



## Explicit Hashin-Shtrikman bounds in 3D linearized elasticity

Krešimir Burazin<sup>a,\*</sup>, Ivana Crnjac<sup>a</sup>, Marko Vrdoljak<sup>b</sup>

<sup>a</sup>*School of Applied Mathematics and Computer Science, University of Osijek*

<sup>b</sup>*Department of Mathematics, University of Zagreb*

**Abstract.** In this paper, we are dealing with Hashin-Shtrikman bounds in the context of linearized elasticity. We give an explicit computation of the upper bound on the primal energy in three space dimensions and the corresponding microstructure that saturates this bound. Due to equivalency between the upper Hashin-Shtrikman bound on the primal energy and the lower Hashin-Shtrikman bound on the complementary energy, the explicit calculation of the latter arises. These calculations have straightforward applications in evaluation of experimental results and numerical schemes regarding composite elastic materials, as well as structural optimization problems.

### 1. Introduction

The term *composite material* is typically used for a material that is produced from two or more constituent materials, which remain separate and distinct on some (micro) length scale. It appears that such materials are prevalent in nature, as well as among engineered materials, a non-exhausting list including some quite distinctive materials, such as sandstone, clouds, bones, wood, concrete, steel and fiberglass. Benefits of composite materials can be deduced already from aforementioned list, but it is worth to emphasize that what gives them their utility is that they often combine (desired) attributes of the constituent materials. Therefore, it is not surprising that composite materials have been extensively studied by scientist and engineers, starting already in works of Poisson [29] and Faraday [13] (for more information on historical developments we refer to [25]), and being today an enormous field of research. Even a brief overview of the field would be overwhelming for the purpose of this paper, and thus we just mention probably the most comprehensive book on the subject, a monograph of Milton [26], which can serve as good starting point for an interested reader, with an extensive list of references.

Properties (chemical or physical) of a composite material typically depend on the corresponding properties of constituents, their ratio and their arrangement within the composite. The constituents are often mixed on a rather *small* scale (microscale), which leads to rapid oscillations (on the length scale of the microstructure) in coefficients describing the composite. This makes governing partial differential equations on the microscale quite difficult to study, both from analytical and numerical perspective. In order to overcome this difficulties, one is typically interested in *locally averaged* or *homogenized* coefficients, which

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\* Corresponding author: Krešimir Burazin

*Email addresses:* [kburazin@mathos.hr](mailto:kburazin@mathos.hr) (Krešimir Burazin), [icrnjac@mathos.hr](mailto:icrnjac@mathos.hr) (Ivana Crnjac), [marko@math.hr](mailto:marko@math.hr) (Marko Vrdoljak)

should describe effective properties of the composite on a macroscale. For the purpose of this paper the term homogenization refers to the framework introduced by Murat and Tartar [27] (see also [16, 33, 34] and [4] for an overview of the method). We shall also restrict ourselves to the equations of linearized elasticity and composites made of only two constituents (phases). A composite material in this setting is a couple  $(\theta, \mathbf{A})$ , where  $\theta$  represents a local fraction of the first phase in a mixture, while  $\mathbf{A}$  is a homogenized elasticity tensor which contains information on how materials are mixed and represents an effective stiffness of the composite.

One of the most prominent problems in the theory of composite materials is a description of all possible mixtures that one can achieve from given constituents (with, or without prescribed ratios of them). It is usually called *G-closure problem* [23], as, mathematically, it consists of finding a closure of a set of classical material in topology of G- (or H-) convergence. Information on G-closure is particularly important in problems of structural optimization, in which one seeks for a composite (usually with prescribed ratios of constituents), that has optimal properties in regard with some criterion. While, unfortunately, this is still an open problem in the context of linearized elasticity, we have on our disposal various bounds on the properties of such generated composite material. A term bounds typically refers to some inequalities that correlate various physical or microstructural quantities of a composite. They are often used in evaluation of various experimental result, as well as numerical schemes for computing coefficients describing composites [26]. Probably the most prominent representative among them are famous Hashin-Shtrikman bounds [19, 20], which have imposed themselves as the benchmark against which most experimental results are compared. Here we use the terminology of Allaire's book [4], and thus use the term *Hashin-Shtrikman bounds* for bounds on effective energy of composite material, which are also known as *energy bounds*.

Explicit calculation of Hashin-Shtrikman bounds is also important for structural optimization, as these bounds prove essential for some numerical methods for optimal design problems [4, 10, 11, 32]. They are well-known in the conductivity setting, where, taken together, they completely characterize the G-closure of two isotropic phases at a fixed volume fraction [24, 27]. In the elasticity setting the situation is more complex. An explicit calculation of the bounds was first done by Gibiansky and Cherkhaev [17] in the context of the elastic plate equation (see also [12]) and by using the translation method. In the two-dimensional linearized elasticity, bounds are calculated in [7] (see also [11]) for the mixture of two isotropic phases, while in the three-dimensional case it was formally done only for the shape optimization problems, where one material is replaced by the void [5, 8, 17, 18].

An explicit calculation of bounds in three space dimensions requires elementary but rather tedious and formidable calculations, and thus, up to date, it remained a task that no one was willing to undertake. In this paper we explicitly calculate the upper Hashin-Shtrikman bound on the primal energy and the lower Hashin-Shtrikman bound on the complementary energy of the three-dimensional elastic composite of two isotropic phases. For the upper bound on the primal energy, we rewrite the minimization problem in the bound (9) as the nonsmooth convex optimization problem, and solve it by using Karush-Kuhn-Tucker conditions [22]. The lower bound on the complementary energy is obtained from the upper bound on the primal energy by the Legendre-Fenchel transformation.

In the rest of this introductory section we briefly recall the framework of mixing two isotropic elastic materials and provide necessities for the main results from the second and the third section. We finish the paper with some concluding remarks.

In the paper we mostly follow the notation from [4]: by  $\text{Sym}_d$  we denote a space of all  $d \times d$  symmetric matrices, and by  $\text{Sym}_d^4$  a space of all symmetric fourth order tensors acting on symmetric matrices. For an open and bounded set  $\Omega \subseteq \mathbf{R}^d$ , which represents an elastic medium, we consider the linearized elasticity system

$$\begin{cases} -\text{div}(\mathbf{A}e(\mathbf{u})) = \mathbf{f} \\ \mathbf{u} \in H_0^1(\Omega; \mathbf{R}^d), \end{cases} \quad (1)$$

where  $e(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^\top)$ . Here, the displacement  $\mathbf{u}$  is uniquely determined by the force density  $\mathbf{f} \in H^{-1}(\Omega; \mathbf{R}^d)$ , while a tensor function  $\mathbf{A} \in L^\infty(\Omega; \text{Sym}_d^4)$  contains information about elastic properties of the material that constitutes  $\Omega$ , called the stiffness tensor. Matrix  $e(\mathbf{u})$  is known as the strain tensor, while  $\mathbf{A}e(\mathbf{u})$

is the stress tensor. We assume that  $\mathbf{A}$  is bounded and coercive, i.e. for some  $0 < \alpha < \beta$  it satisfies (a.e. on  $\Omega$ )

$$\mathbf{A}\xi : \xi \geq \alpha|\xi|^2, \quad \mathbf{A}^{-1}\xi : \xi \geq \frac{1}{\beta}|\xi|^2, \quad \xi \in \text{Sym}_d. \tag{2}$$

We shall focus on domains filled with two well-ordered isotropic elastic phases

$$\begin{aligned} \mathbf{A}_1 &= 2\mu_1\mathbf{I}_4 + \left(\kappa_1 - \frac{2\mu_1}{d}\right)\mathbf{I}_2 \otimes \mathbf{I}_2 \\ \mathbf{A}_2 &= 2\mu_2\mathbf{I}_4 + \left(\kappa_2 - \frac{2\mu_2}{d}\right)\mathbf{I}_2 \otimes \mathbf{I}_2, \end{aligned}$$

where  $\kappa_i - \frac{2\mu_i}{d}$  is known as Lamé’s first parameter. More precisely, for the shear moduli we shall assume  $0 < \mu_1 \leq \mu_2$ , and similarly for the bulk moduli:  $0 < \kappa_1 \leq \kappa_2$ , so that any mixture of them satisfies (2), with  $\alpha = \min\{2\mu_1, d\kappa_1\}$  and  $\beta = \max\{2\mu_2, d\kappa_2\}$ . Therefore, if we denote by  $\chi \in L^\infty(\Omega; \{0, 1\})$  a characteristic function of the part of the domain occupied by  $\mathbf{A}_1$ , then the overall stiffness tensor is defined as

$$\mathbf{A}(\mathbf{x}) = \chi(\mathbf{x})\mathbf{A}_1 + (1 - \chi(\mathbf{x}))\mathbf{A}_2, \quad \mathbf{x} \in \Omega. \tag{3}$$

We are interested in fine mixtures of original materials in prescribed ratio, also known as composite material. To define a composite more precisely, we use the homogenization framework introduced by Murat and Tartar [27], where a composite material is a couple  $(\theta, \mathbf{A})$  that can be obtained as a limit (in  $L^\infty$  weak\* topology for  $\theta$  and H-topology for  $\mathbf{A}$ ) of sequences  $(\chi^n, \mathbf{A}^n)$  satisfying (3). Here,  $\theta$  represents a local fraction of the first phase in a mixture, while  $\mathbf{A}$  is a homogenized elasticity tensor which contains information on how the materials are mixed (see e. g. [4] for more).

