1, $\epsilon_1^* - R(\Delta\epsilon^*)\epsilon^{III} R^T(\Delta\epsilon^*)$ in the exterior phase 1 and ϵ_2^* in phase 2. For this microstructure and displacement field, the average strain is $\bar{\epsilon}$ (c.f., (4.62)) and $W_\chi(u) = \bar{W}_\chi^l(\bar{\epsilon})$ (as the reader can verify). This shows that the lower bound (4.49) is optimal in Regime IV for isotropic α_1 .

(It is easy to see that similar rank-three laminates exist for five other choices of $\epsilon^I, \epsilon^{II}$ and ϵ^{III} in (4.60).) \square

When α_1 is isotropic, the next two examples illustrate the construction of rank-two laminates described in the proof of Theorem 4.32 (Regime III). For simplicity the figures are drawn for a specific choice of σ .

Example 4.33. When α_1 is isotropic, from Lemma 4.8 we can pick $\epsilon_n = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The analogues of Figure 3.1(b) are shown in Figure 4.3 for this choice of ϵ_n . The rank-one cone at the origin (in the space of diagonal 2×2 matrices) is the union of the axes (i.e., $\text{Span}\{\text{Diag}(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix})\} \cup \text{Span}\{\text{Diag}(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix})\}$). The shaded quadrants form

the symmetrized-rank-one cone at the origin (in the space of diagonal 2×2 matrices). It is easy to verify that (3.20) is satisfied. In particular for the rank-two laminate shown in Figure 4.3(a), (3.20b) is

$$\frac{\lambda_1 - \rho}{\lambda_1(1 - \rho)} \text{Diag} \left(\begin{pmatrix} \rho(v_1+v_2) \\ (1-\rho)(v_1+v_2) \end{pmatrix} \right) + \frac{\rho\lambda_2}{\lambda_1(1 - \rho)} \text{Diag} \left(\begin{pmatrix} v_1+v_2 \\ 0 \end{pmatrix} \right) = \text{Diag} \left(\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \right),$$

which implies that $\rho = \lambda_1 \frac{v_1}{v_1+v_2}$; for the rank-two laminate shown in Figure 4.3(b), (3.20b) is

$$\frac{\lambda_1 - \rho}{\lambda_1(1 - \rho)} \text{Diag} \left(\begin{pmatrix} (1-\rho)(v_1+v_2) \\ \rho(v_1+v_2) \end{pmatrix} \right) + \frac{\rho\lambda_2}{\lambda_1(1 - \rho)} \text{Diag} \left(\begin{pmatrix} 0 \\ v_1+v_2 \end{pmatrix} \right) = \text{Diag} \left(\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \right),$$

which implies that $\rho = \lambda_1 \frac{v_2}{v_1+v_2}$.

Example 4.34. When α_1 is isotropic, from Lemma 4.8 we can pick $\epsilon_n = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. The analogues of Figure 3.1(b) are shown in Figure 4.4 for this choice of ϵ_n . The matrices

$$\begin{pmatrix} \frac{v_1}{\sqrt{v_1 v_2}} & \sqrt{\frac{v_1 v_2}{v_2}} \\ \sqrt{\frac{v_1 v_2}{v_2}} & v_2 \end{pmatrix}, \quad \begin{pmatrix} \frac{v_1}{-\sqrt{v_1 v_2}} & -\sqrt{\frac{v_1 v_2}{v_2}} \\ -\sqrt{\frac{v_1 v_2}{v_2}} & v_2 \end{pmatrix}$$

are rank-one. The rank-one cone at the origin in the plane of the figure, i.e., in

$$\text{Span} \left\{ \begin{pmatrix} \frac{v_1}{\sqrt{v_1 v_2}} & \sqrt{\frac{v_1 v_2}{v_2}} \\ \sqrt{\frac{v_1 v_2}{v_2}} & v_2 \end{pmatrix}, \begin{pmatrix} \frac{v_1}{-\sqrt{v_1 v_2}} & -\sqrt{\frac{v_1 v_2}{v_2}} \\ -\sqrt{\frac{v_1 v_2}{v_2}} & v_2 \end{pmatrix} \right\},$$

is the union of the axes, i.e.,

$$\text{Span} \left\{ \begin{pmatrix} \frac{v_1}{\sqrt{v_1 v_2}} & \sqrt{\frac{v_1 v_2}{v_2}} \\ \sqrt{\frac{v_1 v_2}{v_2}} & v_2 \end{pmatrix} \right\} \cup \text{Span} \left\{ \begin{pmatrix} \frac{v_1}{-\sqrt{v_1 v_2}} & -\sqrt{\frac{v_1 v_2}{v_2}} \\ -\sqrt{\frac{v_1 v_2}{v_2}} & v_2 \end{pmatrix} \right\}.$$

