Bounds for effective properties of multimaterial two-dimensional conducting composites, and fields in optimal composites

Andrej Cherkaev

May 6, 2008

Contents

Abstract

The paper suggests exact bounds for the effective conductivity of an isotropic multimaterial composite, which depend only on isotropic conductivities of the mixed materials and their volume fractions. These bounds refine Hashin-Shtrikman bound in the region of parameters where it is loose. The bounds by polyconvex envelope are modifies by taking into account the range of fields in optimal structures. The bounds generalize Nesi bound. The dual upper bound and the anisotropic extension are derived. For three-material composites, bounds for effective conductivity are found in an explicit form. Three-material isotropic microstructures of minimal conductivity that realize the bounds for all values of parameters are found. Optimal structures are laminates of a finite rank. They vary with the volume fractions and experience two topological transitions: For large values of m_1, the domain of material with minimal conductivity is connected, for intermediate values of m_1, no material forms a connected domain, and for small values of m_1, the domain intermediate material is connected.

Keywords Effective properties, multimaterial composites, quasiconvexity, polyconvexity, nonconvex variational problem.

1 Introduction

1.1 Hashin-Shtrikman bounds

Hashin-Shtrikman bounds [18, 19] for effective properties of composites is perhaps the most celebrated result in the theory of composites: most books on composite discuss them, and a Google search on them brings up 42,300 hits. The bounds state that the effective conductivity k_* of any isotropic mixture of several isotropic conducting materials satisfies certain inequalities independently of the structure of a composite. In the two-dimensional case, the lower k_L and upper k_U bounds are

$$k_L \le k_* \le k_U. \tag{1.1}$$

Here

$$k_L = -k_1 + H_0, \quad H_0 = \left(\sum_{i=1}^{N} \frac{m_i}{k_i + k_1} \right)^{-1}, \tag{1.2}$$

$$k_U = -k_N + H_0^U, \quad H_0^U = \left(\sum_{i=1}^{N} \frac{m_i}{k_i + k_N} \right)^{-1}, \tag{1.3}$$

$k_1 < k_2 < \dots k_N$ are conductivities of the materials (materials), and $m_1 \ge 0, \dots, m_N \ge 0$ $(m_1 + \dots + m_N = 1)$ are their volume fractions.

These bounds and their anisotropic extensions are exact for two-material composites (mixtures): There are microstructures that explicitly realize them for all values of k_1, k_2 and m_1 [18, 24, 37]. For multicomponent composites, they are exact only if volume fractions m_i of materials are in certain intervals, but not for all composites. The lower bound is definitely not exact for small fractions m_1 of the "best" material k_1. Indeed, it depends on k_1 even in the limit $m_1 = 0$, as it was pointed by Milton [29]. Clearly, this is impossible because k_1 is not presented in the composite. Therefore the bound is rough and can be improved for sufficiently small m_1. Moreover, the inaccuracy of the multimaterial bound can question the established results for two-material bound. Indeed, an infinitesimal amount of an unaccounted material with lowest conductivity can significantly change the bound. Assume, for example, that two materials with conductivities $k_2 = 1$ and $k_3 = 3$ are mixed in the equal fractions ($m_2 = m_3 = .5$). The lower Hashin-Shtrikman bound (1.2) is $k_L = 1.667$. A formal addition to the mixture a material with conductivity $k_1 = .1$ and *zero* volume fraction $m_1 = 0$ changes the bound to $k_L = 1.5238$. Of course the difference between the two formulations is only semantic. The fact that the Hashin-Shtrikman bound is loose in a region of parameters and is exact outside this region suggests that some inequality constraints are missing in its derivation. These constraints might become active in that region.

1.2 Some previous work

Since Hashin and Shtrikman suggested the bounds for effective properties [18] in 1963, the method was extended in several directions. The contemporary approach to *geometrically independent bounds* was suggested in eighties in [23, 24, 26, 37], generalized in [27, 20, 30, 6] and other papers. Milton [30] called it*translation method*. It allows for obtaining bounds for effective properties of anisotropic conducting, elastic, and viscoelastic composites and polycrystals. For references, we refer to books and reviews [12, 9, 28, 10] and references therein. The approach is based on investigation of nonconvex variational problem that describes the problem of bounds. The references can be found in books [9, 28, 14]. The translation bounds are proven to be exact for two-material mixtures and polycrystals, but not for general multimaterial composite, as it evident from the above example.

The work was done to extend the technique of the bounds to multimaterial composites. Nesi [33] used an additional inequality to improve the bounds. The inequality states (see [5]) states that $\det(\nabla u_a|\nabla u_b) \geq 0$ where u_a and u_b are two solution of conductivity problem in an inhomogeneous periodicity cell, exposed to two different external fields. The inequality is valid independently of optimality of the structure of the composite. Adding this inequality to the translation method, Nesi improved Hashin-Shtrikman bound [33]. Later, the structures have been found in [9] that attain Nesi's bound in an asymptotic case when one material has infinite conductivity. Simultaneously, evidences were provided that the bound is not exact in the general case. It does not satisfy the correct asymptotic. In the current paper, we use several ideas of Nesi's approach.

The mathematical foundations of multiwell bounds were investigated. Smyshlyaev and Willis [34] formulated the three-well problem as the problem for vector-valued H-measures. Bhattacharya and Dolzmann [8] found the quasiconvex hull of multiwell Lagrangian. Talbot, Willis, and Nesi [36] suggested an improvement of Hashin-Shtrikman bounds. Barbarosie [7] expended Milton's structures to the case of infinitely many materials.

The first optimal three-material structure was found by Milton [29] who considered two kinds of Hashin-Shtrikman coated circles [18], mixed together. The structures realize the Hashin-Shtrikman bound (a.k.a the isotropic translation bound) in a region of parameters where the volume fraction m_1 of the best material κ_1 is larger than a threshold value. Lurie and Cherkaev [26] formulated an optimization problem and found the a different type of optimal structures: the multi-layer coated circles. The solution is topologically different from the solution found in [29]. Effective conductivity of both structures realizes the bound in the range where the structures are geometrically possible, and then deviates from the bound. Milton and Kohn [31] extended earlier Milton's result [24] to anisotropic composites by using second-rank matrix laminates. All these structures match the bound in a range of volume fractions $n_1 > m_1^0$ and do not match correct asymptotic when $m_1 \to 0$. This suggested that some unaccounted inequalities become active for small m_1.

Meanwhile, miscellaneous facts concerning optimal multimaterial composites were collected. Cherkaev and Gibiansky [11] found three-component structures of extreme anisotropy whose properties significantly differ from the two-material ones: when the effective conductivity in x-direction is equal to harmonic mean of mixing materials' conductivities, the conductivity in perpendicular direction can be made smaller than arithmetic mean of them. The necessary conditions technique for examining fields in multimaterial composites was worked out [9] following the approach suggested by Lurie [21, 22] and Murat [32] in 1970s. Using this technique, the range of fields in optimal composites were investigated in [9, 13], and constraints on the range of fields in an optimal structure were established.

Gibiansky and Sigmund [15] discovered a new class of three-material structures that significantly expanded the known region of attainability of Hashin-Shtrikman bound. Recently, Albin, Cherkaev, and Nesi found new optimal anisotropic three-material laminates for two-dimensional conductivity, [4, 3]. New optimal three-material structures for three-dimensional conductivity were described by Albin and Cherkaev in [2]. These structures realize Hashin-Shtrikman bounds and anisotropic translation bounds in a larger range than it was known before (they are discussed below, in Section 8.1). Some hints on the optimal values of fields in materials outside of optimality of Hashin-Shtrikman bound were revealed by Albin in [1] by numerical optimization of microstructures.

Contents of the paper In this paper, we suggest new bounds of isotropic effective conductivity that complement Hashin-Shtrikman bounds. We also find structures that realize the bounds of conductivity of three-component composites for all values of volume fractions and conductivities of components. Section 2 describes conductivity of inhomogeneous body and a corresponding variational problem. Section 3 outlines the known bounds (by the polyconvex envelope)and establishes inequalities for the fields in optimal two-component structures. Section 4 introduces new bounds by *localized polyconvexity*, and works out the algebra of new bounds. The constraint for fields in optimal structures is discussed in Section 4.4. These constraints are used in Section 5 to derive an exact lower bound for effective conductivity of a multimaterial conducting composite. Section 6 discusses generalization: the upper bound (Section 6.1) and anisotropic bounds (Section 6.2). Section 7 gives an explicit description of the bound for a three-material composite. Section 8 determines optimal three-material structures which conductivity match the bound. Appendix describes the found parameters of optimal structures in an asymptotic case.

2 Periodic conducting composites

2.1 Equations

Periodic cell Consider the plane divided into periodic system of unit squares. Each periodicity cell Ω, ($\Omega = \{(x_1, x_2):\ 0 \le x_1 \le 1,\ 0 \le x_2 \le 1\} = 1$) is divided into N parts Ω_i, $\Omega = \bigcup \Omega_i$ and each part is occupied with an isotropic conductor of conductivity k_i. Denote the dividing curves between Ω_i and Ω_j as ∂_{ij}. Note that domains Ω_i are not necessary connected.

The variable conductivity $k(x)$ within the cell is

$$k(x) = \sum_{i=1}^{N} \chi_i(x) k_i \tag{2.1}$$

where $x = (x_1, x_2)$ and χ_i is the characteristic function of subdomain Ω_i:

$$\chi_i(x) = \begin{cases} 1 \text{ if } x \in \Omega_i \\ 0 \text{ if } x \notin \Omega_i \end{cases}. \tag{2.2}$$

The area of subdomain Ω_i is called *volume fraction* m_i of material k_i:

$$m_i = \|\Omega_i\| = \int_{\Omega_i} dx = \int_{\Omega} \chi_i \, dx. \tag{2.3}$$

Fractions m_i are assumed to be strictly positive and they sum up to one.

$$m_i > 0, \quad \sum_{i=1}^{N} m_i = 1. \tag{2.4}$$

Conductivity Assume that a homogeneous external field E_a is applied to the composite along x_1-axis causing potential $u_a(x)$ inside. Potential u_a satisfies the following conditions:
(i) u_a is harmonic in connected components of Ω_i, because $k(x) = k_i$ is constant there.

$$\nabla^2 u_a = 0 \text{ in } \Omega_i, \quad \nabla \cdot k(x) \nabla u_a(x) = 0 \text{ in } \Omega, \tag{2.5}$$

We notice that magnitude $|\nabla u_a|$ of a harmonic in Ω_i field u_a reaches its supremum on its boundary $\partial\Omega_i$,

$$\mathrm{arg}\left(\mathrm{sup}_{\mathrm{x}\in\Omega_\mathrm{i}} |\nabla \mathrm{u_a(x)}|\right) \in \partial\Omega_\mathrm{i}, \quad \mathrm{i} = 1, \ldots, \mathrm{N}. \tag{2.6}$$

(ii) Gradient $\nabla u_a(x)$ is Ω-periodic and its average equals to the applied field E_a

$$\int_{\Omega} \nabla u_a \, dx = E_a, \quad \nabla u_a(x) \text{ is } \Omega\text{-periodic}, \tag{2.7}$$

(iii) Conditions on boundaries ∂_{pm} between domains Ω_p and Ω_m, $p, m = 1, \dots N, p \neq m$, are satisfied

$$\left[\frac{\partial u_a}{\partial \tau}\right]_m^p = 0 \quad \text{on } \partial\Omega_{pm}, \tag{2.8}$$

and

$$\left[k\frac{\partial u_a}{\partial n}\right]_m^p = 0, \quad \text{on } \partial\Omega_{pm}. \tag{2.9}$$

Here, $[z(s)]_m^p$ denotes the jump of a function z on the point s at the boundary Ω_{pm},

$$[z(s)]_m^p = \lim_{x\to s, x\in\Omega_p} z(x) - \lim_{x\to s, x\in\Omega_m} z(x)$$

and n and τ are the normal and tangent to ∂_{pm}. Conditions (2.8) and (2.9) express the continuity of potential u_a and normal component of the current, respectively. We assume that n and τ are defined almost everywhere on ∂_{pm}.

Energy The energy Π_a of the periodicity unit cell Ω in an external field E_a is equal to

$$\Pi_a = \frac{1}{2} \inf_{u_a \in \mathcal{U}_a} \left(\int_\Omega \sum_{i=1}^N \chi_i k_i \nabla u_a^T \nabla u_a \, dx \right) \tag{2.10}$$

where

$$\mathcal{U}_a = \left\{ u_a : \int_\Omega \nabla u_a \, dx = E_a, \quad \nabla u_a \text{ is } \Omega\text{-periodic }, u \in W_2^1(\Omega) \right\}. \tag{2.11}$$

2.2 Effective Properties

The energy is a quadratic function of magnitude of applied field E_a,

$$\Pi_a = \frac{1}{2} k_*(\chi)_{11} E_a^T E_a. \tag{2.12}$$

Coefficient $k_*(\chi)_{11}$ represents the overall conductivity of the cell subjected to the field E_a. It is the entry of *effective tensor* $K_*(\chi)$; it depends only on characteristic function $\chi = (\chi_1, \dots, \chi_N)$ of layout. In order to characterize tensor K_* in more details, we compute the sum of energies of a cell subjected to two orthogonal external fields E_a and E_b. In addition to $\Pi_a(u_a)$, we consider the energy Π_b and potential $u_b \in \mathcal{U}_b$ defined similarly to (2.11) but associated with an external field E_b instead of E_a. We also assume that E_b is orthogonal to E_a, $E_a^T E_b = 0$.

The sum of the energies can be written as

$$J(e_0, \chi) = \Pi_a + \Pi_b = \frac{1}{2} \inf_{u \in \mathcal{U}} \int_\Omega \left(\sum_{i=1}^N \chi_i k_i \, \mathrm{Tr}\,(\nabla u^T \nabla u) \, dx \right). \tag{2.13}$$

Here, u is vector of potentials $u = [u_a, u_b]$, $\mathcal{U} = \mathcal{U}_a \bigoplus \mathcal{U}_b$, and ∇u is a 2×2 matrix with columns ∇u_a and ∇u_b,

$$\nabla u = (\nabla u_a | \nabla u_b) = \begin{pmatrix} \frac{\partial u_a}{\partial x_1} & \frac{\partial u_b}{\partial x_1} \\ \frac{\partial u_a}{\partial x_2} & \frac{\partial u_b}{\partial x_2} \end{pmatrix}. \tag{2.14}$$

Entries $(\nabla u)_{ij} = \frac{\partial u_i}{\partial x_j} \in L_2(\Omega)$ are Ω-periodic, and matrix ∇u satisfies integral conditions (see (2.11)):

$$\mathcal{U}: \int_\Omega \nabla u \, dx = e_0, \quad e_0 = (E_a | E_b), \quad E_a^T E_b = 0. \tag{2.15}$$

Here, e_0 is a symmetric matrix of external fields with eigenvalues equal to $|E_a|$ and $|E_b|$ and eigenvectors oriented along x_1 and x_2 axes, respectively.

The left-hand side of (2.13) defines the *effective conductivity tensor* $K_*(\chi)$. It is a quadratic form of $(e_0)_{kj}$ with K_* entries

$$J(e_0, \chi) = \frac{1}{2} \operatorname{Tr} \left[K_*(\chi) e_0 e_0^T \right]. \tag{2.16}$$

Because e_0 is arbitrary and $K_*(\chi)$ that depends only on layout (structure) χ, (2.16) allows for defining K_*.