An important class of composites made of two elastic materials are laminated composites [4, 16]. A simple laminate  $\mathbf{A}$  is made by stacking isotropic phases  $\mathbf{A}_1$  and  $\mathbf{A}_2$  in proportions  $\theta$  and  $(1 - \theta)$  and layers orthogonal to a unit vector  $\mathbf{e} \in \mathbf{R}^d$ . It is represented with the formula

$$\theta(\mathbf{A} - \mathbf{A}_2)^{-1} = (\mathbf{A}_1 - \mathbf{A}_2)^{-1} + (1 - \theta)f_2(\mathbf{e}), \tag{4}$$

where  $f_2(\mathbf{e})$  is a symmetric positive semidefinite fourth order tensor defined by the quadratic form

$$f_2(\mathbf{e})\xi : \xi = \frac{1}{\mu_2} \left( |\xi\mathbf{e}|^2 - (\xi\mathbf{e} \cdot \mathbf{e})^2 \right) + \frac{d}{2\mu_2(d - 1) + d\kappa_2} (\xi\mathbf{e} \cdot \mathbf{e})^2, \quad \xi \in \text{Sym}_d. \tag{5}$$

By repeating this lamination process, with different choices for  $\theta$  and  $\mathbf{e}$ , we get a whole family of laminated materials from phases  $\mathbf{A}_1$  and  $\mathbf{A}_2$ . Explicit formulae for tensor of such composites are known [16] for sequential laminates, where at each stage of lamination, the previous laminate is laminated again with the same pure phase. In this way, if we laminate  $p \in \mathbf{N}$  times with the phase  $\mathbf{A}_2$  in directions  $\mathbf{e}_1, \dots, \mathbf{e}_p$ , the obtained composite is determined by the formula

$$\theta(\mathbf{A} - \mathbf{A}_2)^{-1} = (\mathbf{A}_1 - \mathbf{A}_2)^{-1} + (1 - \theta) \sum_{i=1}^p m_i f_2(\mathbf{e}_i), \tag{6}$$

where  $m_i \geq 0, i = 1, \dots, p$  and  $\sum_{i=1}^p m_i = 1$ , while  $f_2$  is given by (5). We call it a rank- $p$  sequential laminate, with core  $\mathbf{A}_1$  and matrix  $\mathbf{A}_2$ , in proportions  $\theta$  and  $(1 - \theta)$ , respectively, with the lamination directions  $\mathbf{e}_i, i = 1, \dots, p$ .

In particular, we are interested in the G-closure set  $G(\theta)$  of all possible homogenized elasticity tensors which can be obtained by mixing phases  $\mathbf{A}_1$  and  $\mathbf{A}_2$  in the prescribed proportions  $\theta$  and  $(1 - \theta)$ . As already mentioned, the explicit characterization of the G-closure set is still an open problem in the elasticity setting, and thus we rely on some optimal bounds on this set obtained by Hashin-Shtrikman variational principle

[20] and known as Hashin-Shtrikman bounds. They are given as the extremal values of the elastic energy written in terms of strain (primal energy),  $\mathbf{A}\xi : \xi$ , or as the extremal values of the elastic energy written in terms of stress (complementary energy),  $\mathbf{A}^{-1}\sigma : \sigma$ . We start with the Hashin-Shtrikman variational principle for the primal energy [6].

**Proposition 1.1.** *Let  $\xi \in \text{Sym}_d$ . Any homogenized tensor  $\mathbf{A} \in G(\theta)$  satisfies*

$$\mathbf{A}\xi : \xi \geq \mathbf{A}_1\xi : \xi + (1 - \theta) \max_{\eta \in \text{Sym}_d} [2\xi : \eta - (\mathbf{A}_2 - \mathbf{A}_1)^{-1}\eta : \eta - \theta g(\eta)], \tag{7}$$

where  $g(\eta)$  is a nonlocal term given by

$$g(\eta) = \max_{\mathbf{e} \in S^{d-1}} (f_1(\mathbf{e})\eta : \eta), \tag{8}$$

and

$$\mathbf{A}\xi : \xi \leq \mathbf{A}_2\xi : \xi + \theta \min_{\eta \in \text{Sym}_d} [2\xi : \eta + (\mathbf{A}_2 - \mathbf{A}_1)^{-1}\eta : \eta - (1 - \theta)h(\eta)], \tag{9}$$

where  $h(\eta)$  is a nonlocal term given by

$$h(\eta) = \min_{\mathbf{e} \in S^{d-1}} (f_2(\mathbf{e})\eta : \eta), \tag{10}$$

where  $f_2(\mathbf{e})$  is defined by (5) and  $f_1(\mathbf{e})$  is defined with the similar formula, by putting 1 instead of 2 in (5). Furthermore, these upper and lower bounds are optimal and optimality is achieved by a rank- $d$  sequential laminate with the lamination directions given by the extremal vectors in the definition of the nonlocal terms  $g(\eta)$  and  $h(\eta)$ . In particular, lamination directions of the optimal rank- $d$  sequential laminate for the upper bound are also eigendirections of  $\xi$ . ■

Optimality of a bound in the above proposition means that for any  $\xi$  there exist a tensor  $\mathbf{A} \in G(\theta)$  such that equality in (7) (or (9)) is achieved. In the next section we give an explicit calculation for the upper Hashin-Shtrikman bound on primal energy in three space dimensions and find the optimal microstructure that saturates the bound.

## 2. Explicit calculation of the Hashin-Shtrikman upper bound

Our main motivation for undertaking the explicit calculation of the Hashin-Shtrikman bounds lies in our interest in optimal design problems, where, when minimizing the compliance under a prescribed ratio of constituents, the lower Hashin-Shtrikman bound on the complementary energy naturally arises in the necessary conditions of optimality. Based on these conditions, the optimality criteria method is derived for finding a numerical solution. In order to implement the method and have the explicit update of the design variables, we need an explicit computation of the lower Hashin-Shtrikman bound on the complementary energy. However, due to its simplicity, we shall first explicitly calculate the upper Hashin-Shtrikman bound on the primal energy, while the lower bound on the complementary energy can be deduced from this bound by using the Legendre-Fenchel transformation. Beside an explicit computation of the bound, we give the optimal microstructure for the bound, which is also needed for application in optimal design problems.

For the explicit computation of the bound (9), one should first study the nonlocal term  $h(\eta)$ . It is given in the following Lemma [6].