The shaded quadrants form the symmetrized-rank-one cone at the origin (in the plane of the figure). It is easy to verify that (3.20) is satisfied. In particular, enforcing (3.20e), we obtain $\rho = \frac{\lambda_1}{2}$.

Note 4.35. Since $P_i, I_i, i = 1, 2, 3$ defined in (4.57) preserve rank-one-ness and symmetrized rank-one-ness the rank-two and rank-three laminates constructed in the proof of Theorem 4.32 (and in Examples 4.33 and 4.34) also use only rank-one connections. As in two dimensions (c.f., Note 3.13) this is in fact necessary.

To see this, first we observe that in Regimes III and IV at any interface the strain difference $[\![\epsilon]\!]$ is related to the stress difference $[\![\sigma]\!]$ through

$$[\![\sigma]\!] \parallel \beta^* \cdot T^{R*}([\![\epsilon]\!]) \quad (4.63a)$$

and the constant of proportionality is non-zero (c.f., (4.44) and recall that $\alpha_1 \epsilon_n = \beta^* \cdot T^{R*} \epsilon_n$). As before, at any interface with normal $\hat{n} \in \mathbb{R}^3$ we require

$$([\![\sigma]\!])\hat{n} = 0, \quad (4.63b)$$

$$[\![\epsilon]\!] \parallel \hat{m} \otimes_s \hat{n}, \quad (4.63c)$$

for some $\hat{m} \in \mathbb{R}^3$. The following lemma, which is the three-dimensional analogue of Lemma 3.14 shows that (4.63) is equivalent to requiring that $[\![\epsilon]\!] \parallel \hat{n} \otimes \hat{n}$.