Stationarity of $J(e_0, \chi)$. Rank-one connectedness Consider variational problem (2.13). Minimization of $J(e_0, \chi)$ with respect of $u \in \mathcal{U}$ leads to the Euler-Lagrange equations (compare with (2.5), (2.7))

$$\nabla \cdot k(x) \nabla u_j = 0 \text{ in } \Omega, \quad \int_\Omega \nabla u_j dx = E_j, \quad \nabla u_j \text{ are } \Omega\text{- periodic}, \; j = a, b. \tag{2.17}$$

At the dividing curve ∂_{mp} between the domains Ω_m and Ω_p, the vector potential u satisfies the main boundary conditions similar to (2.8)

$$\left[\frac{\partial u}{\partial \tau} \right]_p^m = 0 \quad \text{on } \partial \Omega_{mp} \tag{2.18}$$

and the variational boundary conditions similar to (2.9) which follow from the stationarity of $J(e_0, \chi)$

$$\left[k \frac{\partial u}{\partial n} \right]_p^m = 0, \quad \text{on } \partial \Omega_{mp}. \tag{2.19}$$

These conditions imply the rank-one connectedness of the matrices ∇u and $k \nabla u$ on the opposite sides of boundary ∂_{mp}:

$$\operatorname{rank} \; [\nabla u]_p^m = 1, \quad \operatorname{rank} \; [k \nabla u]_p^m = 1. \tag{2.20}$$

Let denote the set of values of matrices $e = \nabla u$ in Ω_i as Ψ_i,

$$\Psi_i = \{\nabla u(x),\ x \in \Omega_i\} \tag{2.21}$$

Condition (2.20) implies that sets Ψ_m and Ψ_p are *rank-one connected*:

$$\exists e_m \in \Psi_m,\ \exists e_p \in \Psi_p : \ \det(e_m - e_p) = 0 \tag{2.22}$$

Relaxed rank-one connectedness Our goal is to describe optimal composites or optimal subdomains Ω_i that minimize $J(e_0, \chi)$, (2.16). A minimizing sequence may contain domains Ω_i of arbitrary shape and connectedness, moreover, these domains may become infinitely wiggly fractals, as in [6]. Dealing with such sequences, we assume that conditions similar to (2.6) and (2.22) are satisfied even when minimizing structures tend to a fractal. In the last case, we assume relaxed boundary conditions that correspond to the situation when a "larger" domain Ω_i neighbors a fine-scale mixture of other materials, and the scales are separated. Namely, we assume that field e_i at the boundary of Ω_i must be in rank-one connection with a convex combination of the fields in the remaining part of Ω that represent an averaged field at the other side of the boundary. Therefore, Ψ_i sets must satisfy the conditions

$$\exists\ e_i \in \Psi_i,\ \exists\ e_c = \mathcal{C}\left(\bigcup_{k\neq i} \Psi_k\right) : \ \det(e_i - e_c) = 0 \tag{2.23}$$

of *relaxed rank-one connectedness.*

Particularly, relaxed rank-one connectedness corresponds to continuity of a potential in the sequential laminates of any rank. Definition of these sequences of structures (see, for example, [24, 9, 28]) includes an assumption of the separation of scales of laminates of different rank. Inside any laminate scale, the piece-wise constant fields satisfy the boundary and equilibrium conditions. The conditions on the boundary between slices of "smaller scale" laminates of higher ranks are satisfied for the fields averaged in that scales, as in (2.23). The conditions are satisfied in the limit when the ratio of scales tends to zero.

Optimal composites A layout χ (or a limit of a sequence $\{\chi_i^s\}$) that minimizes the energy $J(e_0, \chi)$ with a given external field e_0 is called an *optimal composite.* Minimal energy is still a quadratic function of entries of e_0 and is defined by a tensor K_L of the lower bound (see [9]).

$$\inf_{\chi_i \text{ as in (2.3),(2.4)}} J(e_0, \chi) = \frac{1}{2} \operatorname{Tr}(K_L e_0 e_0^T). \tag{2.24}$$

It is assumed that χ satisfies (2.3), (2.4) or that the compared structures keep the volume fractions.

Effective conductivity tensor K_* of any structure is bounded by K_L as follows

$$e_0^T(K_*(\chi) - K_L)e_0 \geq 0 \quad \forall \chi \text{ as in } (2.3), (2.4), \ \forall e_0. \tag{2.25}$$

The difference $K_*(\chi) - K_L$ is nonnegative defined, in particular

$$\det(K_*(\chi) - K_L) \geq 0 \quad \forall \chi \text{ as in } (2.3), (2.4), \ \forall e_0. \tag{2.26}$$

If $|E_a| = |E_b| = s$ or $e_0 = sI$, optimal structures are isotropic, see for example [9, 28].

$$K_L = k_L I \quad \text{ if } \ e_0 = sI. \tag{2.27}$$

Then, the bound k_L for isotropic conductivity k_* becomes:

$$k_L = \frac{1}{s^2} \inf_{\chi_i} J(sI, \chi). \tag{2.28}$$

Bound k_L depends only on k_i and m_i, it defines the lower isotropic component of *G-closure* - set of all effective tensors of composites with fixed volume fractions m_i of materials, see [23, 24, 9],

$$k_L(m_i, k_i) \leq k_*(\chi) \quad \forall \chi \text{ as in } (2.3). \tag{2.29}$$

2.3 Notations

For the next consideration, it is convenient to introduce a matrix basis for 2×2 matrices $e = \nabla u$. We introduce a convenient basis (see, for example [9, 4])

$$a_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad a_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$a_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad a_4 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Matrices a_i are orthonormal with respect to scalar product $\operatorname{Tr}(a_i a_j^T)$. One can check that $\operatorname{Tr}(a_i a_j^T) = \delta_{ij}$, where δ_{ij} is the Kronecker symbol. Any 2×2 matrix Z is represented by its coefficients in that basis as follows

$$Z = \frac{1}{\sqrt{2}} \left[S(Z)a_1 + D_*(Z)a_2 + D_{**}(Z)a_3 + V(Z)a_4 \right]$$

where

$$S(Z) = \frac{1}{\sqrt{2}} (Z_{11} + Z_{22}), \quad D_*(Z) = \frac{1}{\sqrt{2}} (Z_{11} - Z_{22}),$$
$$D_{**}(Z) = \frac{1}{\sqrt{2}} (Z_{12} + Z_{21}), \quad V(Z) = \frac{1}{\sqrt{2}} (Z_{12} - Z_{21}). \tag{2.30}$$

One can immediately verify that

$$\text{Tr}\,(Z^T Z) = S^2 + D^2 + V^2, \quad \det(Z) = \frac{1}{2}(S^2 + V^2 - D^2) \tag{2.31}$$

where

$$D^2 = D_*^2 + D_{**}^2. \tag{2.32}$$

Notice that $S(Z)$, $D(Z)$ and $V(Z)$ are invariant to rotation of Z.

If Z is symmetric, then $V(Z) = 0$. If Z is proportional to unit matrix, $Z = sI$, then $V(Z) = D(Z) = 0$, and $S(Z) = \sqrt{2}s$.

In particular, matrix ∇u of gradient u is represented as

$$\nabla u = S(\nabla u)a_1 + D_*(\nabla u)a_2 + D_{**}(\nabla u)a_3 + V(\nabla u)a_4$$

where

$$\begin{array}{ll} S(\nabla u) = \frac{1}{\sqrt{2}}\left(\frac{\partial u_a}{\partial x_1} + \frac{\partial u_b}{\partial x_2}\right); & D_*(\nabla u) = \frac{1}{\sqrt{2}}\left(\frac{\partial u_a}{\partial x_1} - \frac{\partial u_b}{\partial x_2}\right), \\ D_{**}(\nabla u) = \frac{1}{\sqrt{2}}\left(\frac{\partial u_a}{\partial x_2} + \frac{\partial u_b}{\partial x_1}\right), & V(\nabla u) = \frac{1}{\sqrt{2}}\left(\frac{\partial u_a}{\partial x_2} - \frac{\partial u_b}{\partial x_1}\right). \end{array} \tag{2.33}$$

Matrix $e = \nabla u$ can be represented by its rotationally invariant components (S, D, V) and the angle of orientation of the labor system.

3 Harmonic Mean and Translation Bounds

3.1 Harmonic Mean Bound

In this section, we recall the derivations of the known bounds for the effective properties and comment on requirements to optimal fields.

Energy of an optimal composite In the notations (2.31), the energy of an isotropic composite is

$$J(e_0, \chi) = J(\sqrt{2}S_0 I, \chi) = k_* S_0^2. \tag{3.1}$$

The energy is equal the sum of energies in the mixed materials. We write, using (2.31)

$$\begin{aligned} k_* S_0^2 &= 2 \inf_{e(x)} \frac{1}{2} \sum_{i=1}^{N} k_i \int_{\Omega_i} \text{Tr}\,\left(e^T(x) e(x)\right) dx \\ &= \inf_{S,D,V} \sum_{i=1}^{N} k_i \int_{\Omega_i} (S^2 + D^2 + V^2) dx. \end{aligned} \tag{3.2}$$

It is convenient to separate the fields in the subdomains Ω_i into their mean values S_i, D_i, V_i and deviations, rewrite the energy as follows:

$$k_* S_0^2 = \min_{S_1, D_i, V_i} \sum_{i=1}^N m_i k_i (S_i^2 + D_i^2 + V_i^2) + \mathcal{N}, \tag{3.3}$$

where

$$S_i = \frac{1}{\|\Omega_i\|} \int_{\Omega_i} S(x)\, dx, \;\; D_i = \frac{1}{\|\Omega_i\|} \int_{\Omega_i} D(x)\, dx, V_i = \frac{1}{\|\Omega_i\|} \int_{\Omega_i} V(x)\, dx, \tag{3.4}$$

$$\mathcal{N} = \inf_{S(x), D(x), V(x) \in \Psi} \sum_{i=1}^N \mathcal{N}_i, \tag{3.5}$$

$$\mathcal{N}_i = k_i \int_{\Omega_i} \left[(S(x) - S_i)^2 + (D_i - D(x))^2 + (V_i - V(x))^2 \right] dx. \tag{3.6}$$

The mean values are subject to integral constraints

$$\sum_{i=1}^N m_i S_i = S_0, \quad \sum_{i=1}^N m_i D_i = 0, \quad \sum_{i=1}^N m_i V_i = 0. \tag{3.7}$$

and deviations are free of them. The only nonhomogeneous constraint in (3.7) is imposed on the average of S-components.

Harmonic mean bound The lower bounds are obtained by enlarging the set of minimizers. If differential constraints (2.17). (2.18) on minimizers are neglected, the minimum decreases. Assume that these constraints are omitted so that $e(x)$ is a matrix with entries $e_{ij} \in L_2(\Omega)$. Then, the energy minimum corresponds to piece-wise constant isotropic fields in each domain Ω_i,

$$S(x) = S_i, \quad D(x) = D_i \quad V(x) = V_i \quad \forall x \in \Omega_i, \quad i = 1, \ldots, N, \tag{3.8}$$

because the integrals in (3.6) are convex functionals of S, D, V. The variational problem becomes an algebraic one: $\mathcal{N} = 0$ in (3.5).

Further, we find:

$$V_i = 0, \quad D_i = 0, \quad i = 1, \ldots, N. \tag{3.9}$$

Minimizing the right-hand side of (3.3) over S_i, subject to (3.7), we compute

$$S_i = \frac{1}{k_i} H_h S_0, \quad i = 1, \ldots, N, \quad H_h = \left(\sum_{i=1}^N \frac{m_i}{k_i} \right)^{-1}. \tag{3.10}$$

Expression (3.2) gives the harmonic mean bound for effective conductivity k_*,

$$k_* \geq k_L^h = H_h. \tag{3.11}$$

Notice that fields (3.8)-(3.9) are not compatible. Since e is constant in Ω_i and proportional to unit matrix, a tangent component of e is discontinuous at the boundaries where S-component jumps, (3.10). This contradicts (2.20) or (2.23). Therefore the bound (3.11) is not attainable by a structure.

3.2 Translation or Hashin-Shtrikman bound

Integral constraint and translated energy A polyconvex envelope [20, 24, 37, 14] is also obtained by neglecting differential constraints $e(x) = \nabla u$, and replacing fields in Ω_i by their averages. However, the differential constraints are indirectly accounted for via quasiaffinity of $\det(\nabla u)$,

$$\det(e_0) = \int_\Omega \det(\nabla u) dx, \ \forall u \in \mathcal{U}. \tag{3.12}$$

Adding this equality, multiplied by a real number t called *translation parameter*, to both sides of (3.2) we write

$$J(e_0, \chi) + t \det(e_0) = \inf_{e(x)=\nabla u} \frac{1}{2} \sum_{i=1}^N \int_{\Omega_i} \left[k_i \ \mathrm{Tr} \left(e^T(x) e(x) \right) + t \det e(x) \right] dx \tag{3.13}$$

We transform the left-hand side of (3.13) to the form

$$J(e_0) + t \det(e_0) = \frac{1}{2}(k_* + t) S_0^2. \tag{3.14}$$

recalling that the applied field $e_0 = \frac{1}{\sqrt{2}} S_0 I$ and the corresponding tensor $K_L = k_L I$ are isotropic.

To obtain the bound, we again relax the right-hand side of (3.13) by omitting the differential constrain $e = \nabla u$ and treating e as a matrix with entries from $L_2(\Omega)$, as before. The minimum in these enlarged class of minimizers is lower, and the equality (3.13) is replaced by an inequality

$$\frac{1}{2}(k_* + t) S_0^2 \geq \frac{1}{2} W_t^{\mathrm{poly}}(e_0) \tag{3.15}$$

where W_t^{poly} is a solution of a finite-dimensional minimization problem

$$W_t^{\mathrm{poly}} = \inf_{e \in \mathcal{E}} \sum_i^N \int_{\Omega_i} \left[(k_i + t) \left(S^2(x) + V^2(x) \right) + (k_i - t) D^2(x) \right] dx. \tag{3.16}$$

(here, decomposition (2.31) is used to transform the right-hand side of (3.13)).

Minimizers S, D, V are subject to integral constraint

$$\mathcal{E} = \left\{ e : \int_\Omega S(x)\, dx = S_0, \quad \int_\Omega D(x)\, dx = 0, \quad \int_\Omega V(x)\, dx = 0 \right\}.$$

W_t^{poly} is a quadratic function of S_0, as the left-hand side of (3.15). Since S_0 is arbitrary, we obtain a family of inequalities

$$k_* \geq k_L = \frac{W_t^{\mathrm{poly}}}{S_0^2} - t \quad \forall t \in R_1. \tag{3.17}$$

that depends on parameter $t \in R$. Translation bound (or polyconvex envelope) corresponds to maximum of right-hand side of (3.17) with respect of t.

Range of translation parameter The integrals in W_t^{poly} (3.16) are bounded as

$$\frac{1}{m_i} \int_{\Omega_i} \Big[(k_i + t) \left(S^2(e(x)) + V^2(e(x)) \right) dx + (k_i - t) D^2(e(x)) \Big]\, dx$$
$$\geq G_i^{poly}(S_i, D_i, V_i, t) \tag{3.18}$$

where S_i, D_i, V_i are defined in (3.4), $i = 1, \dots, N$,

$$G_i^{poly} = \begin{cases} (k_i + t)(S_i^2 + V_i^2) + (k_i - t) D_i^2 & \text{if } 0 < t \leq k_i \\ -\infty & \text{if } t > k_i \end{cases}. \tag{3.19}$$

Indeed, when coefficients $k_i + t$ and $k_i - t$ are nonnegative, the integral in (3.18) is a convex functional of S, D, V. Its minimum is achieved when $S(x), V(x)$ and $D(x)$ are constant in Ω_i and equal to their mean values.

When $k_1 - t = 0$, the right-hand side of (3.18) is independent of $D^2(x)$, $x \in \Omega_1$. The extremal fields $S(x), V(x)$ are constants, as before.

When $k_i - t < 0$, the integral in (3.18) is a concave functional of $D(x)$. The improper infimum of that integral (see (3.19)) corresponds to a unbounded minimizing sequence $\{D^s\}$ such that the magnitude of $\{D^s\}$ tends to infinity while the average of D over Ω_i is zero,

$$\int_{\Omega_i} (D^s)^2 dx \to \infty, \quad \int_{\Omega_i} (D^s) dx = 0.$$

Because of this feature, the lower estimate (3.18) is nontrivial only if $t \in [0, k_1]$.