**Lemma 2.1.** *Let  $\eta_1, \dots, \eta_d$  be the eigenvalues of a symmetric matrix  $\eta$ . Then*

$$h(\eta) = \frac{3}{4\mu_2 + 3\kappa_2} \min \{ \eta_1^2, \dots, \eta_d^2 \}.$$



Let us denote the upper Hashin-Shtrikman bound by

$$f_+(\xi) := \max_{\mathbf{A} \in G(\theta)} \mathbf{A}\xi : \xi.$$

In order to write explicit expressions for bound  $f_+$  in a suitable and more compact form, we shall introduce numbers  $\delta\mu = \mu_2 - \mu_1$ ,  $\delta\kappa = \kappa_2 - \kappa_1$  and  $\gamma_i = 3\kappa_i + 4\mu_i$ ,  $i = 1, 2$ , and define the following linear functions:

$$\begin{aligned} f(x, y, z) &= (1 - \theta)(2\delta\mu(y - z) - 3\delta\kappa(y + 2z)) + \gamma_2(z - x) \\ g(x, y, z) &= -3\delta\mu f(x, y, z) - \gamma_2(3\delta\kappa(x + y + z) - 2\delta\mu(-2x + y + z)) \\ l(x, y, z) &= -27(1 - \theta)\delta\mu\delta\kappa x + \gamma_2(3\delta\kappa(3x - y + z) + \delta\mu(z - y)) \\ m(x, y, z) &= 9(1 - \theta)\delta\kappa x - \gamma_2(2x - y - z). \end{aligned}$$

**Theorem 2.2.** *In three dimensional, well-ordered case, let  $\xi$  be a symmetric matrix with eigenvalues  $\xi_1, \xi_2$  and  $\xi_3$  and corresponding orthonormal eigenvectors  $\mathbf{e}_1, \mathbf{e}_2$  and  $\mathbf{e}_3$ .*

*Then, the upper Hashin-Shtrikman bound on primal energy can be expressed explicitly by exactly one of the following five cases. In each case (except the case D) one is free to take any choice  $(i, j, k) \in \{(1, 2, 3), (2, 3, 1), (3, 1, 2)\}$ .*

A. If

$$\begin{aligned} f(\xi_i, \xi_j, \xi_k)g(\xi_i, \xi_j, \xi_k) &< 0 \\ f(\xi_i, \xi_k, \xi_j)g(\xi_i, \xi_k, \xi_j) &< 0, \end{aligned} \tag{11}$$

then

$$f_+(\xi) = (\theta\mathbf{A}_1 + (1 - \theta)\mathbf{A}_2)\xi : \xi - (1 - \theta)\theta \frac{(2\delta\mu(2\xi_i - \xi_j - \xi_k) + 3\delta\kappa(\xi_i + \xi_j + \xi_k))^2}{3(\theta\gamma_2 + (1 - \theta)\gamma_1)}. \tag{12}$$

This bound is achieved by a simple laminate with the lamination direction  $\mathbf{e}_i$ .

B. If

$$\begin{aligned} \frac{f(\xi_i, \xi_j, \xi_k)}{f(\xi_i, \xi_j, \xi_k) + f(\xi_k, \xi_j, \xi_i)} &\geq 0 \\ \frac{f(\xi_k, \xi_j, \xi_i)}{f(\xi_i, \xi_j, \xi_k) + f(\xi_k, \xi_j, \xi_i)} &\geq 0 \\ m(\xi_j, \xi_k, \xi_i) \left( 27(1 - \theta)\delta\kappa\delta\mu(\xi_j - \xi_i - \xi_k) - l(\xi_k, \xi_i, \xi_j) - l(\xi_i, \xi_k, \xi_j) \right) &> 0, \end{aligned} \tag{13}$$

then

$$\begin{aligned} f_+(\xi) = \mathbf{A}_2\xi : \xi + \frac{2\theta}{3f(1, 0, -1)} \left( -27(1 - \theta)\delta\mu\delta\kappa\xi_j^2 + \right. \\ \left. + \gamma_2(\delta\mu(2\xi_j - \xi_i - \xi_k)^2 + 3\delta\kappa(\xi_i + \xi_j + \xi_k)^2) \right). \end{aligned} \tag{14}$$

This bound can be achieved by the rank-2 sequential laminate with the lamination directions  $\mathbf{e}_i$  and  $\mathbf{e}_k$ , and lamination parameters

$$m_i = \frac{f(\xi_k, \xi_j, \xi_i)}{f(\xi_i, \xi_j, \xi_k) + f(\xi_k, \xi_j, \xi_i)} \quad \text{and} \quad m_k = \frac{f(\xi_i, \xi_j, \xi_k)}{f(\xi_i, \xi_j, \xi_k) + f(\xi_k, \xi_j, \xi_i)}. \tag{15}$$

C. If

$$\begin{aligned}
 l(\xi_i, \xi_j, \xi_k)l(\xi_i, \xi_k, \xi_j) &> 0 \\
 \frac{g(\xi_k, \xi_i, \xi_j)}{\xi_j - \xi_k} &\geq 0 \\
 \frac{g(\xi_j, \xi_i, \xi_k)}{\xi_k - \xi_j} &\geq 0,
 \end{aligned}
 \tag{16}$$

then

$$f_+(\xi) = \mathbf{A}_2 \xi : \xi - \theta \delta \mu \left( \frac{9\delta \kappa \xi_i^2}{3\delta \kappa + \delta \mu} + \frac{\gamma_2(\xi_j - \xi_k)^2}{-3(1 - \theta)\delta \mu + \gamma_2} \right).
 \tag{17}$$

In this case, the bound can be achieved by the rank-2 sequential laminate with the lamination directions  $\mathbf{e}_j$  and  $\mathbf{e}_k$ , and lamination parameters

$$m_j = \frac{g(\xi_k, \xi_i, \xi_j)}{6(1 - \theta)\delta \mu(3\delta \kappa + \delta \mu)(\xi_j - \xi_k)} \quad \text{and} \quad m_k = \frac{g(\xi_j, \xi_i, \xi_k)}{6(1 - \theta)\delta \mu(3\delta \kappa + \delta \mu)(\xi_k - \xi_j)}.
 \tag{18}$$

D If

$$\begin{aligned}
 \frac{m(\xi_1, \xi_2, \xi_3)}{\xi_1 + \xi_2 + \xi_3} &\geq 0 \\
 \frac{m(\xi_2, \xi_1, \xi_3)}{\xi_1 + \xi_2 + \xi_3} &\geq 0 \\
 \frac{m(\xi_3, \xi_2, \xi_1)}{\xi_1 + \xi_2 + \xi_3} &\geq 0,
 \end{aligned}
 \tag{19}$$

then

$$f_+(\xi) = \mathbf{A}_2 \xi : \xi - \theta \frac{\delta \kappa \gamma_2 (\xi_1 + \xi_2 + \xi_3)^2}{-3(1 - \theta)\delta \kappa + \gamma_2}.
 \tag{20}$$

In this case, the bound can be achieved by the rank-3 sequential laminate with the lamination directions  $\mathbf{e}_1$ ,  $\mathbf{e}_2$  and  $\mathbf{e}_3$ , and lamination parameters

$$\begin{aligned}
 m_1 &= \frac{m(\xi_1, \xi_2, \xi_3)}{9(1 - \theta)\delta \kappa(\xi_1 + \xi_2 + \xi_3)}, \quad m_2 = \frac{m(\xi_2, \xi_1, \xi_3)}{9(1 - \theta)\delta \kappa(\xi_1 + \xi_2 + \xi_3)}, \quad \text{and} \\
 m_3 &= \frac{m(\xi_3, \xi_2, \xi_1)}{9(1 - \theta)\delta \kappa(\xi_1 + \xi_2 + \xi_3)}.
 \end{aligned}
 \tag{21}$$

E If

$$\begin{aligned}
 \frac{l(\xi_i, \xi_k, \xi_j)}{\xi_j - \xi_i - \xi_k} &\geq 0 \\
 \frac{27(1 - \theta)\delta \kappa \delta \mu (\xi_j - \xi_i - \xi_k) - l(\xi_i, \xi_k, \xi_j) - l(\xi_k, \xi_i, \xi_j)}{\xi_j - \xi_i - \xi_k} &\geq 0 \\
 \frac{l(\xi_k, \xi_i, \xi_j)}{\xi_j - \xi_i - \xi_k} &\geq 0,
 \end{aligned}
 \tag{22}$$

then

$$f_+(\xi) = \mathbf{A}_2 \xi : \xi - \theta \frac{9\delta \kappa \delta \mu \gamma_2 (\xi_i - \xi_j + \xi_k)^2}{l(1, 0, 1) + l(0, 1, 1)}.
 \tag{23}$$

In this case, the bound can be achieved by the rank-3 sequential laminate with the lamination directions  $\mathbf{e}_i$ ,  $\mathbf{e}_j$  and  $\mathbf{e}_k$ , and lamination parameters

$$m_i = \frac{l(\xi_i, \xi_k, \xi_j)}{27(1 - \theta)\delta\kappa\delta\mu(\xi_j - \xi_i - \xi_k)}, \quad m_j = \frac{27(1 - \theta)\delta\kappa\delta\mu(\xi_j - \xi_i - \xi_k) - l(\xi_i, \xi_k, \xi_j) - l(\xi_k, \xi_i, \xi_j)}{27(1 - \theta)\delta\kappa\delta\mu(\xi_j - \xi_i - \xi_k)}, \quad \text{and}$$

$$m_k = \frac{l(\xi_k, \xi_i, \xi_j)}{27(1 - \theta)\delta\kappa\delta\mu(\xi_j - \xi_i - \xi_k)}. \tag{24}$$