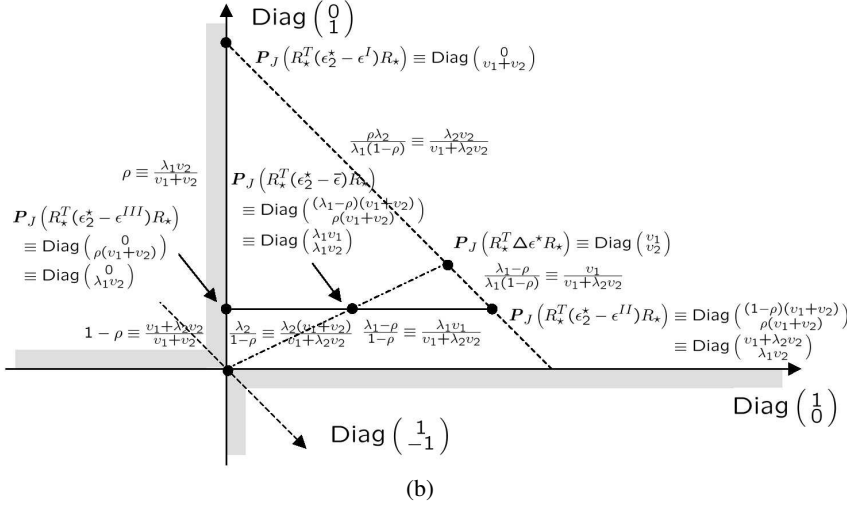
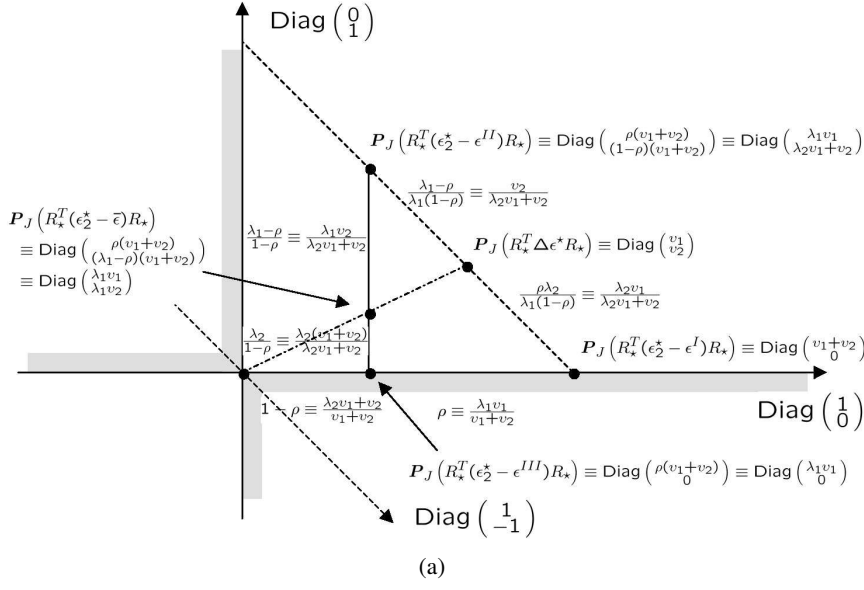
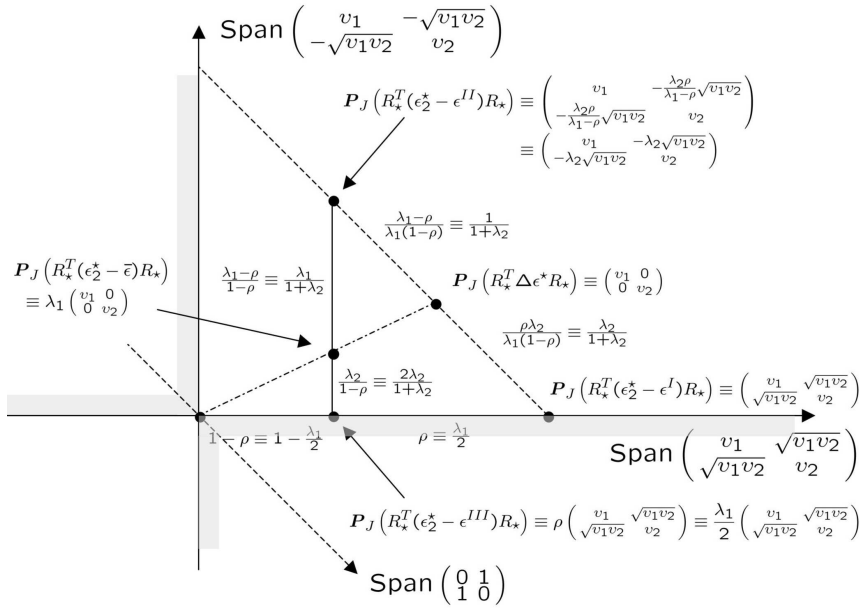


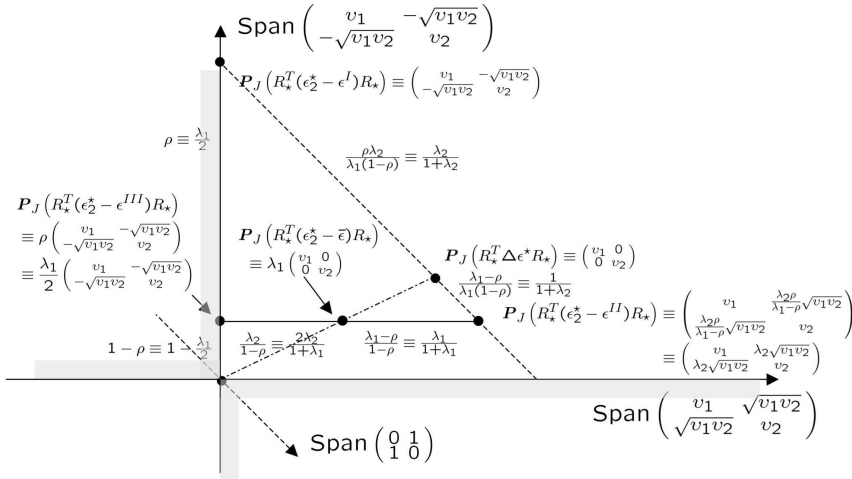
Fig. 4.3. Two optimal rank-two laminates in Regime III (c.f. proof of Theorem 4.32 and Example 4.33).