Translation (Hashin-Shtrikman) bound Let $t \in [0, k_1]$. Proceeding as before, we find that optimal values of D_i and V_i are zeros, $D_i = 0$, $V_i = 0$ and W_t^{poly} becomes

$$W_t^{\text{poly}} = \min_{S_i \in \mathcal{S}} \Gamma, \quad \Gamma = \sum_{i=1}^{N} m_i (k_i + t) S_i^2 \tag{3.20}$$

where

$$\mathcal{S} : \left\{ S_1, \ldots, S_N : \sum_i^N m_i S_i = S_0 \right\}. \tag{3.21}$$

Performing minimization over S_i, we compute optimal values of S_i (compare with (3.10))

$$S_i = \frac{1}{k_i + t} H_0(t) S_0. \tag{3.22}$$

where

$$H_0(t) = \left(\sum_i^N \frac{m_i}{k_i + t} \right)^{-1}. \tag{3.23}$$

Then we compute Γ,

$$\Gamma = H_0(t) S_0^2$$

and arrive at a lower bound (3.17)

$$k_* \geq B(t) \quad \forall t \in [0, k_1]; \quad B(t) = (-t + H_0(t)). \tag{3.24}$$

Finally, we choose $t \in [0, k_1]$ (see (3.19)) to maximize the lower bound $B(t)$. A straightforward calculation shows that optimal value of t is k_1 - the end point of its permitted interval.

$$k_L = \max_{t \in [0, k_1]} (-t + H_0(t)) = -k_1 + H_0(k_1). \tag{3.25}$$

We arrive at the Hashin-Shtrikman bound (1.2) a.k.a. *translation bound.*

Fields in translation-optimal structures If $t = k_1$, the left-hand side of (3.18) is independent of $D(x)$ if $x \in \Omega_1$ because the coefficient $(k_1 - t)$ by D^2 vanishes, and

$$G_i^{poly}(S_1, D, 0, k_1) = \text{ constant}(D).$$

Optimal D-components are

$$\int_{\Omega_1} D(x) dx = 0, \quad D(x) \text{ is undefined } \forall x \in \Omega_1, \tag{3.26}$$

$$D(x) = 0, \ \forall x \in \Omega - \Omega_1. \tag{3.27}$$

The value of $D(x),\ x \in \Omega_1$ can be arbitrary. In order to satisfy the constraint (3.7) on the mean field, the average D_1 must be zero $D_1 = 0$. Optimal S-components are ordered and constant in each subdomain,

$$S_i = \beta_i S_0, \quad \beta_i = \frac{1}{k_i + k_1} H_0(k_1)\ i = 1, \ldots, N. \tag{3.28}$$

Notice that the polyconvex bound admits a minimizer with nonzero D-component in Ω_1, unlike the harmonic mean bound. This flexibility in minimizers makes the bound attainable by a structure in which fields in all but the first material are isotropic and incompatible $D_i, = V_i = 0,\ i = 2, \ldots N$. The D-component of the field in the first material may vary with $x \in \Omega_1$, providing a connectedness between other materials so that (2.20) is satisfied at all interfaces, see [4] and the discussion below. In an optimal structure, domain Ω_1 is placed between the other domains which have mutually incompatible fields.

In other terms, sets $\Psi_i,\ i > 1$ of ranges of ∇u in Ω_i are rank-one connected to Ψ_1 set, see (2.22), (2.23). Indeed, sets $\Psi_i,\ i > 1$, consist of one isotropic matrix each: $\Psi_i = \{\nabla u : \ S = S_i, D = 0, V = 0\}$, but set Ψ_1 consists of all symmetric (V=0) matrices with a fixed trace and arbitrary D-component, $\Psi_1 = \{\nabla u : \ S = S_1, D\text{- arbitrary}, V = 0\}$. The equality (2.18) of the tangent components of ∇u in Ω_1 and a neighboring subdomain Ω_i is expressed as $S_i = S_1 + D_1$ in notations (2.33). By choosing a proper value of D in Ψ_1, one can make sets Ψ_1 and $\Psi_i,\ i > 1$ be rank-one connected.

Remark 3.1 Translation bound assumes a special role of the first phase k_1 because $e \in \Psi_i$ connects all fields. When fraction m_1 of it tends to zero, $m_1 \to 0$, the fields in remaining phases lose connectedness and the bound become loose like the Harmonic mean bound. This causes the paradox of Hashin-Shtrikman bound mentioned in the Introduction. Algebraically, we observe that translation parameter t is less than or equal to k_1 regardless of the volume fraction of k_1. Correspondingly, the bound depends on k_1 even in the limit $m_1 \to 0$.

Remark 3.2 The translation bound for an anisotropic conductivity tensor K_*

$$2\frac{\det K_* - k_1^2}{\operatorname{Tr} K_* - 2k_1} \geq H_0(k_1) \quad \forall K_* \text{ in } G\text{-closure} \tag{3.29}$$

is obtained by the same method (see [24, 31]) and degenerates into (1.2) when $K_* = k_* I$. This time, the average field e is not proportional to the unit matrix, $D(e) \neq 0$, but is related to the degree of anisotropy of bounding tensor K_*. Notice that $B_0(k_1)$ and $H_0(k_1)$ keep their forms if $D_1 \neq 0$ which is the case for anisotropic e_0 and K_* (see below, Section 6.2). In this case, the optimal fields are similar to (3.26), (3.27) but

D-component in Ω_1 has the average equal to $D_1 = \frac{1}{m_1}D(e)$. The D-components in the other materials are zero. The *translation bound* is obtained similarly, it has a form [24],

3.3 Fields in Two-material Optimal Structures

Supporting points Consider a two-material optimal isotropic composite from the material k_m and k_i, $k_m > k_i$. It satisfies the translation bounds: The fields in the structures satisfy conditions (3.26), (3.27), (3.28). Here we show that D-component of the field in Ω_1 is bounded,

$$D^2 \leq (S_i - S_m)^2 \quad \forall \text{ in } \Omega_i. \tag{3.30}$$

In Ω_m, the field is isotropic: $S(x) = S_m = \beta, D(x) = 0, V(x) = 0$. The corresponding potentials are affine functions

$$u_a = \frac{1}{2}\beta_m S_0^2 x_1, \quad u_b = \frac{1}{2}\beta_m S_0^2 x_2, \quad \forall x \in \Omega_m.$$

At the boundary ∂_{im}, the continuity conditions (2.18), (2.19) are satisfied. Since the field in Ω_m is constant and isotropic, the field component S, D, V at Ω_i-side of the boundary satisfies the conditions

$$S - D = S_m, \quad S + D = \frac{k_m}{k_i} S_m, \quad V = 0 \quad \text{on } \partial_{im}$$

or

$$D^2 = (S - S_m)^2, \quad S = \frac{k_i + k_m}{2k_i} S_m, \quad V = 0 \text{ on } \partial_{im} \tag{3.31}$$

showing that $S(\nabla u)$ and $D(\nabla u)$ are constant at the boundary ∂_{im} regardless of the orientation of its normal.

In domain Ω_i, the translation optimality conditions (3.26)-(3.28) state that $S = S_i =$ constant, $V = 0$. Using (2.30), these conditions are represented through potentials u_a, u_b as

$$\frac{\partial u_a}{\partial x_1} + \frac{\partial u_b}{\partial x_2} = 2\beta_i, \quad \frac{\partial u_a}{\partial x_2} - \frac{\partial u_b}{\partial x_1} = 0 \quad \forall x \in \Omega_1. \tag{3.32}$$

Equations (3.32) are reminiscent of Cauchy-Riemann conditions. They state that u_a and u_b can be represented as sum of an affine function of x_1, x_2 and the real and imaginary parts of an analytic in Ω_i function $\hat{u}$ of $x_1 + ix_2$, respectively,

$$u_a = \beta_i x_1 + \Re(\hat{u}), \quad u_a = \beta_i x_2 + \Im(\hat{u}). \tag{3.33}$$

This and similar representations have been used in [38, 28, 17] to find families of optimal structures.

Absolute value $|\nabla\hat{u}|$ of gradient of an analytic function reaches its maximum at the boundary of Ω_i. Using (3.32), we exclude derivatives of u_b and express $\det\nabla u$ through gradient ∇u_a of a harmonic in Ω_i function u_a,

$$\det(\nabla u) = \frac{\partial u_a}{\partial x_1}\left(-\frac{\partial u_a}{\partial x_1} + 2\beta_i\right) - \left(\frac{\partial u_a}{\partial x_2}\right)^2 = -\|\nabla(u_a - \beta_1 x_1)\|^2. \tag{3.34}$$

The right-hand side of (3.34) reaches its minimum at the boundary ∂_{im} and so does $\det(\nabla u)$. Because of decomposition (2.31), $\det(\nabla u) = S^2 + V^2 - D^2$. Optimality conditions require that $V(x) = 0,\ S(x) = S_i =$ constant, $x \in \Omega_i$, therefore

$$\det\nabla u(x) = -D^2(x) + S_i^2 \quad \forall x \in \Omega_i. \tag{3.35}$$

Correspondingly, $D(x)$ reaches its maximum at ∂_{im} which proves (3.30).

Relations (3.26), (3.27),(3.28), and (3.30) state that fields in a two-phase optimal structures are ordered: Difference between fields in Ω_i and Ω_m is nonnegative defined:

$$e(x) - e(y) \geq 0 \Rightarrow \det(e(x) - e(y)) \geq 0 \quad \forall x \in \Omega_i,\ \forall y \in \Omega_m. \tag{3.36}$$

Notice that relation (3.36) holds also for anisotropic two-component optimal structures. Particularly, it holds for second-rank laminates and for simple laminates.

Remark 3.3 [Symmetry of fields in optimal structures] The conclusion of symmetry of the fields ($V = 0$) in optimal structures is based on the orthogonality of applied fields E_1 and E_2 and the symmetry of e_0, $V_0 = 0$. If these fields were non-orthogonal, the consideration would be similar but formulas would be more bulky. The term $\sqrt{S^2 + V^2}$ would replace S in the calculations below.

4 Bound by Localized Polyconvexity

4.1 Boundedness of the Fields in Optimal Structures

Constraints The range of fields $e(x)$ in optimal multimaterial structures is bounded. For example, the constraint $\det e \geq 0$ (see [33, 5]) or

$$S^2 + V^2 \geq D^2 \quad \forall x \in \Omega \tag{4.1}$$

follows from the differential constraints (2.17), (2.18) on the minimizer. The inequality (4.1) holds for all structures, whether they are optimal or not. It is used in Nesi bound [33] to improve Hashin-Shtrikman bound.

The fields in optimal microstructures satisfy certain additional *local optimality conditions* that pointwise restrain the ranges Ψ_i of the fields in optimal composites. These conditions, implemented into the polyconvex envelope procedure, result in better bounds. We call this lower estimate *localized polyconvexity.*

Remark 4.1 An example of constraints are the mentioned local optimality conditions by *structural variation* [21, 22, 32, 9]. They provide uniform inequalities for the fields in an optimal structure. The structural variation is performed by interchanging two infinitesimal elliptical inclusions from materials k_i and k_j. These inclusions are placed in arbitrary points of subdomains Ω_j and Ω_i, respectively, and the increment of $J(\chi, e_0)$ is computed. The increment is nonnegative, if the tested configuration is optimal. This condition leads to an inequality that constrains values of fields $e \in \Psi_i$ and $e \in \Psi_j$ in arbitrary points of Ω_i and Ω_j, respectively. It uniformly restricts the fields in Ω_i and Ω_j.

Ordering and boundedness Fields in the materials in optimal structures are ordered: Norms $\|e_i\| = \sqrt{\operatorname{Tr}(e_i^T e_i)}$ satisfy inequalities

$$\|e_i\| \in [\alpha_{i+1}, \alpha_i] \tag{4.2}$$

where α_i are ordered constants, $0 \le \alpha_N \le \ldots \le \alpha_1 < \infty$. These inequalities can be proven if the variational problem (2.24) is rewritten as a multiwell problem (see, for example [9]) with the Lagrangian

$$F = \min_{i=1,\ldots N} \left\{ \frac{1}{2} k_i \|e_{i+1}\|^2 + \gamma_i \right\}$$

that depends only on e. Here γ_i are Lagrange multipliers by constraints (2.3), ordered as follows $\gamma_1 > \ldots, \gamma_n$. The ordering constrains fields in all materials but the first one.

Field in Ω_1 is bounded as well. Indeed, potential u_a in domain Ω_1 is harmonic, therefore the norm of its gradient reaches its maximum at the boundary $\partial\Omega_1$ (see (2.6)). At the other side of this boundary, where other materials are located, ∇u_a is bounded, see (4.2). The jump conditions (2.18) requires that ∇u_a at $\partial\Omega_1$ is bounded too; therefore it is bounded everywhere in Ω_1. The same is true for ∇u_b. Therefore, $\|e(x)\|^2 = S^2 + D^2 + V^2$ is bounded everywhere in Ω.

Remark 4.2 The boundedness of $\|e(x)\|$ geometrically restricts optimal multiphase microstructures. Particularly, boundaries with corners are excluded and structures where three or more materials meet in isolated points. In such structures, fields are singular in a neighborhood of these special points.

An account for constraints on Ψ_i-sets improves the bounds on effective properties. To derive the bound, we explore a simple lemma.

Lemma 4.1 Let α be a real parameter, Ω a bounded domain, and $v(x)$ - an integrable function in Ω. Assume that $v(x)$ is bounded in Ω and its mean value is fixed,

$$\|v(x)\|_{L_\infty} \le v_{\max}, \quad \frac{1}{\|\Omega\|}\int_\Omega v(x)dx = v_0. \tag{4.3}$$

Here v_0, $v_{\max}$ are real numbers and

$$|v_0| \le v_{\max}. \tag{4.4}$$

Then

$$\min_{v(x)\,\mathrm{as\,in}(4.3)} \left(\frac{1}{\|\Omega\|}\int_\Omega \alpha v^2 dx\right) = \begin{cases} \alpha v_0^2 & \text{if } \alpha \ge 0 \\ \alpha v_{\max}^2 & \text{if } \alpha \le 0 \end{cases}. \tag{4.5}$$

Indeed, if $\alpha \ge 0$, integrant αv^2 is a convex function of v, therefore the minimum in left-hand side is achieved at a constant minimizer $v(x) = v_0$. The value of minimum and the minimizer are independent of $v_{\max}$. If $\alpha \le 0$, integrant αv^2 is a concave function of v, therefore the minimum corresponds to piece-wise constant $v(x)$ that alternates its extreme values

$$v_{\mathrm{opt}}(x) = v_{\max} \text{ or } v_{\mathrm{opt}}(x) = -v_{\max} \quad \forall x \in \Omega.$$

Measures of the subdomains where and $v_{\mathrm{opt}} = -v_{\max}$ are equal to $\|\Omega\|m_A$ and $\|\Omega\|m_B$ respectively. Here $m_A \in [0, 1]$ is a volume fraction of the domain where $v_{\mathrm{opt}} = v_{\max}$ and $m_B = 1 - m_A$. The value of minimum is independent of m_A. The average value of minimizer can be made equal to v_0 by a proper choice of these measures, $m_A = \frac{v_0+v_{\max}}{2v_{\max}}$ Then (4.3) is satisfied.

4.2 Optimal Constrained Fields and Bounds

Assume that ranges Ψ_i of fields in an optimal structure are described by inequalities $\theta_i(S, D, V) \ge 0$. Below in Section 4.4, we describe these constraints. Here, we work out the algebra of the bounds if the constraints are applied. We assume that constraints have the form

$$V = 0, \quad D^2 \le \Theta_i(S) \text{ in } \Omega_i \tag{4.6}$$

where Θ_i are some nonnegative functions. Constraints of ranges of optimal fields Ψ_i can be implemented into the translation bound derivation, similarly to [33].

We return to the scheme of polyconvex envelope for a multiphase composite, $N \ge 3$ accounting for constrained fields in an optimal structure. Assume that fields in an optimal structure are constrained as (4.6) and let us choose translation parameter t in (3.24) larger than k_1, $t > k_1$. Then some terms in the right-hand side of inequality (3.16) become nonconvex and constraints (4.6) become active.

First, assume that $k_1 < t \le k_2$. Consider inequality (3.18) for $i = 1$. Coefficient $(k_1 - t)$ in front of $\int_{\Omega_1} D^2 dx$ in the right-hand side is negative. According to Lemma, the constraint on $D^2 \le \Theta_1(S)$ becomes active and the minimizer takes values

$$D(x) = \pm\Theta_1^{\frac{1}{2}}(S(x)) \quad \forall x \in \Omega_1.$$

The integral of D^2 is estimated as

$$\int_{\Omega_1} D^2 dx \le \int_{\Omega_1} \Theta_1(S) dx = m_1 \Theta_1(S_1).$$

Functions G_i in inequalities (3.18) become

$$G_1 = (k_1 + t)S_1^2 + (k_1 - t)\Theta_1(S_1), \tag{4.7}$$

$$G_i = (k_i + t)S_1^2, \quad i = 2, \ldots, N. \tag{4.8}$$

Next calculation, performed as in (3.20), gives the expression for $H(t) = H_1(t)$ that differs from (3.20) only in the value of G_1 that is defined in (4.8).