*Proof.* In order to find the explicit bound, we need to solve the minimization problem

$$\min_{\eta \in \text{Sym}_3} \left[ 2\xi : \eta + (\mathbf{A}_2 - \mathbf{A}_1)^{-1} \eta : \eta - (1 - \theta)h(\eta) \right]. \tag{25}$$

In the isotropic three-dimensional case function  $h$  can be explicitly written as in Lemma 2.1. Problem (25) can be recognised as a nonsmooth convex minimization problem

$$\min_{\eta \in \text{Sym}_3} \left[ 2\xi : \eta + \max_{i \in \{1,2,3\}} \left\{ (\mathbf{A}_2 - \mathbf{A}_1)^{-1} \eta : \eta - (1 - \theta) \frac{3}{4\mu_2 + 3\kappa_2} \eta_i^2 \right\} \right], \tag{26}$$

where  $\eta_1, \eta_2$  and  $\eta_3$  are eigenvalues of the matrix  $\eta$ . Indeed, by [4, Remark 2.3.17], for any  $i$ , one concludes that the quadratic form  $\Phi_i(\eta) := (\mathbf{A}_2 - \mathbf{A}_1)^{-1} \eta : \eta - (1 - \theta) \frac{3}{4\mu_2 + 3\kappa_2} \eta_i^2$  is nonnegative. That remark is written in a more general situation for the sum of  $p$  energies, but for the single energy the form is even positive. Therefore, in (26) we are dealing with a strictly convex function  $\Phi := \max_{i \in \{1,2,3\}} \Phi_i$  so, by its coercivity, this minimization problem has a unique solution, for any  $\xi$ .

Furthermore, since the phases are isotropic we have

$$(\mathbf{A}_2 - \mathbf{A}_1)^{-1} \eta : \eta = \frac{1}{2\delta\mu} (\eta_1^2 + \eta_2^2 + \eta_3^2) + \left( \frac{1}{9\delta\kappa} - \frac{1}{6\delta\mu} \right) (\eta_1 + \eta_2 + \eta_3)^2.$$

By introducing vector  $\mathbf{b} = [2\xi_1 \quad 2\xi_2 \quad 2\xi_3]^\top$ , constants  $k = \frac{1}{9\delta\kappa} - \frac{1}{6\delta\mu}$  and  $c = \frac{3(1-\theta)}{4\mu_2 + 3\kappa_2}$ , matrix

$$\mathbf{B} = \begin{bmatrix} \frac{1}{2\delta\mu} + k & k & k \\ k & \frac{1}{2\delta\mu} + k & k \\ k & k & \frac{1}{2\delta\mu} + k \end{bmatrix}$$

and employing the classical von Neumann result [28], the minimization over all symmetric  $3 \times 3$  matrices in (25) is equivalent to the three dimensional minimization of the function

$$\mathbf{b} \cdot \eta + \max_{i \in \{1,2,3\}} \left\{ \mathbf{B}\eta \cdot \eta - c\eta_i^2 \right\} \tag{27}$$

over all  $\eta = (\eta_1, \eta_2, \eta_3) \in \mathbf{R}^3$ . Indeed, if we order eigenvalues as  $\xi_1 \geq \xi_2 \geq \xi_3$  and  $\eta_1 \leq \eta_2 \leq \eta_3$ , then [28]  $2\xi : \eta \geq 2 \sum_{i=1}^3 \xi_i \eta_i$ , with equality being achieved when  $\xi$  and  $\eta$  are simultaneously diagonalized, which together with the independence of  $\Phi$  on permutations of its variables implies that (25) is equivalent to minimization of (27) over the subset  $\{\eta_1 \leq \eta_2 \leq \eta_3\}$  of  $\mathbf{R}^3$ . Since  $\sum_{i=1}^3 \xi_i \eta_i \leq \sum_{i=1}^3 \xi_i \eta_{p(i)}$  for any permutation  $p$  of the set  $\{1, 2, 3\}$ , we can remove the ordering constraint from the eigenvalues of  $\eta$  (and consequently from  $\xi$ , as well) and conclude that (25) is equivalent to minimization of (27) over  $\mathbf{R}^3$ . To be precise, if  $\eta^*$  is optimal in (25) then its eigenvalues are optimal in (27) and if  $(\eta_1^*, \eta_2^*, \eta_3^*)$  is optimal in (27), then the matrix  $\eta^*$  with eigenvalues  $\eta_i^*$  and eigenvectors  $\mathbf{e}_i$  is optimal in (25). Since the function  $\eta \mapsto \mathbf{B}\eta \cdot \eta - c\eta_i^2$ , is convex for  $i = 1, 2, 3$  ([4, Remark 2.3.17]), problem (27) is a problem of the nonsmooth convex optimization which

can be solved by using subdifferential calculus. However, by introducing the additional variable, problem (27) is equivalent to the constrained minimization

$$\begin{cases} \mathbf{b} \cdot \eta + t \longrightarrow \min_{(\eta, t) \in \mathbf{R}^4} \\ \mathbf{B}\eta \cdot \eta - c\eta_i^2 \leq t, \quad i = 1, 2, 3, \end{cases} \tag{28}$$

and it can be solved in a more elementary way. We shall obtain the solution of the problem (28) by finding the unique solution  $(\eta_1, \eta_2, \eta_3, t, \lambda_1, \lambda_2, \lambda_3)$  of the Karush-Kuhn-Tucker system:

$$\begin{cases} \mathbf{b} + \sum_{i=1}^3 \lambda_i(2\mathbf{B}\eta - 2c\eta_i\mathbf{f}_i) = 0, \\ 1 - \sum_{i=1}^3 \lambda_i = 0, \\ \lambda_i(\mathbf{B}\eta \cdot \eta - c\eta_i^2 - t) = 0, \quad i = 1, 2, 3, \\ \lambda_i \geq 0, \quad i = 1, 2, 3 \\ \mathbf{B}\eta \cdot \eta - c\eta_i^2 \leq t, \quad i = 1, 2, 3, \end{cases} \tag{29}$$

where  $(\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3)$  denotes the canonical basis of  $\mathbf{R}^3$ .

Before solving the above system, let us show that optimality of the bound is achieved by the sequential laminate  $\mathbf{A}^*$  with lamination parameters  $\lambda_i$ , and lamination directions  $\mathbf{e}_i, i = 1, 2, 3$ , given by formula

$$\theta(\mathbf{A}^* - \mathbf{A}_2)^{-1} = (\mathbf{A}_1 - \mathbf{A}_2)^{-1} + (1 - \theta) \sum_{i=1}^3 \lambda_i f_2(\mathbf{e}_i). \tag{30}$$

Indeed, by multiplying the equation (30) by matrix  $\eta^*$ , we obtain

$$\theta(\mathbf{A}^* - \mathbf{A}_2)^{-1}\eta^* = (\mathbf{A}_1 - \mathbf{A}_2)^{-1}\eta^* + \frac{3(1 - \theta)}{3\kappa_2 + 4\mu_2} \sum_{i=1}^3 \lambda_i \eta_i^* \mathbf{e}_i \otimes \mathbf{e}_i,$$

and by definition of vector  $\mathbf{b}$ , matrix  $\mathbf{B}$  and constant  $c$ , after some calculations, the first two conditions given in (29) imply

$$\theta(\mathbf{A}^* - \mathbf{A}_2)^{-1}\eta^* = \xi,$$

from which it follows

$$\mathbf{A}^* \xi : \xi = \mathbf{A}_2 \xi : \xi + \theta \eta^* : \xi.$$

To prove the assertion, it remains to show that

$$\eta^* : \xi = -(\mathbf{A}_2 - \mathbf{A}_1)^{-1} \eta^* : \eta^* + (1 - \theta)h(\eta^*),$$

which can be obtained by taking inner product with the optimal vector  $\eta^*$  in the first condition in (29).

Let us return now to the solution of Karush-Kuhn-Tucker system (29). Since  $1 - \sum_{i=1}^3 \lambda_i = 0$ , at least one  $\lambda_i, i = 1, 2, 3$  is positive. Therefore, the solution saturates at least one inequality in (28).