Lemma 4.36. Let $\hat{m}, \hat{n} \in \mathbb{R}^3$, $\beta \in \mathbb{R}_+^3$ and $\beta \cdot T(\hat{m} \otimes_s \hat{n}) \neq 0$. Then the following are equivalent.

1. $(\beta \cdot T(\hat{m} \otimes_s \hat{n})) \hat{m} = 0$.
2. $(\beta \cdot T(\hat{m} \otimes_s \hat{n})) \hat{n} = 0$.
3. $\hat{m} \parallel \hat{n}$.



(a)



(b)

Fig. 4.4. Two optimal rank-two laminates in Regime III (c.f. proof of Theorem 4.32 and Example 4.34).

Proof. The equivalence of the first two statements is trivial. Simple calculations show that

$$(\beta \cdot T(\hat{m} \otimes_s \hat{n})) \hat{m} \parallel ((\beta \cdot T)(\hat{m} \otimes \hat{m})) \hat{n},$$

$$\ker((\beta \cdot T)(\hat{m} \otimes \hat{m})) = \text{Span} \{ \hat{m} \}.$$

It immediately follows that $(\beta \cdot T(\hat{m} \otimes_s \hat{n})) \hat{m} = 0 \iff \hat{m} \parallel \hat{n}$. \square

4.10.2. Optimal microstructures. It is clear that Theorem 3.15 holds in three dimensions as well.

Theorem 4.37 (Optimal microstructures). *Assume, renumbering if necessary, that $2 \min(\mu_1, \eta_1) = \gamma_{\alpha_1} \leq \gamma_{\alpha_2}$. Also let*

$$D_{III} := \begin{cases} 1 & \text{if } \mu_1 \neq \eta_1, \\ 2 & \text{if } \mu_1 = \eta_1; \end{cases} \quad D_{IV} := \begin{cases} 2 & \text{if } \mu_1 < \eta_1, \\ 5 & \text{if } \mu_1 = \eta_1, \\ 3 & \text{if } \mu_1 > \eta_1. \end{cases}$$

1. *In Regime 0 any microstructure is optimal. The optimal strain and stress are constant.*
2. *In Regime I the optimal microstructure is either a rank-one laminate, with either of two possible layering directions, or a microstructure made up of these laminates. The optimal strain takes the value ϵ_1^* in phase 1 and ϵ_2^* in phase 2 while the optimal stress is constant.*
3. *In Regime II the optimal microstructure is unique and is a rank-one laminate. The optimal strain takes the value ϵ_1^* in phase 1 and ϵ_2^* in phase 2.*
4. *In Regime III, no rank-one laminate is optimal. The class of optimal microstructures is possibly large (in a sense explained in the proof) and includes at least two rank-two laminates.*

In any optimal microstructure, in phase i , $i = 1, 2$, the strain is confined to an affine subspace of dimension

$$\dim \ker(\alpha_i - \beta_{III} \cdot T^{R_*}) \leq \begin{cases} D_{III} & \text{if } \beta^* < 2 \min(\mu_1, \eta_1), \\ D_{IV} & \text{if } \beta^* = 2 \min(\mu_1, \eta_1); \end{cases}$$

the sum of the dimensions of the affine subspaces is at most

$$\begin{cases} 2 & \text{if } \beta^* < 2 \min(\mu_1, \eta_1), \\ 5 & \text{if } \beta^* = 2 \min(\mu_1, \eta_1). \end{cases}$$

In particular, if phase i is harder than the other phase (i.e., if $\gamma_{\alpha_i} > \gamma_{(\alpha_1, \alpha_2)}$) then the strain is ϵ_i^ in that phase.*

5. *In Regime IV: If $\mu_1 = \eta_1$ then there exists an optimal rank-three laminate; otherwise the lower bound is possibly non-optimal. Whenever the bound is optimal:*
 - (a) *No rank-one laminate is optimal.*
 - (b) *If one phase is harder than the other (i.e., if $\gamma_{\alpha_2} > \gamma_{\alpha_1}$) then no rank-two laminate is optimal.*

(c) In any optimal microstructure the strain in each phase is confined to an affine subspace of dimension at most $\dim \ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)} T) \leq D_{IV}$; the sum of the dimension of the two affine subspaces is at most 5. Moreover, if one phase is harder than the other then the strain in the harder phase is constant.