Finally, the most restricted lower bound k_L is defined by maximum of H_0 and H_1. The bound has the form similar to (3.24):

$$k_L = \max_{t \in [k_1, k_2]} \left(-t + H(t)\right), \quad H(t) = \begin{cases} H_0(t) \text{ if } t = k_1, \\ H_1(t) \text{ if } t \in (k_1, k_2]. \end{cases} \tag{4.9}$$

Notice that H continuously depends on t. Notice also that $t \in [0, k_1)$ are nonoptimal (see (3.25)), therefore these values are not accounted for in (4.9).

Supports of optimal fields. By assumption, optimal fields are symmetric, $V = 0$. When $t < k_2$, the S and D components are

$$\begin{array}{ll} S(x) = S_i, \ D(x) = 0 & \forall x \in \Omega_i, \ i > 2, \\ S(x) = S_1, \ D(x) = \pm\Theta_1^{\frac{1}{2}} & \forall x \in \Omega_1. \end{array} \tag{4.10}$$

The fields are constant and isotropic is all materials but the first. In the first material, D-component of the optimal field is not completely defined: It can take one of two values in each point.

When $t = k_2$, D-component is undetermined in Ω_2, and Ω_2 plays the same role as Ω_1 plays in the translation bound. The optimal fields are

$$\begin{array}{ll} S(x) = S_i, \ D(x) = 0, & \forall x \in \Omega_i, \ i > 2, \\ S(x) = S_1, \ D(x) = \pm\Theta_1^{\frac{1}{2}}, & \forall x \in \Omega_1, \\ S(x) = S_2, \ D(x)^2 \le \Theta_2, \ D_2(x) \text{ is not defined} & \forall x \in \Omega_2. \end{array} \tag{4.11}$$

More than three materials When the number of materials is greater than three, the procedure can be continued. Increase of t leads to increase of the number of active constraints. When $k_r < t \le k_{r+1}$, r constraints are active:

$$G_i = \begin{cases} (k_i + t)S_i^2 - (t - k_i)\Theta_i(S_i) & \text{if } i < r \\ (k_i + t)S_1^2 & \text{if } r \le i \le N \end{cases} \tag{4.12}$$

$$\Gamma_r = \sum_{i=1}^{N} m_i G_i = \sum_{i=1}^{N} m_i \left[(k_i + t)S_i^2\right] - \sum_{i=1}^{r} m_i (t - k_i)\Theta_i(S_i), \tag{4.13}$$

and

$$H_r(t) = \min_{S_i \in S, S_0 = 1} \Gamma_r. \tag{4.14}$$

Bound (3.24) for the effective properties corresponds to the maximum over t of the obtained expressions. It becomes

$$k_L = \max_{r=0,\dots,N-1} B_r, \tag{4.15}$$

$$B_r = \max_{t \in [k_r, \le k_{r+1}]} \left(-t + H_r(t)\right). \tag{4.16}$$

Optimal fields are symmetric, $V(x) = 0$. They are either isotropic (D-component is zero) or they belong to the boundary of the permitted region ($|D|$-component is maximal). If $t = k_r$, the D-component is undetermined in Ω_r.

$$\begin{array}{ll} S(x) = S_i,\ D(x) = 0, & x \in \Omega_i,\ i = r+1, \dots, N \\ S(x) = S_i,\ D(x)^2 = \Theta_i, & x \in \Omega_i\ i = 1, \dots, r-1 \\ S(x) = S_i,\ \begin{cases} D(x)^2 = 0 & \text{if } t < k_r \\ D(x)^2 < \Theta_2 & \text{if } t = k_r \end{cases}, & x \in \Omega_r \end{array} \tag{4.17}$$

These fields are shown at Figure 1.

This procedure excludes optimal values of D. The optimal values S_i can be found from the finite-dimensional optimization problem (4.14).

Remark 4.3 In localized polyconvexity, the pointwise constraints Θ_i on the optimal fields in Ω_i become active everywhere in these sets when $t > k_i$. The points of Ω_i are undistinguishable because the differential constraints are not account for.

4.3 Nesi bounds

Nesi [33] used the inequality (4.1) to improve Hashin-Shtrikman bounds. It leads to constraints

$$\Theta_i = \Theta_i^\eta = S_i^2, \quad i = 1, \dots N. \tag{4.18}$$

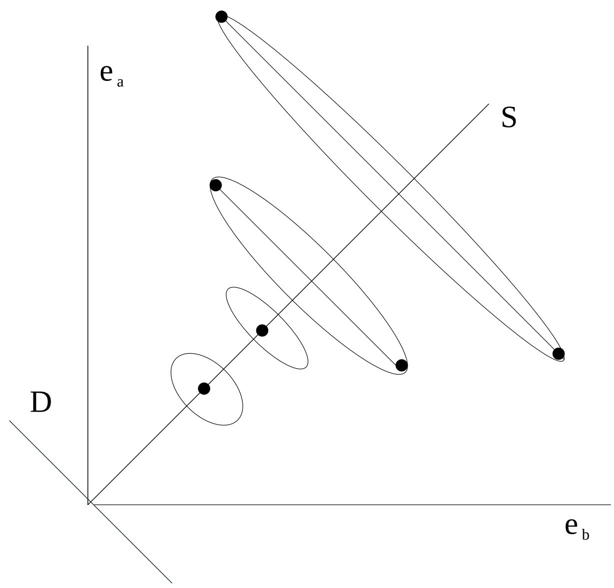

Figure 1: Cartoons of the sets of supports (represented by ellipses) and locations of supports (small circles) in the localized polyconvexification procedure. Case $N = 4$, $k_2 < t < k_3$

and bound (4.15) becomes a Nesi-type bound, as follows. When $t \in (k_n, k_{n+1}]$, $(n < N-2)$, we compute from (4.13), (4.1)

$$G_i = \begin{cases} 2k_i S_i^2 & \text{if } i < n \\ (k_i + t)S_i^2 & \text{if } n \le i \le N \end{cases}$$

minimize Γ (4.13) over S_i and obtain

$$H_n = \left(\sum_{i=1}^{n} \frac{m_i}{2k_i} + \sum_{i=n+1}^{N} \frac{m_i}{t + k_i} \right)^{-1}.$$

The bound has the form (4.15). In Nesi bounds, the optimal D-fields satisfy the relations

$$|D_i| = \begin{cases} S_i & \text{if } i < n \\ 0 & \text{if } i > n \end{cases},$$

and

$$|D_n| = \begin{cases} 0 & \text{if } t \le k_{n+1} \\ \text{undefined} & \text{if } t = k_{n+1} \end{cases}.$$

Nesi bound is better than translation bound when volume fraction m_1 is smaller than a threshold. However, its asymptotic $m_1 \to 0$ does not show the expected limit: Hashin-Shtrikman bound for the remaining materials. However, we show in Section 7 that the bound becomes asymptotically exact when $k_n \to \infty$.

Remark 4.4 Nesi bound is generally not achievable by a structure. Indeed, according to the bound, an optimal field satisfies the relation $|D_1| - S_1 = 0$, or $\det(e_(x)) = 0$ almost everywhere in Ω_1. This condition implies that $\det(\nabla u) = 0$ or that ∇u_a and ∇u_b are collinear almost everywhere in Ω_1. Then, solutions u_a and u_b are linearly dependent contrary to (2.15). Therefore, condition (4.1) cannot be satisfied if $k_n < \infty$ and the bound cannot be exact.

4.4 Extremal constraints

Algebraic form of constraints Geometry of domains Ω_i can be arbitrary, therefore the constraints on Ψ_i do not depend on a point's position in these domains. In particular, it cannot depend on the distance to the boundary, its curvature, connectedness of Ω_i, etc, since these can be arbitrary chosen to minimize the energy; the points in optimal Ω_i domains are undistinguishable. Constraints on Ψ_i are expressed only through the values of e in Ω_i.

Sets Ψ_i depends only on rotational invariants S, V and D of field $e(x)$ and are independent of orientation of its eigenvectors. This feature follows from isotropy of composites: An optimal structure can be composed of several arbitrarily rotated fragments of overall isotropic structure, combined in a larger scale. All the fields are scaled by magnitude S_0 of external field and effective properties are independent of it.

Assume that sets Ψ_i are described by inequalities $\bar{\theta}_i(e) \geq 0$. The constraints have the forms

$$\bar{\theta}_i(S, D, V, M) \geq 0 \text{ or } D^2 \leq \bar{\Theta}_i(S, V, M) \quad \text{in } \Omega_i \tag{4.19}$$

where M is the vector of volume fractions, $M = (m_1, \dots m_N)$. $\bar{\theta}_i$ are homogeneous functions of S, D, V,

$$\bar{\theta}_i(S, D, V, M) \geq 0 \Rightarrow \bar{\theta}_i(\gamma S, \gamma D, \gamma V, M) \geq 0, \ \forall \gamma > 0.$$

We can assume that $S_0 = 1$. The constraints assume the form

$$\bar{\theta}_i(S, D, V, M) \geq 0 \quad \text{in } \Omega_i. \tag{4.20}$$

Optimality of constraints The translation-type bounds by localized polyconvexity in Section 4.1 monotonically depend on constraints Θ_i, see (4.14) (the exception is Hashin-Shtrikman bound where the constraints are nor active). The bound k_L in (4.14) decreases when Θ_i increases,

$$\frac{\partial k_L}{\partial \Theta_i} \leq 0, \quad i = 1, \ldots, N. \tag{4.21}$$

The translation bound corresponds to the absence of the constraints and is the least restrictive. Nesi bound is more restrictive, it uses inequalities (4.1). It is asymptotically ($k_N \to \infty$), see Section 8.2. This bound could be further improved if Θ_i are smaller, see Remark 4.4. The toughest bound corresponds to the smallest $\Theta_i \geq 0$. The anisotropic component D of the field is unrestricted by the mean field and should be made as small as possible, see (3.6).

The conditions (2.18), (2.20) of continuity of potential u at the boundaries imply that $\Theta_i > 0$ for some i that is any structure necessarily includes some fields with nonzero D-components. Constraints must allow for relaxed rank-one connectedness of the sets: Inequalities (2.23) should are satisfied for all Ψ_i. For continuity of the potentials at the interfaces, it is *sufficient* to require that the sets Ψ_i contain relaxed rank-one connected matrices.

Generally, $\bar{\theta}_i$ might depend on volume fractions M. We request that constraints (4.19) are independent of M and assume the form

$$\theta_i(S, D, V) = \bigcup_M \bar{\theta}_i(S, D, V, M) \geq 0 \quad \forall x \in \Omega_i. \tag{4.22}$$

This assumption does not decreases Ψ_i-sets because the inequality (4.22) is valid for all volume fractions.

Particularly, (4.22) is satisfied for less-than-N materials composite, namely for any two-material composites from materials k_i and k_p, $i, p = 1, \ldots, N$, $k_i < k_p$. The two-material problem is an asymptotic of the general one, that corresponds to vanishing of all volume fractions but two, $m_j \to 0$, $j \neq i, p$. Referring to (3.26)-(3.28), (3.30), we require that Ψ_p contains the point $[S_p, D_i = 0, V = 0]$, and Ψ_i contains the point $[S_i, D_i = S_i - S_p, V = 0]$, or

$$\theta_p(S_p, 0, 0) \geq 0, \quad \theta_i(S_i, \pm(S_i - S_p), 0) \geq 0, \ 1 \leq i < p \leq N. \tag{4.23}$$

The minimal of all sets that satisfy conditions (4.19)-(4.23) are follows.

1. The nonsymmetric V-component of e is zero everywhere (see Remark 3.3),

$$V(x) = 0 \ \text{ in } \Omega. \tag{4.24}$$

2. Field in Ω_N is constant and isotropic, $e_N = \frac{1}{\sqrt{2}}\beta_N I$. Ψ_N consists on one point:

$$S_N = \beta_N, \quad D = 0. \tag{4.25}$$

3. The smallest Ψ_i-set, rank-one connected with Ψ_N (4.25) contains the field e such that $\det(e(x) - \beta_N I) = 0$. The corresponding constraint is

$$D^2 \le \Theta_i(S) = (S - \beta_N)^2, \quad \forall S, D \in \Psi_i, \ i = 1. \dots, N-1. \tag{4.26}$$

Notice that (4.26) is stronger than (4.18) and coincides with it when $\beta_N = 0$ or $k_N = \infty$.

Uniform connectedness We call sets $\Psi_1, \dots \Psi_N$ *uniformly connected* if any pair of them contains rank-one connected matrices, see Figure 2,

$$\exists e(x), \ x \in \Omega_i, \ \ \exists e(y), \ y \in \Omega_j : \ \det(e(x) - e(y)) = 0, \ \forall i, j = 1, \dots, N. \tag{4.27}$$

In terms of microstructures, the constrains do not prevent any two subregions Ω_i and Ω_j from being neighbors in the structure. Sets Ψ_i defined by (4.24), (4.25), (4.26) are uniformly connected. Moreover, it is easy to see that they form a *minimal uniformly connected set* of fields. Notice that the ranges Ψ_1 and Ψ_N are independent of properties k_i of intermediate materials. Notice also that the ranges of intermediate materials belong to the convex envelope of Ψ_1 and Ψ_N,

$$\Psi_i \in \mathcal{C}\left(\Psi_1, \Psi_N\right), \ i = 2, \dots, N-1. \tag{4.28}$$

This feature is expected because each intermediate material can be equivalently replaced by a mixture of the extreme materials k_1 and k_N, $k_i \in G-\text{closure}(k_1, k_N)$.

Remark 4.5 The corresponding constraints for anisotropic K_* could be different: (4.22) may be refined if its dependence of $D_0 \neq 0$ is accounted for.

Remark 4.6 The conditions of contacts between materials in an optimal structure are investigated in [9] (Chapter 9). This technique is a development of the structural variation technique suggested by Lurie in [22]. They are obtained by comparing the jump conditions (2.18), (2.19) with an increment of functional J caused by *structural variation* in a neighborhood of an optimal boundary. Conditions of an optimal contact coincide with the above conditions (4.25) and (4.26).

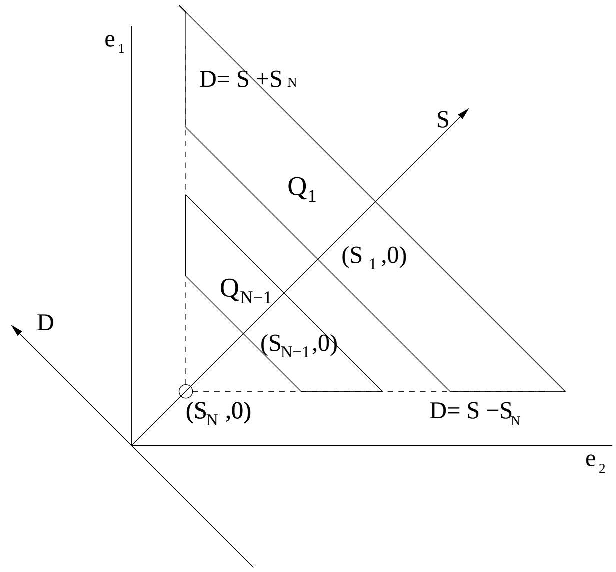

Figure 2: Uniformly connected sets Q_i of ranges of fields in materials k_i

5 New Lower Bound

5.1 First bound by localized polyconvexity

Here we work out the bounds of Section 4.2 using the constraints (4.26). Assume that $k_1 < t \le k_2$ and substitute $\Theta_1 = (S_1 - S_N)^2$ into inequalities (4.7), (4.8). We have

$$\begin{aligned} G_1 &= (k_1 + t)S_1^2 + (k_1 - t)(S_1 - S_N)^2 \\ &= 2\,k_1 S_1^2 + (k_1 - t)\,(-2S_1 + S_N)\,S_N, \\ G_i &= (k_i + t)S_i^2, \quad i = 2, \dots, N. \end{aligned}$$

The value of Γ (see (4.13)) in the interval $k_1 < t \le k_2$ is denoted as Γ_1 where index 1 points to left end of the interval $(k_1, k_2]$ of variation of t. It is equal to

$$\begin{aligned} \Gamma_1 &= \Gamma|_{t\in(k_1,k_2]} = 2m_1 k_1 S_1^2 + \sum_{i=2}^{N-1} m_i (k_i + t) S_i^2 \\ &- 2m_1(k_1 - t)S_1 S_N + (m_N(k_N + t) + m_1(k_1 - t))\,S_N^2 \end{aligned} \tag{5.1}$$

or in the vector form

$$\Gamma_1 = S^T(R_1 + Y_1 P^T)S.$$

Here S is vector of components of the fields in materials, $S^T = (S_1, \ldots, S_N)$, R_1 is a diagonal $N \times N$ matrix

$$R_1 = \mathrm{diag}(m_1(2k_1), m_2(k_2+t), \ldots, m_N(k_N+t) + m_1(k_1-t)), \tag{5.2}$$

and Y_1 and P are N-dimensional vectors with the entries

$$(Y_1)_j = \begin{cases} -2m_1(k_1-t) & \text{if } j=1 \\ 0 & \text{if } j=2,\ldots,N \end{cases}, \tag{5.3}$$

$$(P)_j = \begin{cases} 0 \text{ if } j=1,\ldots,N-1 \\ 1 \text{ if } j=N \end{cases}. \tag{5.4}$$

A rank-one nonsymmetric matrix Y_1P^T has only one nonzero entry $(Y_1P^T)_{1N} = -2m_1(k_1-t)$ that corresponds to term $-2m_1(k_1-t)S_1S_N$ in right-hand side of (5.1).