- I. Assume that  $t = \mathbf{B}\eta \cdot \eta - c\eta_1^2$  and  $\mathbf{B}\eta \cdot \eta - c\eta_i^2 < t, i = 2, 3$ . This implies  $\lambda_2 = \lambda_3 = 0$  and  $\lambda_1 = 1$ . From condition  $\mathbf{b} + 2\mathbf{B}\eta - 2c\eta_1\mathbf{f}_1 = 0$ , we get the unique solution

$$\begin{aligned} \eta_1 &= \frac{3\delta\mu f(\xi_1, \xi_3, \xi_2) + g(\xi_1, \xi_3, \xi_2)}{3(\theta\gamma_2 + (1 - \theta)\gamma_1)} \\ \eta_2 &= \frac{-3\delta\mu f(\xi_1, \xi_3, \xi_2) + g(\xi_1, \xi_3, \xi_2)}{3(\theta\gamma_2 + (1 - \theta)\gamma_1)} \\ \eta_3 &= \frac{-3\delta\mu f(\xi_1, \xi_2, \xi_3) + g(\xi_1, \xi_2, \xi_3)}{3(\theta\gamma_2 + (1 - \theta)\gamma_1)}. \end{aligned} \tag{31}$$



Since  $\mathbf{B}\eta \cdot \eta - c\eta_i^2 < t, i = 2, 3$ , this  $\eta$  must satisfy inequalities  $|\eta_i| > |\eta_1|, i = 2, 3$ . Inequality  $|\eta_1| < |\eta_2|$  can be expressed from (31) in terms of  $\xi_1, \xi_2$ , and  $\xi_3$  as

$$f(\xi_1, \xi_3, \xi_2)g(\xi_1, \xi_3, \xi_2) < 0 \tag{32}$$

while inequality  $|\eta_1| < |\eta_3|$  can be expressed as

$$f(\xi_1, \xi_2, \xi_3)g(\xi_1, \xi_2, \xi_3) < 0. \tag{33}$$

In this case we have the bound

$$f_+(\xi) = (\theta\mathbf{A}_1 + (1 - \theta)\mathbf{A}_2)\xi : \xi - (1 - \theta)\theta \frac{(2\delta\mu(2\xi_1 - \xi_2 - \xi_3) + 3\delta\kappa(\xi_1 + \xi_2 + \xi_3))^2}{3(\theta\gamma_2 + (1 - \theta)\gamma_1)},$$

which corresponds to the subcase of part A of the theorem with  $(i, j, k) = (1, 2, 3)$ . The bound is achieved with the simple laminate with lamination direction  $\mathbf{e}_1$ . The case when only equality  $t = \mathbf{B}\eta \cdot \eta - c\eta_2^2$  is achieved and the case when only equality  $t = \mathbf{B}\eta \cdot \eta - c\eta_3^2$  is achieved can be obtained by symmetry, which gives all possible cases of part A in the theorem.

II. Let us now assume that  $\mathbf{B}\eta \cdot \eta - c\eta_1^2 < t$ , and  $\mathbf{B}\eta \cdot \eta - c\eta_i^2 - t = 0, i = 2, 3$ . This implies  $\lambda_1 = 0, \lambda_2 \geq 0, \lambda_3 \geq 0$  and  $|\eta_2| = |\eta_3|$ . If  $\eta_2 = \eta_3$ , the first two conditions in KKT system imply

$$\begin{aligned} \eta_1 &= \frac{-3\delta\mu m(\xi_1, \xi_2, \xi_3) - 27(1 - \theta)\delta\kappa\delta\mu(\xi_1 - \xi_2 - \xi_3) + l(\xi_2, \xi_3, \xi_1) + l(\xi_3, \xi_2, \xi_1)}{6(-\gamma_2 + (1 - \theta)(3\delta\kappa + \delta\mu))} \\ \eta_2 &= \frac{3\delta\mu m(\xi_1, \xi_2, \xi_3) - 27(1 - \theta)\delta\kappa\delta\mu(\xi_1 - \xi_2 - \xi_3) + l(\xi_2, \xi_3, \xi_1) + l(\xi_3, \xi_2, \xi_1)}{3(-\gamma_2 + (1 - \theta)(3\delta\kappa + \delta\mu))} \end{aligned} \tag{34}$$

$$\begin{aligned} \lambda_2 &= \frac{f(\xi_3, \xi_1, \xi_2)}{f(\xi_2, \xi_1, \xi_3) + f(\xi_3, \xi_1, \xi_2)} \\ \lambda_3 &= \frac{f(\xi_2, \xi_1, \xi_3)}{f(\xi_2, \xi_1, \xi_3) + f(\xi_3, \xi_1, \xi_2)}. \end{aligned}$$

Condition  $\mathbf{B}\eta \cdot \eta - c\eta_1^2 < t$  implies  $|\eta_2| < |\eta_1|$  which is equivalent to

$$m(\xi_1, \xi_2, \xi_3)(27(1 - \theta)\delta\kappa\delta\mu(\xi_1 - \xi_2 - \xi_3) - l(\xi_2, \xi_3, \xi_1) - l(\xi_3, \xi_2, \xi_1)) > 0.$$

The above inequality together with conditions  $\lambda_2 \geq 0$  and  $\lambda_3 \geq 0$  give conditions for the part B when  $(i, j, k) = (3, 1, 2)$ . The Hashin-Shtrikman bound in this case is given with

$$\begin{aligned} f_+(\xi) &= \mathbf{A}_2\xi : \xi + \frac{2\theta}{3f(1, 0, -1)} \left( -27(1 - \theta)\delta\mu\delta\kappa\xi_1^2 + \right. \\ &\quad \left. + \gamma_2(\delta\mu(2\xi_1 - \xi_2 - \xi_3)^2 + 3\delta\kappa(\xi_1 + \xi_2 + \xi_3)^2) \right), \end{aligned} \tag{35}$$

and the optimality is achieved by rank-2 sequential laminate with lamination parameters  $\lambda_2$  and  $\lambda_3$  given in (34) and lamination directions  $\mathbf{e}_2$  and  $\mathbf{e}_3$ .

On the other hand, if  $\eta_2 = -\eta_3$ , we get

$$\begin{aligned} \eta_1 &= -\frac{9\delta\kappa\delta\mu\xi_1}{3\delta\kappa + \delta\mu} \\ \eta_2 &= \frac{\delta\mu\gamma_2(\xi_2 - \xi_3)}{3(1 - \theta)\delta\mu - \gamma_2} \\ \lambda_2 &= \frac{g(\xi_3, \xi_1, \xi_2)}{6(1 - \theta)\delta\mu(3\delta\kappa + \delta\mu)(\xi_2 - \xi_3)} \\ \lambda_3 &= \frac{g(\xi_2, \xi_1, \xi_3)}{6(1 - \theta)\delta\mu(3\delta\kappa + \delta\mu)(\xi_3 - \xi_2)}. \end{aligned} \tag{36}$$

In this case condition  $|\eta_2| < |\eta_1|$  is equivalent to

$$l(\xi_1, \xi_2, \xi_3)l(\xi_1, \xi_3, \xi_2) > 0,$$

which together with  $\lambda_2 \geq 0$  and  $\lambda_3 \geq 0$  gives conditions of case C for triplet  $(i, j, k) = (1, 2, 3)$ . The Hashin-Shtrikman bound in this case reads

$$f_+(\xi) = \mathbf{A}_2\xi : \xi - \theta\delta\mu \left( \frac{9\delta\kappa\xi_1^2}{3\delta\kappa + \delta\mu} + \frac{\gamma_2(\xi_2 - \xi_3)^2}{-3(1 - \theta)\delta\mu + \gamma_2} \right), \tag{37}$$

and it is achieved by rank-2 sequential laminate with lamination parameters  $\lambda_2$  and  $\lambda_3$  from (36) and directions  $\mathbf{e}_2$  and  $\mathbf{e}_3$ . Cases when strict inequality  $\mathbf{B}\eta \cdot \eta - c\eta_2^2 < t$  is valid, with equality in other two inequalities and when strict inequality  $\mathbf{B}\eta \cdot \eta - c\eta_3^2 < t$  is valid, with equality in other two inequalities go analogously, and together with presented case give all possible cases of parts B and C of the theorem.