Proof. The proof for the statement pertaining to Regime 0 remains unchanged except that (4.44) is used instead of (3.8).

In Regime I, from Corollary 4.28, $v_2(\Delta\epsilon^*) = 0$ and $v_1(\Delta\epsilon^*)v_3(\Delta\epsilon^*) < 0$. Thus from Lemma 3.11, we find $\hat{m} \nparallel \hat{n} \in \mathbb{R}^3$ such that $\Delta\epsilon^* \parallel \hat{n} \otimes_s \hat{n}$. It follows that the strain and thus the microstructure is either of two rank-one laminates (with layering direction \hat{m} or \hat{n}) or a microstructure of these laminates. Finally from (4.52) and (4.44), $\Delta\sigma^* = 0$: the stress is constant.

In Regime II, from Corollary 4.28, $v_2(\Delta\epsilon^*) = 0$ and $v_1(\Delta\epsilon^*)v_3(\Delta\epsilon^*) = 0$ so that from Lemma 3.11, we find unique (upto scaling) $\hat{n} \in \mathbb{R}^3$ such that $\Delta\epsilon^* \parallel \hat{n} \otimes \hat{n}$. It follows that the strain and thus the microstructure is a unique rank-one laminate with layering direction \hat{n} .

The proof for the statement pertaining to Regime III remains unchanged except that $\ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)} T)$ must be replaced as indicated. The inequalities follows from Corollary 4.15, Lemma 4.17, Note 4.3 and Note 4.30.

We turn to Regime IV. If, when one phase is harder than another, in any optimal microstructure the strain is constant in the harder phase, then the non-existence of optimal rank-two laminates follows from Lemma 4.38 below. The rest of the statement follows by a reasoning almost identical to that for Regime III; that $\sum_{i=1}^2 \dim \ker(\alpha_i - \gamma_{(\alpha_1, \alpha_2)} T) \leq 5$ follows from Notes 4.3 and 4.30. \square

Lemma 4.38. *Let $n \geq 3$. Let ϵ (viewed as a linear operator on \mathbb{R}^n) be either negative- or positive-definite. Then ϵ and 0 cannot form the two rank-two laminates schematically shown in Figures 4.5 and 4.6. I.e., neither the following*

$$\exists \mu \in (0, 1), \exists \epsilon', \epsilon'' \in \mathbb{R}_{sym}^{n \times n}, \mu\epsilon' + (1 - \mu)\epsilon'' = \epsilon, \quad (4.64a)$$

$$\exists \hat{m}', \hat{n}' \in \mathbb{R}^n, \quad \epsilon' = \hat{m}' \otimes_s \hat{n}', \quad (4.64b)$$

$$\exists \rho \in (0, 1), \exists \hat{m}, \hat{n} \in \mathbb{R}^n, \quad \rho\epsilon' - \epsilon'' = \hat{m} \otimes_s \hat{n} \quad (4.64c)$$

nor the following

$$\exists \mu \in (0, 1), \exists \epsilon', \epsilon'' \in \mathbb{R}_{sym}^{n \times n}, \mu\epsilon' + (1 - \mu)\epsilon'' = \epsilon, \quad (4.65a)$$

$$\exists \hat{m}', \hat{n}' \in \mathbb{R}^n, \quad \epsilon' = \hat{m}' \otimes_s \hat{n}', \quad (4.65b)$$

$$\exists \hat{m}'', \hat{n}'' \in \mathbb{R}^n, \quad \epsilon'' = \hat{m}'' \otimes_s \hat{n}'' \quad (4.65c)$$

can hold.

Proof. Assume on the contrary that either (4.64) or (4.65) holds. Either of these, along with Lemma 3.11 implies: $\exists \rho_-, \rho_+, \rho'_-, \rho'_+ \geq 0, v_-, v_+, v'_-, v'_+ \in \mathbb{R}^n$ such that

$$\epsilon = -\rho_- v_- \otimes v_- + \rho_+ v_+ \otimes v_+ - \rho'_- v'_- \otimes v'_- + \rho'_+ v'_+ \otimes v'_+$$