Quadratic form Γ_1 is assumed to be nonnegative. This assumption corresponds to symmetric part of matrix $R_1 + Y_1P^T$ being nonnegative defined. Solving the last condition for m_N we arrive at a condition

$$m_N \geq m_1 \frac{2t(t-k_1))}{(k_1+t)(k_N+t)} \quad \forall t \in (k_1, k_2]. \tag{5.5}$$

The inequality is the strongest, if $t = k_2$. Here, we assume this inequality to be true (for three-material composites, the opposite case of small m_N corresponds to the optimality of the Hashin-Shtrikman bound, as it can be checked from the corresponding formulas in Section 7).

We normalize the mean field, $S_0 = m_1S_1 + \ldots + m_NS_N = 1$ or, in the vector form,

$$M^TS = 1, \quad M^T = (m_1, \ldots m_N). \tag{5.6}$$

and minimize Γ_1 over vector $S = (S_1, \ldots S_N)$. Performing minimization, we find vector S_{opt} of optimal fields

$$S_{\mathrm{opt}}(t) = H_1(R_1 + Y_1P^T)^{-1}M \quad \text{and } \min_S \Gamma_1 = \frac{1}{H_1} \tag{5.7}$$

where

$$H_1 = \frac{1}{M^T(R_1 + Y_1P^T)^{-1}M}. \tag{5.8}$$

Finally, we substitute (5.7) into bound (4.15), (4.16) and obtain

$$k_L^{(1)} = \max_{t \in (k_1, k_2]} (-t + H_1.) \tag{5.9}$$

Accounting for (5.2), (5.3), and (5.4), we compute $\frac{1}{H_1}$,

$$\begin{aligned}\frac{1}{H_1} &= \sum_{i=2}^{N-1} \frac{m_i}{k_i + t} \\ &+ \frac{(k_1 - t)m_1^2 + (k_N + 2k_1 - t)m_1 m_N + 2k_1 m_N^2}{(k_1^2 - t^2)m_1 + 2k_1(k_N + t)m_N}.\end{aligned} \tag{5.10}$$

Observe that H_1 degenerates into H_0 (1.2) when $t = k_1$. Therefore this bound is no less restrictive than Hashin-Shtrikman bound (1.2).

Supporting sets The supporting sets of the pairs (S, D) for the optimal fields (5.7) are

$$\begin{aligned}\Psi_1 &= \{S_1, \pm(S_1 - S_N)\} \\ \Psi_2 &= \begin{cases} \{S_2, 0\} & \text{if } t \in (k_1, k_2) \\ \{S_2, D\},\ D \leq S_1 - S_N & \text{if } t = k_2 \end{cases} \\ \Psi_i &= \{S_i, 0\},\ i = 3, \dots, N\end{aligned} \tag{5.11}$$

where S_i are as in (5.7).

Formulas (5.11) imply that field e in Ω_1 is always in the rank-one contact with $e_N = S_N I$ in an optimal structure. In Ω_1, the $D(x)$-component is not defined pointwise. It is only required that $D(x)$ alternates values $\pm(S_1 - S_N)$ and its mean value is zero

$$\int_{\Omega_1} D(e_1)dx = D_0 = 0. \tag{5.12}$$

When $t_{\text{opt}} = k_2$, the bound keeps its form, and S-components of the optimal fields are still computed by (5.7) but the D-component Ω_2 becomes undefined. Its mean value satisfies the constraint

$$\int_{\Omega_1} D(e)dx + \int_{\Omega_2} D(e)dx = D_0 = 0. \tag{5.13}$$

Remark 5.1 Nonzero values of $D(x)$ in Ω_2 provide the continuity of potential u at the interfaces when the uniformly bounded field ∇u in Ω_1 can no longer connect domains of other materials with isotropic fields, because volume fraction m_1 is too small. In that case, the D component of the field in Ω_2 becomes non-zero.

5.2 Next bounds

In general case ($N \geq 4$), calculations are similar. Assume that

$$t \in (k_r, k_{r+1}] \tag{5.14}$$

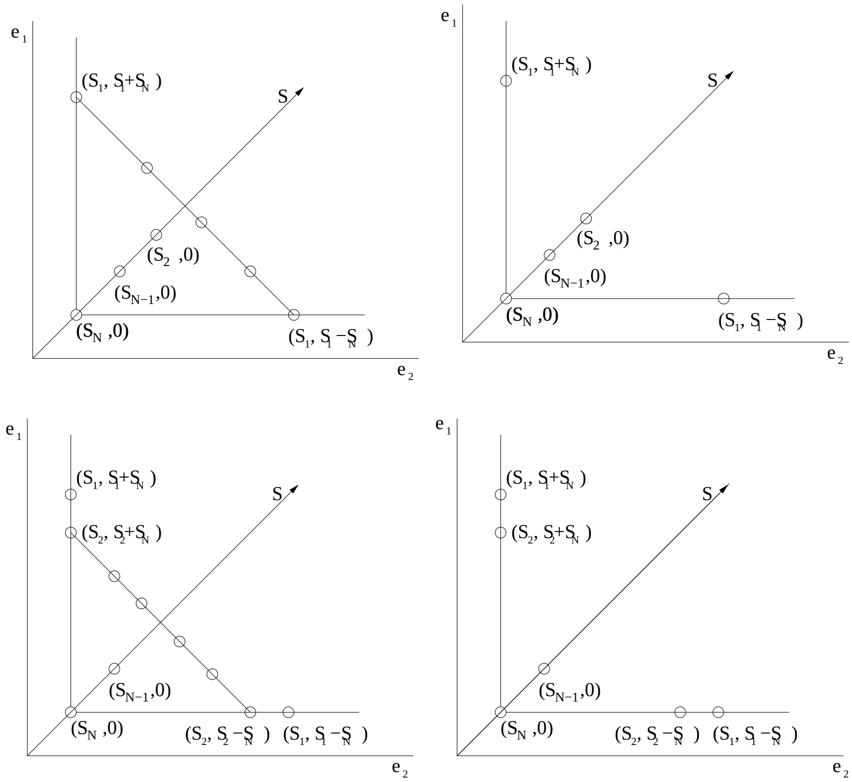

Figure 3: Eigenvalues of supporting fields e_i (5.11) that correspond to the bounds. Top left: Hashin-Shtrikman bound ($t = k_1$). Top right: first bound, $k_1 < t_0 < k_2$. Bottom left: second bound, $t = k_2$. Bottom right: $k_2 < t_0 < k_3$

where $r = 2, \ldots, N-2$. Terms $(k_i - t)D_i^2$, $i - 1, ..., r$ become concave and corresponding constraints $(D_i)^2 \le (S_i - D_i)^2$, $i = 1, ...r$ become active.

We compute as in (4.12)

$$G_{ri} = \begin{cases} (k_i + t)S_i^2 + (k_i - t)\,(S_i - S_i)^2 & \text{if } i = 1, \ldots, r \\ (k_i + t)S_i^2 & \text{if } i = r+1, \ldots, N \end{cases} \tag{5.15}$$

where first index r refers to interval $(k_r, k_{r+1}]$ of t and the second index i – to the material k_i. Then, we compute Γ as in (4.13)

$$\Gamma_r = \sum_{i=1}^{N} m_i(k_i + t)S_i^2 - \sum_{i=1}^{r} m_i(t - k_i)\,(S_i - S_N)^2$$

or in the vector form

$$\Gamma_r(t) = S_r^T(R_r + Y_r P^T)S_r$$

where R_r - diagonal matrix with components $(R_r)_{ii}$

$$(R_r)_{ii} = \begin{cases} 2m_i k_i & \text{if } i = 1, \ldots, r \\ m_i(k_i + t) & \text{if } i = r+1, \ldots, N-1 \\ \rho_r & \text{if } i = N \end{cases},$$

$$\rho_r = m_N(k_N + t) + \sum_{i=1}^{r} m_i(k_i - t), \tag{5.16}$$

P is defined in (5.4), and Y_r is a vector with coordinates

$$(Y_r)_i = \begin{cases} 2m_i(k_i - t) & \text{if } i = 1, \ldots, r \\ 0 & \text{if } i = r+1, \ldots, N \end{cases}. \tag{5.17}$$

To compute the bounds, we again fix $t \in (k_r, k_{r+1}]$ and perform minimization over the components S_i that are constrained as in (5.6) assuming positive definiteness of $(R_r + Y_r P^T)$,

$$(R_r + Y_r P^T) > 0. \tag{5.18}$$

Remark 5.2 For three-material mixtures, either (5.18) is satisfied, or Hashin-Shtrikman bound holds. However, for the more-than-three-material composites, this condition might become active, when simultaneously m_1 and m_N are sufficiently small. We do not work out the details of this case here.

Vector S_{opt} of optimal fields in the materials is

$$S_{\text{opt}}(t) = H_r (R_r + Y_r P^T)^{-1} M$$

where

$$H_r(t) = \frac{1}{M^T (R_r + Y_r P^T)^{-1} M}. \tag{5.19}$$

Thus, the problem of bounds is reduced to a finite-dimensional problem of constrained optimization: It remains to compute optimal t for each interval (5.14) and compare results:

Theorem 5.1 Effective conductivity k_* of any N-material composite that satisfies (5.18) is bounded from below by k_L,

$$k_L = \max_{r=1,\ldots,N-1} \left[\max_{t \in (k_{r-1}, k_r]} (-t + H_r(t)) \right] \tag{5.20}$$

where $k_0 = 0$.

When $m_1 \to 0$, the bound (5.20) tends to the bound for the remaining $N-1$ materials, unlike to Hashin-Shtrikman bounds (1.2).

5.3 Simplification of the Bound Form

Term $\frac{1}{H_r} = M^T (R_p + Y_p)^{-1} M$ can be simplified using Sherman-Morrison formula

$$(R_r + Y_r P^T)^{-1} = R_r^{-1} + \frac{1}{1 + Y_r^T R_r^{-1} P} R_r^{-1} Y_r P^T A^{-1}. \tag{5.21}$$

We compute

$$\frac{1}{H_r} = M^T R_r^{-1} M + \frac{(M^T R_r^{-1} Y_r)(P^T R_r^{-1} M)}{1 + Y_r R_r^{-1} P}. \tag{5.22}$$

Using definitions of R_r, M, Y_r, we compute

$$\begin{aligned} M^T R_r^{-1} M &= \sum_{i=1}^{r} \frac{m_i}{2k_i} + \sum_{i=r+1}^{N-1} \frac{m_i}{k_i + t} + \frac{m_N^2}{\rho_r}, \\ M^T R_r^{-1} Y_r &= 2 \sum_{i=1}^{r} m_i \frac{k_i - t}{k_i}, \quad Y_r^T R_r^{-1} P = 0, \quad P^T R_r^{-1} M = \frac{m_N}{\rho_r}. \end{aligned}$$

Substituting these terms into (5.22), we obtain an explicit formula

$$\frac{1}{H_r} = \sum_{i=1}^{r} \frac{m_i}{2k_i} + \frac{m_N^2}{\rho_r} + \sum_{i=r+1}^{N-1} \frac{m_i}{k_i + t} + 2 \frac{m_N}{\rho_r} \sum_{i=1}^{r} \frac{m_i}{k_i}(k_i - t).$$

Collecting the coefficients by m_i, we compute

$$\frac{1}{H_r(t)} = \sum_{i=1}^{r} \frac{m_i}{2k_i}\left(1 - \frac{4m_N(k_i - t)}{\rho_r}\right) + \sum_{i=r+1}^{N-1} \frac{m_i}{k_i + t} + \frac{m_N^2}{\rho_r} \tag{5.23}$$

where ρ_r is defined in (5.16). Expression (5.23) should be substituted into expression (5.20) for the bound.

Asymptotic When the optimal value of t_0 of translator t is $t_0 = k_1$, the bound becomes Hashin-Shtrikman bound. Indeed, we compute (5.23) in this case:

$$r = 0, \quad \rho = m_N(k_N + k_1), \quad H(k_1) = H_0(k_1) = \left(\sum_{i=1}^{N} \frac{m_i}{k_i + k_1}\right)^{-1}.$$

Substituting this expression into k_L, we obtain the Hashin-Shtrikman bound (1.2).

When $k_N = \infty$, we compute $\rho_r = \infty$, and H_r becomes as in Nesi bound

$$H_r(t) = \left(\sum_{i=1}^{r-1} \frac{m_i}{2k_i} + \sum_{i=r}^{N-1} \frac{m_i}{t + k_i}\right)^{-1}. \tag{5.24}$$

6 Generalizations

6.1 Upper (Dual) bound

The dual bound $k_U \geq k_*$ is found by the same procedure. It is enough to recall that any divergencefree field $j = (j_1, j_2)$ is a turned 90° gradient, $j = R\nabla u_{\text{dual}}$ where R is the matrix of 90° rotation, and u_{dual} is a dual scalar potential. The energy of the type $F = \frac{1}{k} j^T j$ where $\nabla \cdot j = 0$ can be represented as $F = \frac{1}{k}(\nabla u_{\text{dual}})^T (R^T R) \nabla u_{\text{dual}}$. Since $R^T R = I$, the form of energy becomes similar to the one used in derivation of the lower bound. Therefore, the lower bound $k_* \geq k_L(k_1, \dots k_N, m_1, \dots, m_N, t)$ where k_L is defined in (5.20), implies the dual bound

$$\frac{1}{k_*} \geq k_L\left(\frac{1}{k_N}, \dots, \frac{1}{k_1}, m_N, \dots, m_1, \frac{1}{t}\right) \tag{6.1}$$

obtained by the substitution

$$k_i \leftrightarrow \frac{1}{k_{N-i+1}} \quad m_i \leftrightarrow m_{N-i+1}, \quad t \leftrightarrow \frac{1}{t} \tag{6.2}$$

that preserves the ordering of conductivities $\frac{1}{k_N} < \dots, \frac{1}{k_1}$ and their fractions. The dual bound can be rewritten as the upper bound for k_*,

$$k_* \le k_U, \quad \text{where } k_U = \frac{1}{k_L\left(\frac{1}{k_N}, \dots, \frac{1}{k_1}, m_N, \dots, m_1, \frac{1}{t}\right)}. \tag{6.3}$$

6.2 Bounds for anisotropic composites

The bound for anisotropic effective conductivity K_* is derived by a similar procedure, using (2.25), (2.26). This time, it is not assumed that the external field e_0 and the corresponding optimal effective tensor K_* are isotropic, $D_0 \neq 0$. The anisotropy of the average field e_0 changes the left-hand side of (3.15) but it does not change the right-hand side of this estimate and supporting sets Ψ_i, if the level of anisotropy D_0/S_0 is small enough, see Remark 3.2.

Indeed, assume for example that $t \in (k_1, k_2)$. The D component of the field in Ω_1 still alternates the same supporting points $\pm(S_1 - S_N)$ but this time it has a nonzero mean value $\hat{D}_1 \in [-(S_1 - S_N), (S_1 - S_N)]$. The fractions (measures) of the supports are chosen to provide the equality $D_0 = m_1 \hat{D}$, see (5.12), (5.13). If D_0 is close to zero, $m_1|D_0| \le S_1 - S_N$, the supports Ψ_i are the same as in isotropic case. In this range, the bound is derived similarly to the isotropic case. Here, we do not work out the details of the constraints on the range of D_0.