III. It remains to examine the case when  $t = \mathbf{B}\eta \cdot \eta - c\eta_1^2 = \mathbf{B}\eta \cdot \eta - c\eta_2^2 = \mathbf{B}\eta \cdot \eta - c\eta_3^2$ , which implies that  $\lambda_1, \lambda_2, \lambda_3 > 0$  and  $|\eta_1| = |\eta_2| = |\eta_3|$ . If  $\eta_1 = \eta_2 = \eta_3$ , the first two conditions in (29) give

$$\begin{aligned} \eta_1 &= \frac{\delta\kappa(3\kappa_2 + 4\mu_2)(\xi_1 + \xi_2 + \xi_3)}{3(1 - \theta)\delta\kappa - \gamma_2} \\ \lambda_1 &= \frac{m(\xi_1, \xi_2, \xi_3)}{9(1 - \theta)\delta\kappa(\xi_1 + \xi_2 + \xi_3)} \\ \lambda_2 &= \frac{m(\xi_2, \xi_1, \xi_3)}{9(1 - \theta)\delta\kappa(\xi_1 + \xi_2 + \xi_3)} \\ \lambda_3 &= \frac{m(\xi_3, \xi_1, \xi_2)}{9(1 - \theta)\delta\kappa(\xi_1 + \xi_2 + \xi_3)}. \end{aligned} \tag{38}$$

The bound in this case reads

$$f_+(\xi) = \mathbf{A}_2\xi : \xi - \theta \frac{\delta\kappa\gamma_2(\xi_1 + \xi_2 + \xi_3)^2}{-3(1 - \theta)\delta\kappa + \gamma_2}, \tag{39}$$

which, together with conditions  $\lambda_1 \geq 0$ ,  $\lambda_2 \geq 0$  and  $\lambda_3 \geq 0$  give conditions for case D of the theorem. Optimality of the bound is achieved with rank-3 sequential laminate with lamination parameters  $\lambda_1$ ,  $\lambda_2$  and  $\lambda_3$  given in (38) and lamination directions given with the eigenvectors  $\mathbf{e}_1$ ,  $\mathbf{e}_2$  and  $\mathbf{e}_3$  of matrix  $\xi$ .

On the other hand, if we assume that  $\eta_1 = -\eta_2 = \eta_3$ , again, from the first two conditions in (29) we get

$$\begin{aligned} \eta_1 &= \frac{9\delta\kappa\delta\mu\gamma_2(\xi_2 - \xi_1 - \xi_3)}{l(1, 0, 1) + l(0, 1, 1)} \\ \lambda_1 &= \frac{l(\xi_1, \xi_3, \xi_2)}{27(1 - \theta)\delta\kappa\delta\mu(\xi_2 - \xi_1 - \xi_3)} \\ \lambda_2 &= \frac{27(1 - \theta)\delta\kappa\delta\mu(\xi_2 - \xi_1 - \xi_3) - l(\xi_1, \xi_3, \xi_2) - l(\xi_3, \xi_1, \xi_2)}{27(1 - \theta)\delta\kappa\delta\mu(\xi_2 - \xi_1 - \xi_3)} \\ \lambda_3 &= \frac{l(\xi_3, \xi_1, \xi_2)}{27(1 - \theta)\delta\kappa\delta\mu(\xi_2 - \xi_1 - \xi_3)}. \end{aligned} \tag{40}$$

The bound in this case is given with

$$f_+(\xi) = \mathbf{A}_2\xi : \xi - \theta \frac{9\delta\kappa\delta\mu\gamma_2(\xi_1 - \xi_2 + \xi_3)^2}{l(1, 0, 1) + l(0, 1, 1)}, \tag{41}$$

and together with conditions  $\lambda_1 \geq 0$ ,  $\lambda_2 \geq 0$  and  $\lambda_3 \geq 0$  we get case E of the theorem with  $(i, j, k) = (1, 2, 3)$ . Optimality of the bound is achieved with rank-3 sequential laminate with lamination parameters  $\lambda_1$ ,  $\lambda_2$  and  $\lambda_3$  given in (40) and lamination directions given with the eigenvectors  $\mathbf{e}_1$ ,  $\mathbf{e}_2$  and  $\mathbf{e}_3$  of matrix  $\xi$ . Cases when  $\eta_1 = \eta_2 = -\eta_3$  and  $-\eta_1 = \eta_2 = \eta_3$  go analogously, and these cases cover all possible cases of part E and complete the proof of the theorem. □

**Remark 2.3.** As presented, the complete solution of the KKT system can be calculated explicitly, by hands, but due to very long expressions we also checked the solution via symbolic computation with Mathematica. The software is also used as a verification tool for the lower Hashin-Shtrikman bounds on the complementary energy in Theorem 3.1.

### 3. Lower Hashin-Shtrikman bound on complementary energy

The complementary energy plays an important role in studying optimal design problem for compliance minimization [8]. Using Theorem 2.2 and the Legendre-Fenchel transformation in Theorem 3.1 we give an explicit lower Hashin-Shtrikman bound on the complementary energy. For completeness, let us describe this procedure in more detail.

For the moment, let us fix  $\theta \in [0, 1]$  and denote the lower bound on complementary energy by

$$f_-^c(\sigma) := \min_{\mathbf{A} \in G(\theta)} \mathbf{A}^{-1} \sigma : \sigma.$$

For a quadratic positive definite functional  $\frac{1}{2} \mathbf{A} \xi : \xi$ , the conjugate function (or its classical Legendre transform) reads  $\frac{1}{2} \mathbf{A}^{-1} \sigma : \sigma$ , i.e.

$$\frac{1}{2} \mathbf{A} \xi : \xi = \max_{\sigma \in \text{Sym}_d} \left[ \sigma : \xi - \frac{1}{2} \mathbf{A}^{-1} \sigma : \sigma \right], \tag{42}$$

so by taking maximum over  $\mathbf{A} \in G(\theta)$ , and interchanging two maximizations, we have

$$\frac{1}{2} f_+(\xi) = \max_{\sigma \in \text{Sym}_d} \left[ \sigma : \xi - \frac{1}{2} f_-^c(\sigma) \right], \tag{43}$$

meaning that  $\frac{1}{2} f_+$  and  $\frac{1}{2} f_-^c$  are conjugate functions [7]. Note that the upper bound  $f_+$  is strongly convex (on  $\text{Sym}_d$ ) since  $f_+(\xi) - \alpha |\xi|^2 = \max_{\mathbf{A} \in G(\theta)} [\mathbf{A} \xi : \xi - \alpha |\xi|^2]$  is convex and positive, while  $f_-^c$  is also convex, obtained by

$$\frac{1}{2} f_-^c(\sigma) = \max_{\xi \in \text{Sym}_d} \left[ \sigma : \xi - \frac{1}{2} f_+(\xi) \right]. \tag{44}$$

Moreover, by [32, Theorem 26.3], due to the strict convexity of  $f_+$ , its conjugate  $f_-^c$  is smooth (differentiable) on the whole  $\text{Sym}_d$ . Analogously, one can conclude that  $f_-^c$  is strongly convex, which implies that  $f_+$  is smooth, although one concludes the same by [31, Theorem 23.5] (see also the original paper [30]). This enables us to speak about gradients of  $f_+$  and  $f_-^c$  instead of their subdifferentials, which makes the calculation of  $f_-^c$  simple. Indeed, (43) implies Fenchel-Young inequality (see also the original paper [14] on conjugates)

$$\frac{1}{2} f_-^c(\sigma) + \frac{1}{2} f_+(\xi) \leq \sigma : \xi,$$

and, for given  $\sigma \in \text{Sym}_d$ , the equality is obtained for some  $\xi \in \text{Sym}_d$ . Of course, due to differentiability, this  $\xi$  is given by  $\nabla f_+(\xi) = \sigma$ , or equivalently  $\nabla f_-^c(\sigma) = \xi$ . In other words,  $\nabla f_+$  is a surjection on  $\text{Sym}_d$  (but also an injection, due to strict convexity of  $f_+$ ).

Moreover, since the primal upper bound  $f_+(\xi)$  is expressed in terms of the eigenvalues  $(\xi_1, \xi_2, \xi_3)$  of a matrix  $\xi$ , by another application of von Neumann result it follows that  $f_-(\sigma)$  is expressed in terms of the eigenvalues  $(\sigma_1, \sigma_2, \sigma_3)$ , while  $\sigma$  and  $\xi$  (connected by  $\nabla f_+(\xi) = \sigma$ , which also holds in terms of their eigenvalues) are simultaneously diagonalizable.