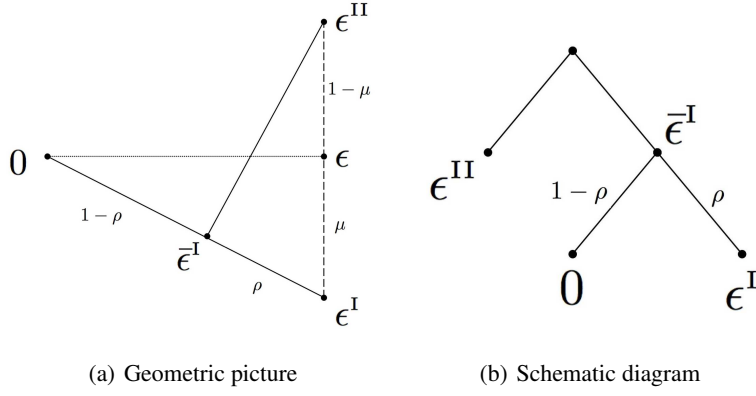


Fig. 4.5. Geometric and schematic diagrams of a rank-two laminate. In the geometric diagram solid lines represent strain compatible directions; dotted lines represent strain incompatible directions; and dashed lines represent directions that need not be strain incompatible.

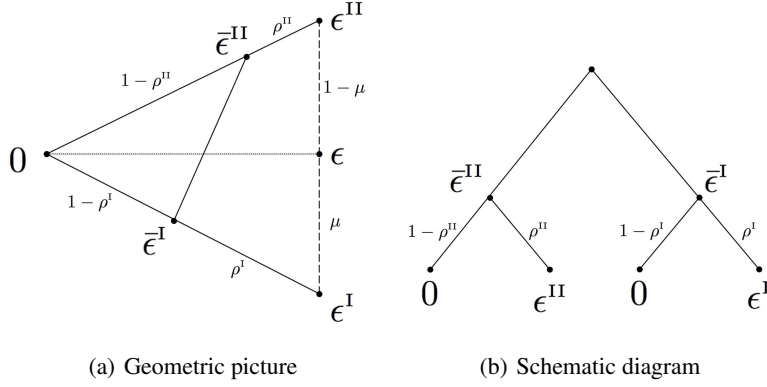


Fig. 4.6. Geometric and schematic diagrams of a rank-two laminate. In the geometric diagram solid lines represent strain compatible directions; dotted lines represent strain incompatible directions; and dashed lines represent directions that need not be strain incompatible.

Let $w_+ \in \text{Span}\{v_-, v'_-\}^\perp$ and $w_- \in \text{Span}\{v_+, v'_+\}^\perp$. Then

$$\begin{aligned} (\epsilon w_-) \cdot w_- &= -\rho_-(v_+ \cdot w_-)^2 - \rho'_-(v'_+ \cdot w_-)^2 \leq 0, \\ (\epsilon w_+) \cdot w_+ &= \rho_+(v_+ \cdot w_+)^2 + \rho'_+(v'_+ \cdot w_+)^2 \geq 0. \end{aligned}$$

This contradicts ϵ being either negative- or positive-definite.

5. Ancillary results.

5.1. The uniform traction problem.

We now turn to the uniform traction problem (1.9) for W given by (1.2). From (1.9), in two dimensions,

$$\begin{aligned}
 \overline{W}_\lambda^\sigma(\bar{\sigma}) &= \inf_{\langle \chi_i \rangle = \lambda_i} \inf_{\bar{\epsilon} \in \mathbb{R}_{\text{sym}}^{2 \times 2}} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_\Omega \sum_{i=1}^2 \chi_i(x) W_i(\epsilon(x)) - \langle \bar{\sigma}, \bar{\epsilon} \rangle \, dx \\
 &= \inf_{\bar{\epsilon} \in \mathbb{R}_{\text{sym}}^{2 \times 2}} \inf_{\langle \chi_i \rangle = \lambda_i} \inf_{u|_{\partial\Omega} = \bar{\epsilon} \cdot x} \int_\Omega \sum_{i=1}^2 \chi_i(x) W_i(\epsilon(x)) \, dx - \langle \bar{\sigma}, \bar{\epsilon} \rangle \\
 &= \inf_{\bar{\epsilon} \in \mathbb{R}_{\text{sym}}^{2 \times 2}} \max_{\beta \in [0, \gamma(\alpha_1, \alpha_2)]} (W_\lambda(\beta, \bar{\epsilon}) - \langle \bar{\sigma}, \bar{\epsilon} \rangle) \\
 &\geq \max_{\beta \in [0, \gamma(\alpha_1, \alpha_2)]} \min_{\bar{\epsilon} \in \mathbb{R}_{\text{sym}}^{2 \times 2}} (W_\lambda(\beta, \bar{\epsilon}) - \langle \bar{\sigma}, \bar{\epsilon} \rangle). \tag{5.1}
 \end{aligned}$$