Assume that D_0 is "small" in the following sense

$$m_1|D_0| \le S_1 - S_N. \tag{6.4}$$

Then, the bounds allow for an extension to anisotropic composites. Since supporting sets Ψ_i are the same as in isotropic case, the expressions for H_r is also the same. Repeating the derivation of the bound, we transform the left-hand side of (3.16) assuming that $D_0 \neq 0$ and K_* is an anisotropic tensor with eigenvalues k_1^* and k_2^*. The translated effective energy (3.14) becomes

$$J_0(K_*, e_0) + t \det(e_0) = \frac{1}{2} k_1^*(S_0 + D_0)^2 + \frac{1}{2} k_2^*(S_0 - D_0)^2 + t(S_0^2 - D_0^2)$$

and the bound (3.15) becomes

$$\frac{1}{2} k_1^*(S_0 + D_0)^2 + \frac{1}{2} k_2^*(S_0 - D_0)^2 + t(S_0^2 - D_0^2) - H_r(t) S_0^2 \ge 0, \tag{6.5}$$

where $H_r(t)$ is defined in (5.19). This inequality is satisfied for all S_0, D_0 if the above quadratic form is nonnegative, see (2.25), (2.26). The nonnegativity is equivalent to the requirement that matrix

$$\begin{pmatrix} k_1^* + k_2^* + 2t - 2H_r(t) & k_1^* - k_2^* \\ k_1^* - k_2^* & k_1^* + k_2^* - 2t \end{pmatrix} \ge 0. \tag{6.6}$$

it nonnegative defined. The nonnegativity of the determinant of this matrix leads to inequalities

$$2\frac{k_1^* k_2^* - t^2}{k_1^* + k_2^* - 2t} \geq H_r(t), \ \forall t \in (k_{r-1}, k_r], \ \forall r = 1, \dots, N-1. \tag{6.7}$$

Equivalently, it can be rewritten in the form

$$\frac{1}{k_1^* - t} + \frac{1}{k_2^* - t} \leq \frac{2}{H_r(t) - 2t}, \ \forall t \in (k_{r-1}, k_r], \ \forall r = 1, \dots, N-1. \tag{6.8}$$

that is familiar for the bounds of two-component composites, [25, 9, 28]. The bound degenerate into (5.20), when tensor K_* is isotropic ($k_1^* = k_2^* = k_*$).

The bound is valid for all effective tensors K_* but may not be exact. Indeed, if assumption (6.4) is not valid, additional constraints must be imposed on the set of admissible fields. The new constraints make the inequalities more restricted and can only increase the lower bound (6.7).

Bound (6.7) can be complemented by the dual bound obtained as in Section 6.1. Together, they define a bounded domain in the plane of eigenvalues of K_* - the outer bound of the G-closure of multicomponent mixtures.

7 Bounds for three-material composites

7.1 Explicit bounds

For three-material mixtures, it is possible to explicitly compute optimal translation parameter t and the bound. When $N = 3$, bound (5.20) takes form

$$k_* \geq k_L = \max_{t \in [k_1, k_2]} \left(-t + H_1(t)\right) \tag{7.1}$$

where

$$\frac{1}{H_1(t)} = \frac{m_1}{2k_1} + \frac{m_2}{k_2 + t} + \frac{(m_1(k_1 - t) + 2k_1 m_3)^2}{2k_1(2k_1 m_3(k_3 + t) + m_1(k_1^2 - t^2))}. \tag{7.2}$$

Optimal value t_0 of t in (7.1) are computed by solving the equation

$$\frac{d}{dt}\left(-t + H_1(t)\right)\bigg|_{t = t_{\text{st}}} = 0 \tag{7.3}$$

for t. The bulky calculation performed by Maple gives the following:

$$t_0(m_1) = \begin{cases} k_1 & \text{if } \ m_{11} \leq m_1 \leq 1 \\ -k_2 + \frac{\sqrt{m_2}(1 - \sqrt{m_2})}{m_1} Z_1 & \text{if } \ m_{12} \leq m_1 \leq m_{11} \\ k_2 & \text{if } \quad 0 \leq m_1 \leq m_{12} \end{cases}. \tag{7.4}$$

Here,

$$
\begin{aligned}
m_{11} &= 2\sqrt{m_2}(1-\sqrt{m_2})\frac{k_1(k_3-k_2)}{(k_3-k_1)(k_1+k_2)} && (7.5)\\
m_{12} &= \frac{1-\sqrt{m_2}}{4k_2(k_3-k_1)}Z_0 && (7.6)\\
Z_0 &= \left(2k_2(k_3-k_1)+\sqrt{m_2}(k_1+k_2)(2k_3-k_1-k_2)-\sqrt{Z_2}\right) && (7.7)\\
Z_1 &= \frac{2m_3k_1(k_3-k_2)-m_1(k_2^2-k_1^2)}{(m_1k_1+m_2k_2+m_3k_3)-k_1-\sqrt{m_2}(k_2-k_1)} && (7.8)\\
Z_2 &= 4k_2^2(k_3-k_1)^2+4\sqrt{m_2}Z_3+m_2Z_4 && (7.9)\\
Z_3 &= (k_2(k_1-k_2)(k_1-k_3)(k_1-k_2+2k_3) && (7.10)\\
Z_4 &= (k_1-k_2)^2(k_1^2+6k_1k_2-4k_1k_3-4k_2k_3+4k_3^2+k_2^2) && (7.11)
\end{aligned}
$$

When $t_0 = k_1$, bound (7.2) degenerates into Hashin-Shtrikman bound. This happens when $m_1 \geq m_{11}$, see (7.4). Notice that if $m_2 = 0$ (a composite is made of two components) then $m_{11} = 0$, which shows that the Hashin-Shtrikman bound is exact everywhere, as expected.

The critical parameters m_{11} and m_{12} are found as solutions of the equations

$$
\begin{aligned}
t_{\rm st}(k_1,k_2,k_3,m_1,m_2) &= k_1, && (7.12)\\
t_{\rm st}(k_1,k_2,k_3,m_1,m_2) &= k_2, && (7.13)
\end{aligned}
$$

respectively; $t_{\rm st}$ is the solution of (7.3). Solving (7.12) for m_1, we obtain boundary $m_1 = m_{11}(m_2, k_1, k_2, k_3)$ of a region where the new bound replaces the Hashin-Shtrikman bound. Similarly, a solution to (7.13) defines the second boundary $m_1 = m_{12}(m_2, k_1, k_2, k_3)$ where the new bound changes its form. We check that $\frac{m_{12}}{m_{11}} \leq 1$ for all values of parameters.

To find the explicit expressions for effective properties bounds, we substitute the optimal values t_0 into bound (7.1), (7.2). The results are as follows.

Theorem 7.1 The effective conductivity k_* of a two-dimensional isotropic composite of three isotropic materials with conductivities $k_1 < k_2 < k_3$ taken in the fractions m_1, m_2 and m_2, $m_1+m_2+m_3 = 1$, is bounded from below by the bound $k_L = B(m_1, m_2)$:

$$k_* \geq B(m_1, m_2) \tag{7.14}$$

where

$$B(m_1, m_2) = \begin{cases} B_1 & \text{if } m_{11} \leq m_1 \leq 1 \\ B_2 & \text{if } m_{11} \leq m_1 \leq m_{12} \\ B_3 & \text{if } \ 0 \leq m_1 \leq m_{12} \end{cases} . \tag{7.15}$$

Here

$$B_1 = -k_1 + \left(\frac{m_1}{2k_1} + \frac{m_2}{k_1+k_2} + \frac{m_3}{k_1+k_3}\right)^{-1} \tag{7.16}$$

$$B_2 = k_2 + (1-\sqrt{m_2})^2 \frac{Z_5}{Z_6} \tag{7.17}$$

$$B_3 = -k_2 + \left(\frac{m_2}{2k_2} + Z_7\right)^{-1} \tag{7.18}$$

and

$$\begin{aligned} Z_5 &= m_1 k_1^2 - m_1 k_2^2 + 2m_3 k_1 (k_3 - k_2) \\ Z_6 &= \left[(1-\sqrt{m_2})^2 + (1 - m_1 - \sqrt{m_2})^2\right] k_1 + m_1 (1-\sqrt{m_2})^2 k_2 + m_1 m_3 k_3 \\ Z_7 &= \frac{(k_1-k_2)m_1^2 + (2k_1 - k_2 + k_3) m_1 m_3 + 2k_1 m_3^2}{(k_1^2 - k_2^2) m_1 + 2k_1 (k_2+k_3) m_3}. \end{aligned}$$

$B(m_1, m_2)$ is a continuously differentiable function of m_1 and m_2.

The regions of the optimality of B_i are shown in Figure 4.

7.2 Asymptotics

Case $m_1 \to 1$. If $m_1 = 0$, then $t_0 = k_2$ the $B(t_0)$ becomes

$$B|_{m_1=0}(k_2) = \frac{m_2}{2k_2} + \frac{m_3}{k_2+k_3}$$

and the bound becomes a Hashin-Shtrikman bound for a two-component mixture of k_2 and k_3, as expected.

Case $k_3 = \infty$. If $k_3 = \infty$, the formulas are simpler, but the problem still preserves its form. This case coincides with the bounds by Nesi [33] computed for $k_3 = \infty$.

Theorem 7.2 The effective conductivity k_* of a two-dimensional isotropic composite of two isotropic materials with conductivities k_1, k_2 and an ideal conductor $k_3 = \infty$ taken in the fractions m_1 m_2 and m_3, respectively, is bounded from below by the bound $k_L = B^\infty(m_1, m_2)$:

$$k_* \geq B^\infty(m_1, m_2) \tag{7.19}$$

where

$$B^\infty(m_1, m_2) = \begin{cases} B_1{}^\infty & \text{if } m_{11}^\infty \leq m_1 \leq 1 \\ B_2{}^\infty & \text{if } m_{12}^\infty \leq m_1 \leq m_{11}^\infty \\ B_3{}^\infty & \text{if } \ 0 \leq m_1 \leq m_{12}^\infty \end{cases}. \tag{7.20}$$

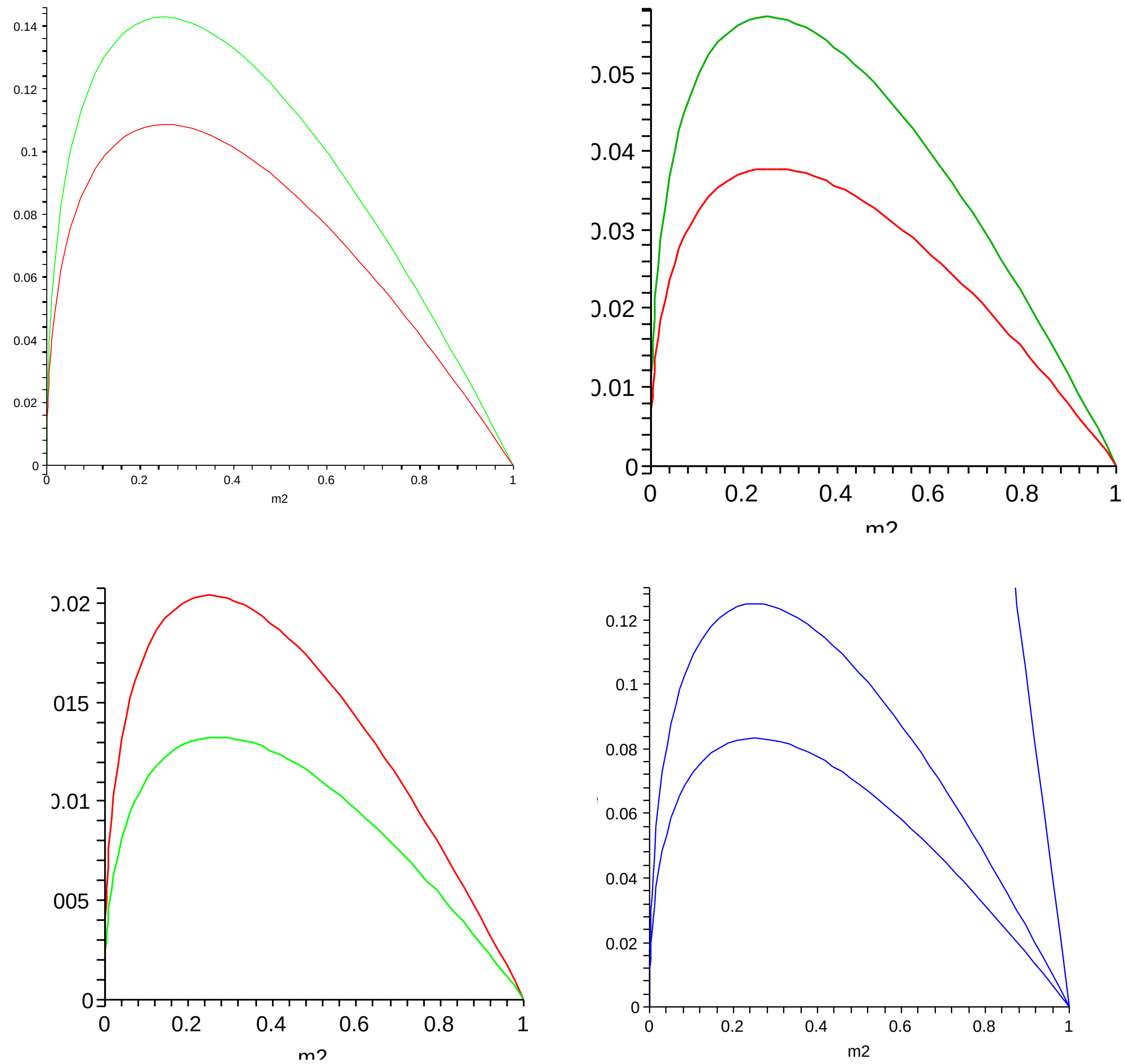

Figure 4: Regions of optimality of B_1, B_2, B_3-bounds in the plane m_1, m_2, $m_2 \le 1 - m_1$, (see (7.24)). Conductivities are $k_1 = 1, k_3 = 8$. Upper left fields: $k_1 = 1, k_2 = 2, k_3 = 8$, upper right field - $k_1 = 1, k_2 = 4, k_3 = 8$, lower left field - $k_1 = 1, k_2 = 6, k_3 = 8$, lower right field - $k_1 = 1, k_2 = 3, k_3 = \infty$. Top regions - bound B_1, intermediate regions - bound B_2, bottom regions - bound B_3. Condition $m_1 + m_2 \le 1$ is assumed (shown in the lower right field).

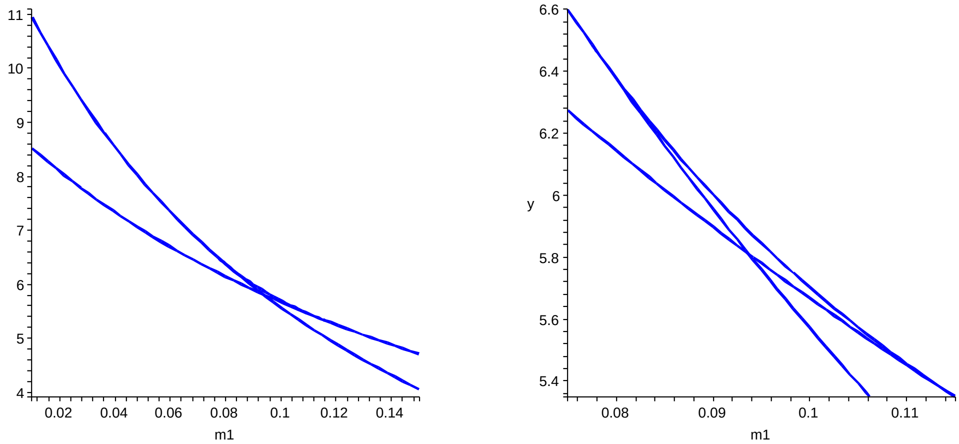

Figure 5: Bounds for parameters $k_1 = 1, k_2 = 3, k_3 = \infty, m_2 = .4$. **Left:** Lower bound $B(m_1, .4)$ (see (7.20)). The three shown curves correspond to B_1, B_2, B_3. **Right:** Magnified region where all three bounds are active. Notice that the bound is smooth everywhere.