Let us also note that any microstructure which saturates the upper primal bound  $f_+(\xi)$  also saturates the lower dual bound  $f_-(\sigma)$ , for the corresponding  $\sigma$ . Indeed, if  $\mathbf{A}^*$  saturates  $f_+(\xi)$ , then by (42) we have

$$\frac{1}{2}\mathbf{A}^*\xi : \xi = \sigma^* : \xi - \frac{1}{2}(\mathbf{A}^*)^{-1}\sigma^* : \sigma^*,$$

where  $\sigma^* = \mathbf{A}^*\xi$ . On the other hand

$$\frac{1}{2}\mathbf{A}^*\xi : \xi = f_+(\xi) = \sigma : \xi - \frac{1}{2}f_-(\sigma) \geq \sigma^* : \xi - \frac{1}{2}f_-(\sigma^*),$$

where  $\nabla f_+(\xi) = \sigma$ , which implies  $\frac{1}{2}(\mathbf{A}^*)^{-1}\sigma^* : \sigma^* \leq \frac{1}{2}f_-(\sigma^*)$ . This is possible only by equality, i.e.  $\mathbf{A}^*$  is an optimal microstructure for the lower dual bound  $f_-(\sigma^*)$ . Consequently,  $\sigma = \nabla f_+(\xi) = \sigma^* = \mathbf{A}^*\xi$ .

An analogous calculation proves the contrary statement: any microstructure which saturates the lower dual bound  $f_-(\sigma)$  also saturates the upper primal bound  $f_+(\xi)$ , for the corresponding  $\xi$ .

Therefore, from Theorem 2.2, we can easily get an explicit lower Hashin-Shtrikman bound on the complementary energy and the corresponding optimal microstructure. Let us introduce numbers  $\zeta = \mu_2 - \theta\delta\mu$ ,  $\vartheta = \kappa_2 - \theta\delta\kappa$ ,  $\rho = \kappa_1\mu_2 - \kappa_2\mu_1$ , and linear functions

$$\begin{aligned} n(x, y, z) &= 6(1 - \theta)\zeta\mu_2\delta\kappa z + \kappa_1\zeta\gamma_2(z - y) - 2(1 - \theta)\mu_2\rho(x - y) \\ o(x, y, z) &= 6(1 - \theta)\mu_2\delta\kappa(x - y - z) + \kappa_1\gamma_2(2x - y - z) \\ p(x, y, z) &= 6(1 - \theta)\delta\kappa\delta\mu\zeta(3\kappa_2 + \mu_2)z - 2\zeta\rho(3\kappa_2 + \mu_2)(x + y + z) + 3\zeta(3\kappa_1\kappa_2\delta\mu + \\ &\quad + 4\mu_1\mu_2\delta\kappa)(y + z) + 6\zeta\rho\mu_2z - 6\mu_1\mu_2\rho(x - y) \\ q(x, y, z) &= -2(1 - \theta)\delta\kappa\delta\mu(3\kappa_2 + \mu_2)(\gamma_2(x - z) + 3\mu_2(-x + y + z)) + \\ &\quad + \gamma_2(-2\mu_1\delta\kappa(3\kappa_2(x - z) + \mu_2(x + y + z)) + \kappa_1\mu_2\delta\mu(z - y)). \end{aligned}$$

**Theorem 3.1.** *In three dimensional, well-ordered case, let  $\sigma$  be a symmetric matrix with eigenvalues  $\sigma_1, \sigma_2$  and  $\sigma_3$  and corresponding orthonormal eigenvectors  $\mathbf{e}_1, \mathbf{e}_2$  and  $\mathbf{e}_3$ .*

*Then, the lower Hashin-Shtrikman bound on complementary energy can be expressed explicitly by exactly one of the following five cases. In each case (except the case D) one is free to take any choice  $(i, j, k) \in \{(3, 2, 1), (2, 1, 3), (1, 3, 2)\}$ .*

A. If

$$\begin{aligned} n(\sigma_i, \sigma_j, \sigma_k)p(\sigma_i, \sigma_j, \sigma_k) &< 0 \\ n(\sigma_j, \sigma_i, \sigma_k)p(\sigma_j, \sigma_i, \sigma_k) &< 0, \end{aligned} \tag{45}$$

then

$$\begin{aligned} f_-(\sigma) = \mathbf{A}_2^{-1}\sigma : \sigma + \frac{\theta}{9\kappa_2\mu_2\zeta(3\kappa_1\kappa_2\zeta + 4\mu_1\mu_2\vartheta)} &\left( 9\delta\mu\kappa_2\mu_2\zeta(\kappa_1 + 3(1 - \theta)\delta\kappa)\sigma_k^2 + \right. \\ &+ \zeta(3\kappa_1\kappa_2\delta\mu(3\kappa_2 + \mu_2) + \mu_1\mu_1\delta\kappa\gamma_2)(\sigma_i + \sigma_j + \sigma_k)^2 + 9\mu_1\mu_2\kappa_2\delta\mu\vartheta(\sigma_j - \sigma_i)^2 - \\ &\left. - 9\kappa_1\kappa_2\delta\mu\zeta(3\kappa_2\sigma_j\sigma_i + (3\kappa_2 + 2\mu_2)\sigma_k(\sigma_j + \sigma_i)) \right). \end{aligned} \tag{46}$$

*This bound is achieved by a simple laminate with the lamination direction  $\mathbf{e}_k$ .*

B. If

$$\begin{aligned} \frac{n(\sigma_i, \sigma_j, \sigma_k)}{n(\sigma_i, \sigma_j, \sigma_k) + n(\sigma_i, \sigma_k, \sigma_j)} &\geq 0 \\ \frac{n(\sigma_i, \sigma_k, \sigma_j)}{n(\sigma_i, \sigma_j, \sigma_k) + n(\sigma_i, \sigma_k, \sigma_j)} &\geq 0 \\ o(\sigma_i, \sigma_j, \sigma_k)(q(\sigma_j, \sigma_i, \sigma_k) + q(\sigma_k, \sigma_i, \sigma_j)) - \\ -6(1 - \theta)\delta\kappa\delta\mu\mu_2(-9\kappa_2\sigma_i + (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k)) &< 0, \end{aligned} \tag{47}$$

then

$$\begin{aligned} f_-^c(\boldsymbol{\sigma}) = \mathbf{A}_2^{-1}\boldsymbol{\sigma} : \boldsymbol{\sigma} + \frac{\theta}{36\kappa_2\mu_2(3\zeta(\kappa_1\kappa_2 + \mu_2\vartheta) + \mu_1\mu_2\vartheta)} &\left(27(1 - \theta)\mu_2\kappa_2\delta\kappa\delta\mu(-\sigma_i + \sigma_j + \sigma_k)^2 + \right. \\ \left. + \gamma_2(\mu_2\delta\kappa(3\zeta + \mu_1)(\sigma_i + \sigma_j + \sigma_k)^2 + 3\kappa_1\kappa_2\delta\mu(2\sigma_i - \sigma_j - \sigma_k)^2)\right). \end{aligned} \tag{48}$$

This bound can be achieved by the rank-2 sequential laminate with the lamination directions  $\mathbf{e}_j$  and  $\mathbf{e}_k$ , and lamination parameters

$$m_j = \frac{n(\sigma_i, \sigma_j, \sigma_k)}{n(\sigma_i, \sigma_j, \sigma_k) + n(\sigma_i, \sigma_k, \sigma_j)} \quad \text{and} \quad m_k = \frac{n(\sigma_i, \sigma_k, \sigma_j)}{n(\sigma_i, \sigma_j, \sigma_k) + n(\sigma_i, \sigma_k, \sigma_j)}. \tag{49}$$

C. If

$$\begin{aligned} \frac{p(\sigma_i, \sigma_j, \sigma_k)}{\sigma_k - \sigma_j} &\geq 0 \\ \frac{p(\sigma_i, \sigma_k, \sigma_j)}{\sigma_j - \sigma_k} &\geq 0 \\ q(\sigma_i, \sigma_j, \sigma_k)q(\sigma_i, \sigma_k, \sigma_j) &> 0, \end{aligned} \tag{50}$$

then

$$\begin{aligned} f_-^c(\boldsymbol{\sigma}) = \mathbf{A}_2^{-1}\boldsymbol{\sigma} : \boldsymbol{\sigma} + \frac{\theta\delta\mu}{9\kappa_2\mu_2(\zeta(3\kappa_2 + \mu_2) + 3\mu_1\mu_2)} &\left(\left(\mu_2(\sigma_i + \sigma_j + \sigma_k) + \right. \right. \\ \left. \left. + 3\kappa_2(-\sigma_i + \sigma_j + \sigma_k)\right)^2 + 9\kappa_2^2(\sigma_i(\sigma_j + \sigma_k) - 3\sigma_j\sigma_k) + 3\kappa_2\mu_2(4\sigma_i^2 + \right. \\ \left. + \sigma_i(\sigma_j + \sigma_k) - 12\sigma_j\sigma_k) + \frac{\mu_2(-4\mu_1\delta\kappa + \kappa_1\delta\mu)}{4\theta\delta\kappa\delta\mu(3\kappa_2 + \mu_2) - 4\kappa_2\mu_2(3\delta\kappa + \delta\mu)} &\left(3\kappa_2(2\sigma_i - \right. \right. \\ \left. \left. - \sigma_j - \sigma_k) + 2\mu_2(\sigma_i + \sigma_j + \sigma_k)\right)^2\right). \end{aligned} \tag{51}$$