From Lemma 3.5, Lemma 3.6 and a saddle point theorem [ET76, Prop. II.2.4, pg. 176], (5.1) is in fact an equality. The analogous expression in three dimensions is obtained by replacing $[0, \gamma(\alpha_1, \alpha_2)]$ with $\cap_{R \in SO(3)} B_{(\alpha_1, \alpha_2)}(R)$ and $\mathbb{R}_{\text{sym}}^{2 \times 2}$ with $\mathbb{R}_{\text{sym}}^{3 \times 3}$; and using Lemmas 4.24 and 4.25 instead of Lemmas 3.5 and 3.6. Note that

$$\begin{aligned}
 W_i(\epsilon) - \langle \bar{\sigma}, \epsilon \rangle &= \frac{1}{2} \langle \alpha_i(\epsilon - \epsilon_i^\top), (\epsilon - \epsilon_i^\top) \rangle + w_i - \langle \bar{\sigma}, \epsilon \rangle \\
 &= \frac{1}{2} \langle \alpha_i \epsilon, \epsilon \rangle - \langle \alpha_i(\epsilon_i^\top + \alpha_i^{-1} \bar{\sigma}), \epsilon \rangle \\
 &\quad + \frac{1}{2} \langle \alpha_i(\epsilon_i^\top + \alpha_i^{-1} \bar{\sigma}), (\epsilon_i^\top + \alpha_i^{-1} \bar{\sigma}) \rangle \\
 &\quad + w_i - \langle \alpha_i \epsilon_i^\top, \bar{\sigma} \rangle - \frac{1}{2} \langle \alpha_i^{-1} \bar{\sigma}, \bar{\sigma} \rangle.
 \end{aligned}$$

Thus with the substitutions

$$\epsilon_i^\top \mapsto \epsilon_i^\top + \alpha_i^{-1} \bar{\sigma} \tag{5.2a}$$

$$w_i \mapsto w_i - \langle \alpha_i \epsilon_i^\top, \bar{\sigma} \rangle - \frac{1}{2} \langle \alpha_i^{-1} \bar{\sigma}, \bar{\sigma} \rangle \tag{5.2b}$$

$\overline{W}_\lambda(\beta, \bar{\epsilon}) - \langle \bar{\sigma}, \bar{\epsilon} \rangle$ can be put in the same form as $\overline{W}_\lambda(\beta, \bar{\epsilon})$. The lower bounds in §3.1.5 and §4.9, the proofs of optimality of the lower bound in §3.2.1 and §4.10.1, and remarks on the optimal microstructures in §3.2.2 and §4.10.2 remain valid with the appropriate substitutions from (5.2). In particular, this independently shows that (5.1) is in fact an equality.

Performing the minimization in (3.5b) without the constraint $\lambda_1 \epsilon_1 + \lambda_2 \epsilon_2 = \bar{\epsilon}$, we obtain, in two dimensions,

$$\alpha_1(\epsilon_1^* - \epsilon_1^\top) + \beta \lambda_2 T(\epsilon_2^* - \epsilon_1^*) = \bar{\sigma}, \tag{5.3a}$$

$$\alpha_2(\epsilon_2^* - \epsilon_2^\top) - \beta \lambda_1 T(\epsilon_2^* - \epsilon_1^*) = \bar{\sigma}. \tag{5.3b}$$

Similarly, in three dimensions, beginning with (4.12b), we obtain,

$$\alpha_1(\epsilon_1^* - \epsilon_1^T) + \lambda_2 \beta \cdot T^{R*}(\epsilon_2^* - \epsilon_1^*) = \bar{\sigma}, \quad (5.4a)$$

$$\alpha_2(\epsilon_2^* - \epsilon_2^T) - \lambda_1 \beta \cdot T^{R*}(\epsilon_2^* - \epsilon_1^*) = \bar{\sigma}. \quad (5.4b)$$