Here,

$$B_1{}^\infty = -k_1 + \left(\frac{m_1}{2k_1} + \frac{m_2}{k_1 + k_2}\right)^{-1} \tag{7.21}$$

$$B_2{}^\infty = k_2 + 2\frac{k_1}{m_1}(1 - \sqrt{m_2})^2 \tag{7.22}$$

$$B_3{}^\infty = -k_2 + \left(\frac{m_1}{2k_1} + \frac{m_2}{2k_2}\right)^{-1} \tag{7.23}$$

and

$$m_{11}^\infty = \frac{2k_1}{k_2 + k_1}(\sqrt{m_2} - m_2), \quad m_{12}^\infty = \frac{k_1}{k_2}(\sqrt{m_2} - m_2). \tag{7.24}$$

Bound $B_2{}^\infty$ corresponds to an optimal value t_0^∞ of the translator t,

$$t_0^\infty = 2k_1\frac{\sqrt{m_2} - m_2}{m_1} - k_2.$$

8 Optimal three-material structures

8.1 Structures for Hashin-Shtrikman bound

Hashin-Shtrikman bound for multimaterial composites is realizable if volume fraction m_1 is above a threshold, $m_1 \geq m_{11}$: There exist structures with conductivity

k_L. In these structures, the fields are constant and isotropic in all materials but k_1. The conditions (2.18) allow for rank-one contact between the fields in k_1-material and fields in other materials, but rank-one contact between these other materials is not permitted.

Coated circles The coated circles assembly suggested by Milton [29] is constructed in two steps. Firstly, a structure with circular inclusions one of from materials $k_2, .., k_N$ surrounded by an annuls from k_1 is built. These are Hashin-Shtrikman coated circles. The fractions of material k_1 in these coated circles is chosen so that all two-material coated circles have the same isotropic effective properties k_*, which is possible only if $k_1 < k_* \leq k_2$ and implies a constraint $m_1 \in [m_{10}, 1]$ on minimal needed amount of m_1: It must be larger than a threshold m_{10}. Secondly, the obtained two-materials composites of same effective conductivity are mixed together in a larger scale; obviously, the effective conductivity does not change.

The fields inside the inclusions from $k_2, \ldots, k_N$ are constant and isotropic $S_i = \beta_i,\ D_i = 0,\ V_i = 0,\ i = 2, \ldots, N$ in agreement with the translation bound, see (3.26)-(3.28). The fields in annuls filled with k_1 vary with its radius r. One can check, however, that $S = \text{ constant}(r), V = 0$, and that $D(r)$ decreases when r increases, see for example [28]. The maximum value of $D(r_0)$ is achieved in the inner radius r_0 of an annulus that satisfies the contact condition between materials k_1 and k_j: at this line, constraint (4.26) is satisfied as equality $D(r_0) = S_1 - S_j$. There is no outer boundary for annuli in this assembly: The coated circles fill in the plane with infinitely many scales.

Similar structures Another optimal structure of multicoated circles was found by Lurie and Cherkaev in [26]. The multicoated structure consists of several inscribed annuli. The cental circle is occupied with k_N, next annulus with k_1, next annulus with k_{N-1}, next again with k_1, etc. Volume fractions of k_1 in annuli are chosen so that fields in annuli between them are constant. The structure also realizes Hashin-Shtrikman bound and is subject to the same constraint $m_1 \in [m_{10}, 1]$.

Two-material Vigdergauz structures [38, 17] are similar to coated circles. They are periodic assembles of inclusions from k_i of optimal shape in the envelope of k_1. These two-material structures also can be expended to the multimaterial case, using two well-separated scales. A smaller scale corresponds to solutions of periodic Vigdergauz problems for all pairs k_1 and k_i, $i = 2, \ldots, N$. A larger scale is used to mix these composites together as in Milton scheme. The same constraint applies.

Multiscale laminates: Geometry A different type of optimal structures is *multiscale laminate* by Albin, Cherkaev, and Nesi [4] and suggested earlier *rectangular blocks* by Gibiansky and Sigmund [15]. These structures and the fields in the

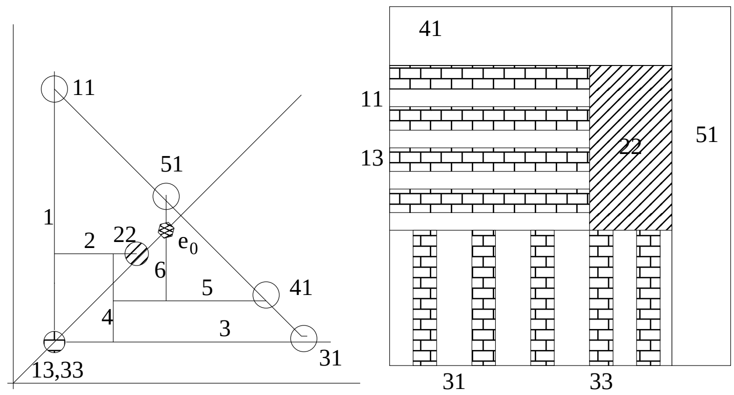

Figure 6: Right: Cartoon of an optimal laminate three-material structure, , see [4]. The case $m_1 \geq m_{11}$ (Hashin-Shtrikman bound). The two-digit labels on layers show the order of laminating (first digit) and the material (second digit). Left: Eigenvalues of corresponding supporting fields in an optimal three-material composite. Circles denote fields in layers, lines denote a connected path. The small stripped circle denotes the average isotropic field e_0. Digits on lines show the order of lamination.

layers are depicted in Figure 6. The structures are optimal in a region of parameters $m_1 \in [m_{11}, 1]$ that is greater than the region of optimality of coated circles, $m_{11} < m_{10}$. Moreover, we show here that multiscale laminate structures are optimal everywhere where Hashin-Shtrikman bound is optimal.

Remark 8.1 The laminate of a rank [9] is a multiscale sequence of microstructures (laminates within laminates) that corresponds to indefinite increase of the ratio of the thickness of laminates of different scales. The effective conductivity of that sequence tends to its limit k_* in the sense of G-convergence.

The central element of the optimal structures is the T^2-structures introduced in [4], see Figure 6, center. They are as follows. The laminate of materials k_1, and k_3 is formed with volume fractions ν_{11} and $\nu_{13} = 1 - \nu_{11}$. The tangent is oriented along x_1 -axis. This laminate is labeled “1”; the label corresponds to the first index of the volume fractions ν_{1p}, second index p refers to material k_p. At the second step, this composite is laminated in an orthogonal direction with a layer of k_2; the layers are oriented along x_2-axis. This layer is labeled “2” and the volume fractions of the added layer of k_2 is denoted ν_{22}. We call the resulting second-rank laminate [9] the *T-structure* and denote it as $\mathcal{L}_{13,2}$.

Next, the T-structure is laminated in x_1 direction with another laminate of materials k_1 and k_3. This laminate is labeled “3” and the volume fractions of materials in it are denoted as ν_{31} and $\nu_{33} = 1 - \nu_{11}$ respectively. The layers are oriented along x_2, orthogonal to the layer with T-structure. We call this structure T^2-*structure* and denote it $\mathcal{L}_{13,2,13}$. The relative volume fractions of the two fragments are called ν_4 - the fraction of the T-structure, and $1 - \nu_4$ - the fraction of the added laminate. Finally, the T^2-structures are sequentially laminated by the two orthogonal layers of k_1, forming the structure $\mathcal{L}_{13,2,13,1,1}$.

Multiscale laminates: Rank-one connections The fields in optimal structures depend on fractions of materials in the layers. In all orthogonal laminates, fields are symmetric ($V_2 = V_3 = 0$). In the optimal structures, the fractions must be chosen so that the fields in Ω_2 and Ω_3 are isotropic ($D_2 = D_3 = 0$), S-component of the field in is constant in each subdomain, and the ratio between S-components is as prescribed in the bound, see (3.22).

In laminates, field $e = \nabla u$ is represented by the pair (e_a, e_b) of its eigenvalues, the eigenvectors of e are directed along or across laminates. Laminate structure can realize the translation optimality conditions (3.26)-(3.28) as follows. A laminate labeled "1" connects field (β_1, β_3) in the first material with isotropic field (β_3, β_3) in third material. The fields are rank-one connected. The average field in the laminate is (e_μ, β_3) where $e_\mu = \mu\beta_3 + (1-\mu)\beta_1$ and $\mu \in (0, 1)$ is the volume fraction of the third material.

T-structure is formed when the obtained composite is laminated with layer of k_2. We request that D-component of the field in k_2 is zero, or that it has a form (β_2, β_2). These fields in the structure are compatible if fraction μ is so chosen that field (e_μ, β_3) is in rank-one contact with the field (β_2, β_2) in k_2: $k_\mu = \mu\beta_3 + (1-\mu)\beta_1 = \beta_2$. Parameters β_i are related by (3.28).

T^2-structure is formed when the T-structure is laminated in an orthogonal direction with another laminate of k_1 and k_3. The volume fractions of the materials in the added laminate must be chosen so that field in k_1 is equal to (β_3, β_1) and field in k_3 - to (β_3, β_3) and the added laminate and the T-structure are in rank-one connection. Then, S-component of the field in k_1 is constant everywhere in the structure, and field in k_3 is constant and isotropic everywhere.

Finally, the assembly is twice laminated with k_1 in two orthogonal directions. The fields in them must have the form $(y_a, \beta_1 - y_a)$ and $(y_b, \beta_1 - y_b)$, respectively, where y_a and y_b are real parameters. Then S-component of the field is constant. The volume fractions of the added layers are chosen so that the whole structure is isotropic ($D_0 = 0$). The fields are shown in Figure 6.

The above-listed conditions for the fields in laminates form a system of equations for the unknown volume fractions of layers. If the system has a solution, the optimal structure is found. The solvability conditions restrict the range of volume fraction m_1 as $m_1 \geq m_{11}$, see [4]. The described structure realizes Hashin-Shtrikman bound

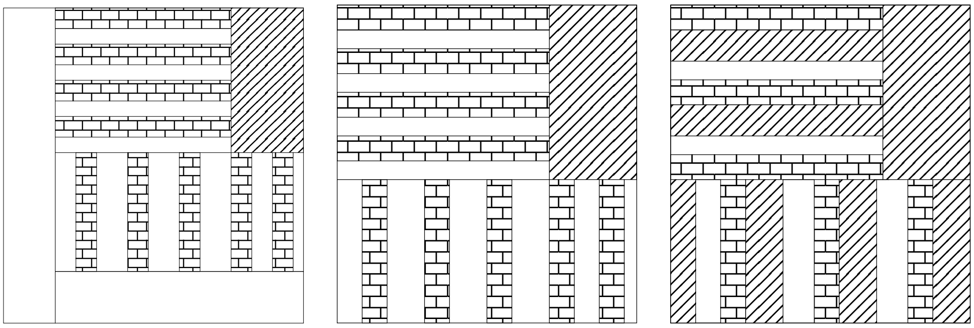

Figure 7: Left, Center, Right: Cartoons of optimal structures for the bounds B_1, B_2, B_3, respectively. Observe the topological change when the amount of k_1 decreases: The Ω_1 domain in the left structure is connected, no domains are connected in the structure in the center, and domain Ω_2 in the right structure is connected. When $m_1 \to 0$, the right structure degenerates into a two-material second rank laminate with k_2 (envelope) and k_3 (inclusions), laminated with laminates of k_2 and k_3.

because sufficient conditions (3.27), (3.28), and (4.26) are satisfied everywhere.

Remark 8.2 Optimal structures of *rectangular blocks*, suggested earlier by Gibiansky and Sigmund in [15] are similar to the described here laminates. The square cell of periodicity Ω is divided into four rectangular domains, filled with either pure materials or laminates. The effective properties of laminates in the rectangles are chosen so that the separation of variables in (2.17) is possible, and the solution $u(x_1, u_b)$ is piece-wise affine. Gibiansky and Sigmund [15] proved optimality of this construction: It realizes Hashin-Shtrikman bound in the interval $m_1 \in [m_{11}, 1]$.

8.2 New optimal three-material structures

We demonstrate here that the obtained bounds are exact by showing optimal laminate structures with conductivities equal to the bound k_L.

Theorem 8.1 The bound (7.19)-(7.24) is exact in each point: There exist laminates of a finite rank that realize the bounds.

Optimal structures that realize the new bounds are shown in Figure 7. Fields in the neighboring subdomains are rank-one connected, which provides for continuity of the potential. In optimal structures, fields e_{ij} in layers satisfy sufficient conditions (5.11):

1. Gradients ∇u_a and ∇u_b are orthogonal everywhere in Ω, $V = 0$.

2. Field is isotropic and constant everywhere in Ω_3, $D = 0$ and $S = \beta_3$.
3. S-component of field in Ω_1 is constant, $S = \beta_1$ and this field is always in rank-one contact with the third material, $D = \pm(\beta_1 - \beta_3)$.
4. If $m_{12} < m_1 < m_{11}$, the field in Ω_2 is isotropic: $D(x) = 0$, $S(x) = \beta_2$. If $m_1 \le m_{12}$, then $S(x) = \beta_2$ is constant, but $D(x)$ varies in different layers of k_2.

The fields are shown in Figure 3.

Optimal microstructures for B_3 The sequential laminates that realize the bound (7.18) $k_L = B_3$ are $\mathcal{L}_{123,2,123}$-structures. They are constructed by the following iterative scheme:

(1) The laminate of materials k_1, k_2 and k_3 is formed with volume fractions ν_{11}, ν_{12} and $\nu_{13} = 1 - \nu_{11} - \nu_{12}$. The tangent is oriented along x_1 -axis. The layers are labeled $11, 12, 13$, respectively

(2) The obtained composite is laminated in the orthogonal direction with a layer of k_2 oriented along x_2-axis, forming a T-*structure*. This layer is labeled 22, and the structure - $\mathcal{L}_{123,2}$

(3) The obtained T-structure is laminated in x_1 direction with another laminate of materials k_1, k_2 and k_3. The layers in this last laminate are labeled $31, 32, 33$, respectively. The volume fractions of materials in that laminate are denoted as ν_{31}, ν_{32} and $\nu_{33} = 1 - \nu_{11} - \nu_{12}$ respectively, and the layers are oriented along x_2. The relative volume fractions of the two fragments are ν_4 – the fraction of the T-structure, and $(1 - \nu_4)$ – the fraction of the lastly added laminate. We denote this structure as $\mathcal{L}_{123,2,123}$. The total volume fractions of k_1 and k_2 are

$$m_1 = (1 - \nu_4)\nu_{31} + \nu_4(1 - \nu_2)\nu_{11}, \tag{8.1}$$

$$m_2 = (1 - \nu_4)\nu_{32} + \nu_4(1 - \nu_2)\nu_{12} + \nu_4\nu_2. \tag{8.2}$$

Volume fractions of layers in an optimal structure are chosen to satisfy the optimality conditions listed above, as it is shown in Appendix.

A different optimal structure for B_3 The shown optimal structures are not unique. There are several ways to joint optimal fields by a rank-one path. Another type of optimal structures that realizes B_3-bound for very small m_1 is found in [9] for the case $k_3 = \infty$. This structure is $\mathcal{L}_{123,2}$-laminate of the second rank in which the layers of all three materials are laminated in an orthogonal direction with a layer of k_2. This laminate can be isotropic if m_1 is sufficiently small

$$m_1 \in [0, m_{120}^{\infty}], \quad m_{120}^{\infty} = \frac{m_2(1 - m_2)}{1 + m_2}\left(\frac{k_1}{k_2}\right).$$

Notice that $m_{120}^{\infty} < m_{12}^{\infty}$, see (7.24). The effective conductivity of optimal $\mathcal{L}_{123,2}$ and $\mathcal{L}_{123,2,123}$ laminates coincide, but the last one is optimal in a larger range of m_1.

Optimal structures for B_2 Optimal structures that realize the intermediate bound B_2 are special T^2-structures (Figure 7, center field) of the type $\mathcal{L}_{13,2,13}$. In them, fractions ν_{12} and ν_{32} are zero, $\nu_{12} = 0 \quad \nu_{32} = 0$ so that k_2-material is placed in the second layer only. In the range $m_{12} < m_1 < m_{11}$, structural parameters (volume fractions of laminates) can be chosen to satisfy the optimality conditions in Theorem 8.1, as it is shown in Appendix.