This bound can be achieved by the rank-2 sequential laminate with the lamination directions  $\mathbf{e}_j$  and  $\mathbf{e}_k$ , and lamination parameters

$$\begin{aligned} m_j = \frac{p(\sigma_i, \sigma_j, \sigma_k)}{6(1 - \theta)\delta\mu(3\kappa_2\delta\kappa\zeta + \mu_2\delta\mu\vartheta)(\sigma_k - \sigma_j)} \quad \text{and} \\ m_k = \frac{p(\sigma_i, \sigma_k, \sigma_j)}{6(1 - \theta)\delta\mu(3\kappa_2\delta\kappa\zeta + \mu_2\delta\mu\vartheta)(\sigma_j - \sigma_k)}. \end{aligned} \tag{52}$$

D. If

$$\begin{aligned} \frac{-o(\sigma_1, \sigma_2, \sigma_3)}{\sigma_1 + \sigma_2 + \sigma_3} &\geq 0 \\ \frac{-o(\sigma_2, \sigma_1, \sigma_3)}{\sigma_1 + \sigma_2 + \sigma_3} &\geq 0 \\ \frac{-o(\sigma_3, \sigma_2, \sigma_1)}{\sigma_1 + \sigma_2 + \sigma_3} &\geq 0, \end{aligned} \tag{53}$$

then

$$f_-^c(\sigma) = \mathbf{A}_2^{-1} \sigma : \sigma + \theta \frac{\delta\kappa\gamma_2(\sigma_1 + \sigma_2 + \sigma_3)^2}{9\kappa_2(4\mu_2(1 - \theta)\delta\kappa + \kappa_1\gamma_2)}. \tag{54}$$

In this case, the bound can be achieved by the rank-3 sequential laminate with the lamination directions  $\mathbf{e}_1, \mathbf{e}_2$  and  $\mathbf{e}_3$ , and lamination parameters

$$\begin{aligned} m_1 &= \frac{-o(\sigma_1, \sigma_2, \sigma_3)}{6(1 - \theta)\delta\kappa\mu_2(\sigma_1 + \sigma_2 + \sigma_3)}, \quad m_2 = \frac{-o(\sigma_2, \sigma_1, \sigma_3)}{6(1 - \theta)\delta\kappa\mu_2(\sigma_1 + \sigma_2 + \sigma_3)}, \quad \text{and} \\ m_3 &= \frac{-o(\sigma_3, \sigma_2, \sigma_1)}{6(1 - \theta)\delta\kappa\mu_2(\sigma_1 + \sigma_2 + \sigma_3)}. \end{aligned} \tag{55}$$

E. If

$$\begin{aligned} \frac{1}{9\kappa_2\sigma_i - (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k)} &\left( q(\sigma_j, \sigma_i, \sigma_k) + q(\sigma_k, \sigma_i, \sigma_j) - \right. \\ &\left. -6(1 - \theta)\delta\kappa\delta\mu\mu_2 \left( -9\kappa_2\sigma_i + (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k) \right) \right) \geq 0 \\ &\frac{q(\sigma_j, \sigma_i, \sigma_k)}{-9\kappa_2\sigma_i + (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k)} \geq 0 \\ &\frac{q(\sigma_k, \sigma_i, \sigma_j)}{-9\kappa_2\sigma_i + (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k)} \geq 0, \end{aligned} \tag{56}$$

then

$$f_-^c(\sigma) = \mathbf{A}_2^{-1} \sigma : \sigma + \frac{\theta\delta\kappa\delta\mu\gamma_2(3\kappa_2(-2\sigma_i + \sigma_j + \sigma_k) + \mu_2(\sigma_i + \sigma_j + \sigma_k))^2}{9\kappa_2\mu_2(4(1 - \theta)\delta\kappa\delta\mu(3\kappa_2 + \mu_2)^2 + \gamma_2(12\kappa_2\mu_1\delta\kappa + \mu_2\kappa_1\delta\mu))}. \tag{57}$$

In this case, the bound can be achieved by the rank-3 sequential laminate with the lamination directions  $\mathbf{e}_i, \mathbf{e}_j$  and  $\mathbf{e}_k$ , and lamination parameters

$$\begin{aligned} m_i &= \frac{1}{6(1 - \theta)\delta\kappa\delta\mu\mu_2(9\kappa_2\sigma_i - (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k))} \left( q(\sigma_j, \sigma_i, \sigma_k) + \right. \\ &\left. + q(\sigma_k, \sigma_i, \sigma_j) - 6(1 - \theta)\delta\kappa\delta\mu\mu_2 \left( -9\kappa_2\sigma_i + (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k) \right) \right) \\ m_j &= \frac{q(\sigma_j, \sigma_i, \sigma_k)}{6(1 - \theta)\delta\kappa\delta\mu\mu_2(-9\kappa_2\sigma_i + (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k))} \quad \text{and} \\ m_k &= \frac{q(\sigma_k, \sigma_i, \sigma_j)}{6(1 - \theta)\delta\kappa\delta\mu\mu_2(-9\kappa_2\sigma_i + (3\kappa_2 + \mu_2)(\sigma_i + \sigma_j + \sigma_k))}. \end{aligned} \tag{58}$$

**Remark 3.2.** The special case where one material is replaced by void is studied in [5, Theorem 2.6]. The same result is recalled in [4, Theorem 2.3.36] with notations which are better suited to ours, so it is easier to verify the resemblance to the results of Theorem 3.1.

More precisely, one is able to directly associate the studied cases:

Theorem 3.1	Theorem 2.3.36 from [4]
A	never occurs
$B, (i, j, k) = (1, 3, 2)$	(2.159)
$B, (i, j, k) = (3, 2, 1)$	(2.157)
$C, (i, j, k) = (3, 2, 1)$	(2.160)
D	(2.156)
$E, (i, j, k) = (1, 3, 2)$	(2.158).

Other cases from [4, Theorem 2.3.36] are obtained symmetrically, by replacing  $\sigma$  by  $-\sigma$ , and they also correspond to particular cases of Theorem 3.1.

**Remark 3.3.** The classical upper Hashin-Shtrikman bound [20] on bulk moduli of isotropic elastic composites can also be recovered from Theorems 2.2 and 3.1 by taking  $\xi$  (or  $\sigma$ ) equal to the identity matrix.

#### 4. Concluding remarks

In this paper, we explicitly calculated the upper Hashin-Shtrikman bound on the primal energy and the lower Hashin-Shtrikman bound on the complementary energy of a composite material obtained by mixing two well-ordered isotropic phases in three space dimensions. Additionally, we described sequential laminates that saturate these bounds. Our explicit calculations of Hashin-Shtrikman bounds smooth path to further results in theory and applications involving the bounds and the G-closure problem. To be more specific, by explicitly computing the upper bound we have also obtained new (partial) results on G-closure, in the sense that we specified the maximum value of the linear function  $\mathbf{A} \mapsto \mathbf{A}\xi : \xi$ ,  $\mathbf{A} \in G_\theta$ , for every strain  $\xi$ . Thus, one is able to reveal a part of the boundary of the set  $G_\theta$ . Additionally, bounds on energy are useful on their own. Probably the most obvious application of the energy bounds is for finding solutions in structural optimization problems involving compliance as a design criterion [4, 10, 11, 32]. Up to now, the most prominent contribution of homogenization method in 3D optimal design problems was restricted to finding designs of optimal shape, where one of the two constituting materials is replaced by a void [4, 5]. Thus, our results are expected to have applications to compliance minimization optimal design problem in the same spirit as it was recently done in 2D case [11]. Other potential applications include the modelling of the damage accumulation [15], as well as the coherent phase transitions [21]. As a draw back, we pinpoint that our results are restricted to the well-ordered case. In two space dimensions the non-well-ordered case was treated by so called *translation method* [7]. However, in three space dimensions the situation is more delicate, and, while the lower bound (7) is obtained (but not explicitly calculated) in [9], the optimal upper bound, to the best of our knowledge, is not yet known.

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