Thus, as in (3.8) and (4.44),

$$\Delta \sigma^* = \begin{cases} \beta T \Delta \epsilon^* & \text{in two dimensions,} \\ \beta \cdot T^{R*} \Delta \epsilon^* & \text{in three dimensions.} \end{cases}$$

Explicit expressions for the optimal strains and stresses in three dimensions can be obtained by solving (5.4):

$$\begin{aligned} \epsilon_1^* &= \alpha_1^{-1} \left(I - \beta \cdot T^{R*} (\lambda_1 \alpha_2^{-1} + \lambda_2 \alpha_1^{-1}) \right)^{-1} \\ &\quad \left((I - \beta \cdot T^{R*} \alpha_2^{-1}) \bar{\sigma} - \lambda_2 \beta \cdot T^{R*} (\Delta \epsilon^T) \right) + \epsilon_1^T, \end{aligned} \quad (5.5a)$$

$$\begin{aligned} \epsilon_2^* &= \alpha_2^{-1} \left(I - \beta \cdot T^{R*} (\lambda_1 \alpha_2^{-1} + \lambda_2 \alpha_1^{-1}) \right)^{-1} \\ &\quad \left((I - \beta \cdot T^{R*} \alpha_1^{-1}) \bar{\sigma} + \lambda_1 \beta \cdot T^{R*} (\Delta \epsilon^T) \right) + \epsilon_2^T; \end{aligned} \quad (5.5b)$$

and

$$\begin{aligned} \sigma_1^* &= \left(I - \beta \cdot T^{R*} (\lambda_1 \alpha_2^{-1} + \lambda_2 \alpha_1^{-1}) \right)^{-1} \\ &\quad \left((I - \beta \cdot T^{R*} \alpha_2^{-1}) \bar{\sigma} - \lambda_2 \beta \cdot T^{R*} (\Delta \epsilon^T) \right), \end{aligned} \quad (5.6a)$$

$$\begin{aligned} \sigma_2^* &= \left(I - \beta \cdot T^{R*} (\lambda_1 \alpha_2^{-1} + \lambda_2 \alpha_1^{-1}) \right)^{-1} \\ &\quad \left((I - \beta \cdot T^{R*} \alpha_1^{-1}) \bar{\sigma} + \lambda_1 \beta \cdot T^{R*} (\Delta \epsilon^T) \right), \end{aligned} \quad (5.6b)$$

$$\Delta \sigma^* = \left(I - \beta \cdot T^{R*} (\lambda_1 \alpha_2^{-1} + \lambda_2 \alpha_1^{-1}) \right)^{-1} \beta \cdot T^{R*} (\Delta (\alpha^{-1}) \bar{\sigma} + \Delta \epsilon^T) \quad (5.6c)$$

Likewise explicit expressions for the optimal strains and stresses in two dimensions can be obtained by solving (5.3). These can also be obtained by formally substituting βT for $\beta \cdot T^{R*}$ in (5.5) and (5.6).

5.2. Applications

We discuss the applications of these results to the study of Nickel super-alloys used in turbine blades and other high temperature applications in [CB]. These materials are made by quenching an off-stoichiometric alloy and spinodal decomposition results in a two-phase solids (e.g., NiAl and Ni₃Al, which are both cubic with different elastic moduli and whose stress-free strains differ by a dilatation) with fixed phase fractions. The microstructure subsequently evolves (by diffusional mass transport) to minimize a combination of interfacial and elastic energies. The late stages of this process are controlled by elastic energy. The microstructure can further evolve during applications due to the presence of stress. There has been considerable numerical and experimental effort to study this problem. Unfortunately the experiments are difficult and the computations expensive. In particular, the computational expense limits the number of particles leading to uncertainty as

to whether the system is in a metastable state. The results we prove here and the consequent insights into optimal elastic microstructures provide a benchmark to evaluate the computations. Our results on applied stress also provide insight into the possible change of microstructure with stress.

Conclusion

In this paper we have studied the relaxation of a two-well energy under fixed phase fractions. From a mathematical standpoint, the methods we use follow closely those that have been used before. However, we find a surprising extension to three dimensions. The method also provides a lower bound when the moduli are anisotropic; however it is not clear at this point whether this bound is optimal. Similarly, the extension of such methods to more than two wells remain open.

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