Asymptotic When $m_1 \to 0$, the structure degenerates into an optimal two-material composite $\mathcal{L}_{23,2,23}$. It realizes Hashin-Shtrikman bound for (k_2, k_3)-composite. Indeed, the T-structure (regions "1" and "2") become *matrix laminate* $\mathcal{L}_{23,2}$ that realizes the translation bound (3.29) see [24, 9]. Lamination of this structure with a laminate $\mathcal{L}_{23}$ keeps it translation-optimal, see [4]. An appropriate choice of parameters brings the structure to an isotropy. The limiting structure is of the type of "haired sphere" structures, described in [2].

When $m_2 \to 0$ or $m_3 \to 0$, the optimal structure degenerates into $\mathcal{L}_{13,1,1}$ and $\mathcal{L}_{2,1,1}$, respectively. These are equivalent to second-rank matrix laminates that are optimal for two-material (k_1, k_3)- and (k_1, k_2)-composites, respectively.

8.3 Connectedness of subdomains in optimal composites

We comment on topology the optimal periodic structures that realize the bounds. The periodic elements of them are shown in Figure 7. There are three types of structures that differ by the connected domain and two topological transitions between these types. When m_1 decrease from one to zero, the enveloping material changes from k_1 to k_2 in the following way.

When $m_1 > m_{11}$ (bound B_1), structure $\mathcal{L}_{13,2,13,1,1}$ is optimal. In the structure, a part of k_1 in the outer layers forms a connected domain. The T^2-structures form inclusions in that domain. The inclusions are composed as follows: the nucleus is made from an intermediate material k_2, and the periphery is a laminate from k_1 and k_3; the layers are directed toward the core, providing a path for the current between an outer boundary and the nucleus.

Below the threshold m_{11}, the outer layers of k_1 disappears and the T^2-inclusions are joined together. In the region $m_{12} < m_1 < m_{11}$ (bound B_2), structure $\mathcal{L}_{13,2,13}$ is optimal. In that structure, none of materials occupies a connected domain, but (k_1, k_3)-layers connect Ω-periodic nuclei of k_2. The optimal composite resembles Schulgasser's optimal polycrystals [35] with the nuclei.

Below the second threshold $m_1 < m_{12}$ (bound B_3), structure $\mathcal{L}_{123,2,123}$ is optimal. In it, a layer of k_2 is added to the (k_1, k_3)-laminate that surrounds the nuclei. Thus, domain Ω_2 percolates and becomes connected. Domains Ω_1 and Ω_3 become inclusions. The field in Ω_3 remains constant and isotropic.

Acknowledgement The author is thankful to Dr. Nathan Albin, Professors Graeme Milton and Vincenzo Nesi and anonymous reviewers for stimulating comments and discussions, and Ms.Yuan Zhang for checking calculations and comments on the manuscript. The work is supported by NSF through grant DMS-0707974.

9 Appendix. Calculation of parameters of optimal laminates

Expression for effective properties Here we show the optimal structural parameters for the structures that realize the bound B (7.14) for all values of parameters. Volume fractions of layers in an optimal structure are chosen so that the optimality conditions of Section 8.2 are satisfied. The calculation were performed by Maple. Here we show the results of the calculation of the optimal parameters for the asymptotic case $k_3 = \infty$ when the bound has the form (7.19). The general case of finite k_3 is similar, but the formulas are much bulkier and not too instructive. They are obtained by applying the same Maple procedure.

Assume that the structure is subjected to a pair of isotropic external fields $e_0 = I$. In orthogonal structures. the fields $e = \nabla u$ in layers are form a diagonal matrix. This matrix is represented by a two-dimensional vector of eigenvalues $e_{nm} = (e_{nm}[1], e_{nm}[2])$ where indices n and m show the material in a layer and the position of the layer in a structure, respectively. Their eigenvectors of e_{nm} are co-directed with laminate direction, so the matrices e_{nm} are completely defined by the vector of their eigenvalues. The average field e_0 is assumed to be $e_0 = I$. Applying rank-one conditions on the boundaries, we find fields in $\mathcal{L}_{123,2,123}$ $(k_3 = \infty)$

$$e_{11} = \begin{pmatrix} \frac{k_2}{\nu_4(\nu_{11}k_2+\nu_{12}k_1)} \\ 0 \end{pmatrix}, \quad e_{31} = \begin{pmatrix} 0 \\ \frac{k_2}{\nu_{31}k_2+\nu_{32}k_1} \end{pmatrix}, \tag{9.3}$$

$$e_{12} = \begin{pmatrix} \frac{k_1}{\nu_4(\nu_{11}k_2+\nu_{12}k_1)} \\ 0 \end{pmatrix}, \quad e_{22} = \begin{pmatrix} \frac{1}{\nu_4} \\ \frac{1}{\nu_2} \end{pmatrix}, \quad e_{32} = \begin{pmatrix} 0 \\ \frac{k_1}{\nu_{31}k_2+\nu_{32}k_1} \end{pmatrix}, \tag{9.4}$$

$$e_{13} = e_{33} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{9.5}$$

Optimal parameters for B_1-structures The structures that realize Hashin-Shtrikman bound (Figure 7, left field) are orthogonal laminates of the type $\mathcal{L}_{13,2,13,1,1}$.

They are mentioned above, in Section 8.1 and are described in details in[4]. They consists of inclusions sequentially laminated by two orthogonal layers of the amount $m_1 - m_{11}$ of k_1. The inclusions are T^2-structures $\mathcal{L}_{13,2,13}$ in which the amount of the k_1-material is equal to m_{11}.

Optimal parameters for B_2-structures These optimal structures that realize the intermediate bound B_2 are T^2-structures (Figure 7, center field) of the type $\mathcal{L}_{13,2,13}$. In them:

1. The fractions ν_{12} and ν_{32} are zero, $\nu_{12} = 0 \quad \nu_{32} = 0$ so that k_2 is placed in the second layer only. It forms nuclei inclusions joined by directors: laminates from k_1 and k_3. Constraint (8.1) becomes $m_2 = \nu_2\nu_4$ and the effective conductivities k_1^* and k_2^* in x_1 and x_2 directions, respectively, become linear combinations of k_1 and k_2

$$k_1^* = \frac{1}{\nu_2\nu_{31}} \left[(\nu_2 - \nu_2\nu_4 + \nu_4\nu_{32})k_1 + \nu_4\nu_{32}k_2\right], \tag{9.6}$$

$$k_2^* = \frac{1}{\nu_4\nu_{11}} \left[(1 + \nu_2\nu_{12} - \nu_2)k_1 + \nu_2\nu_{11}k_2\right]. \tag{9.7}$$

2. S-component is constant in Ω_1, that is $e_{11}[1] = e_{13}[2]$ in (9.3), which implies $\nu_{31} = \nu_{11}\nu_4$, see (9.3).
3. D-component is zero in Ω_2, that is $e_{22}[1] = e_{22}[2]$ in (9.4), which implies $\nu_2 = \sqrt{m_2} \quad \nu_4 = \sqrt{m_2}$, see (9.4)..
4. The structure are isotropic, or $k_1^* = k_2^*$ (see (9.6), (9.7)).

We choose volume fractions of laminates to satisfy the above conditions and (8.1), (8.2). Solving the corresponding equations for fractions ν_{mn}, we compute their optimal values denoted as v_{mn}

$$v_2 = v_4 = \sqrt{m_2}, \quad v_{31} = \frac{m_1}{2(1 - \sqrt{m_2})}, \quad v_{11} = \frac{\nu_{31}}{\sqrt{m_2}}. \tag{9.8}$$

Energy densities W_1 and W_2 in the first and second materials, respectively, are

$$W_1 = \frac{1}{2}k_1\left(e_{11}^2 + e_{31}^2\right) = k_1\left(\frac{1 - \sqrt{m_2}}{m_1}\right)^2 \|e_0\|^2,$$

$$W_2 = \frac{1}{2}k_2\|e_{22}^2\| = \frac{k_2}{2m_2}\|e_0\|^2.$$

The average energy $m_1W_1 + m_2W_2$ defines the effective conductivity k_*. One checks that $k_* = B_2^\infty$. Therefore, the bound is exact.

Optimal parameters for B_3-structures These are the T^2-structures (see Figure 7, right field) of the type $\mathcal{L}_{123,2,123}$ that satisfy (8.1), (8.2). Effective properties of these structures are expressed through the structural parameters as

$$k_1^* = \frac{k_2}{\nu_{31}k_2 + \nu_{32}k_1}\frac{1}{\nu_2}\left((\nu_2 - \nu_2\nu_4 + \nu_4\nu_{32})k_1 + \nu_4\nu_{32}k_2\right), \tag{9.9}$$

$$k_2^* = \frac{k_2}{\nu_{12}k_1 + \nu_{11}k_2}\frac{1}{\nu_4}\left((1 + \nu_2\nu_{12} - \nu_2)k_1 + \nu_2\nu_{11}k_2.\right). \tag{9.10}$$

The optimality conditions are

1. S-component is constant in Ω_1, that is $e_{11}[1] = e_{31}[2]$ in (9.3), implying

$$\nu_{31}k_2 + \nu_{32}k_1 = \nu_4(\nu_{11}k_2 + \nu_{12}k_1). \tag{9.11}$$

2. S-component is constant in Ω_2, that is

$$e_{12}[1] + e_{12}[2] = e_{22}[1] + e_{22}[2] = e_{32}[1] + e_{32}[2]$$

   One of these equalities follows from (9.11), the other implies

$$\frac{k_1}{\nu_{31}k_2 + \nu_{32}k_1} = \frac{1}{\nu_2} + \frac{1}{\nu_4}.$$

3. The structure is isotropic, $k_1^* = k_2^*$ in (9.10), (9.9).

Solving for structural parameters ν_p, we obtain a family of isotropic structures that have the same optimal effective property $k_* = B_3^\infty$. Therefore the bound B_3^∞ is exact.

Nonuniqueness Optimal structures $\mathcal{L}_{123,2,123}$ are not unique. There is a freedom in choosing of volume fractions. Namely, fraction ν_{23} is not defined by optimality conditions, that is the distribution of k_2 between the inner and outer layers is not unique. We put $\nu_{32} = P\nu_4\nu_{12}$ where P is a parameter and obtain

$$v_2 = v_4 = \frac{m_1k_2 + m_2k_1}{k_1}, \tag{9.12}$$

$$v_{31} = \frac{P}{1+P}\frac{m_1k_1}{(k_1 - \tilde{k})} + \frac{1-P}{1+P}\frac{\tilde{k}}{2k_2}, \tag{9.13}$$

$$v_{11} = \frac{k_1}{P+1}\left(\frac{m_1k_1}{k_1\hat{k} - \hat{k}^2} + \frac{P-1}{2k_2}\right). \tag{9.14}$$

Here, $\hat{k} = m_2 k_1 + m_1 k_2$. The range of P is obtained from the conditions $v_{31} \geq 0$ and $v_{11} \geq 0$. Solving for P, we obtain

$$P \in \left[P_0, \frac{1}{P_0}\right], \quad P_0 = 1 - \frac{8k_2 m_1 k_1}{k_1^2 - \hat{k}^2}. \tag{9.15}$$

We also check that the optimal effective conductivity k_* is independent of P. For definiteness, we may request that the average field in the Ω_1 and Ω_2 is isotropic, which corresponds to $P = 1$.

Transition points We expect that v_{12} and v_{32} vanish when $m_1 = m_{12}$ because at that point the bound become $k_L = B_2$ and corresponding optimal structure becomes $\mathcal{L}_{13,2,13}$ as described above. To confirm this feature, we introduce a nonnegative parameter $\mu_1 = m_{12} - m_1 \geq 0$, instead of m_1, and calculate optimal volume fractions v_{12} and v_{32}:

$$v_{12} = \mu_1 \frac{k_2}{P+1}\left(\frac{\sqrt{m_2}}{k_1\sqrt{m_2} - \mu_1 k_2} - \frac{1+\sqrt{m_2}}{(-1+\sqrt{m_2})k_1 - \mu_1 k_2}\right), \tag{9.16}$$

$$v_{32} = \mu_1 \frac{P\, k_2\, \left(2\, k_1 \sqrt{m_2} - \mu_1\, k_2\right)}{(P+1)\, k_1\, \left(k_1(1-\sqrt{m_2}) + \mu_1\, k_2\right)}. \tag{9.17}$$

We observe that both fractions ν_{32} and ν_{12} vanish when $\mu_1 = 0$ and the structure becomes a B_2-type structure. At the point of this topological transition, the current densities through k_1 and k_2 are equal, $k_1|e_{11}| = k_2|e_{22}|$. A similar calculation for the transition point m_{11} is performed in [4]. It shows that external layers disappear in $\mathcal{L}_{13,2,13,1,1}$-structure when $m_1 \to m_{11} + 0$.

References

[1] N.Albin. Optimality of the translation bounds for linear conducting composites in two and three dimensions. PhD thesis, University of Utah, 2006.

[2] N. Albin, A. Cherkaev. Optimality conditions on fields in microstructures and controllable differential schemes (2006)- In: Inverse Problems, Multi-Scale Analysis, and Effective Medium Theory. Habib Ammari and Hyeonbae Kang - eds. Series: Contemporary Mathematics No 408, American Mathematical Society, 2006, pp 137-150.

[3] N. Albin, A. Cherkaev, and V. Nesi. A class of optimal two-dimensional multimaterial conducting laminates (2005)- In: IUTAM Symposium on Topological Design Optimization of Structures, Machines and Materials Status and Perspectives, v. 137, Springer 2006.

[4] N.Albin, A. Cherkaev, and V. Nesi. New optimal structures of three-phase conducting composites in 2D. J. Mech. Phys. Solids, 2007. In print.

[5] G. Alessandrini and V. Nesi. Univalent σ-Harmonic Mappings. Archive for Rational Mechanics and Analysis, V. 158, 2, 155-171

[6] M. Avellaneda, A. Cherkaev, L.Gibiansky, G.W.Milton, M. Rudelson. Complete characterization of possible isotropic effective tensors of polycrystals in planar elasticity (orthotropic monocrystal). Journal of Mechanics and Physics of Solids 44(7) 1179-1218.

[7] C. Barbarosie. Shape optimization of periodic structures, Computational Mechanics, 30, p. 235-246, 2003

[8] K. Bhattacharya and G. Dolzmann. Relaxation of some multi-well problems. Proc. Roy. Soc. Edinburgh Sect. A, 2001,

[9] A. Cherkaev. Variational methods for structural optimization. Springer NY 2000.

[10] A.Cherkaev. Approaches to nonconvex variational problems of mechanics In: Nonlinear homogenization and its applications to composites, polycrystals and smart materials. P.Ponte Castaneda, J.J.Telega and B. Gamblin eds., Kluwer 2004. pp. 65-106. (NATO Science Series, Mathematics, Physics and Chemistry v. 170)

[11] A. Cherkaev and L. Gibiansky. Extremal structures of multiphase composites. Int. J. of Solids and Structures JSS 33(18), 2609-2623.

[12] A. Cherkaev and R. V. Kohn, (editors) Topics in the mathematical modelling of composite materials. Progress in Nonlinear differential equations and their applications 31. Birkhuser, Boston (1997).

[13] A. Cherkaev and I. Kucuk. Detecting stress fields in an Optimal Structure Parts I and II Int.J Struct. Opt. January 2004, pp 1-24.

[14] B. Dacorogna. Direct Methods in the Calculus of Variations (Applied Mathematical Sciences). Springer, NY, 1989.

[15] L.Gibiansky and O. Sigmund. Multiphase composites with extremal bulk modulus. J. Mech. Phys. Solids 48 (2000), no. 3, 461–498.

[16] L.V.Gibiansky, G.W.Milton, and J.G.Berryman, On the effective viscoelastic moduli of two-phase media. Proc. R. Soc. London, Ser. A 455, 2117 (1999).

[17] Y. Grabovsky and R. V. Kohn. Microstructures minimizing the energy of a two phase elastic composite in two space dimensions. Parts1, 2. JMPS, 43, 6, (1995) pp.933–972",

[18] Z. Hashin and S. Shtrikman. A variational approach to the theory of effective magnetic permeability of multiphase materials. J. Appl. Phys. 33 (1962) 3125–3131.

[19] Z. Hashin and S. Shtrikman. A variational approach to the theory of the elastic behavior of multiphase materials. J. Mech. Phys. Solids, 1963.

[20] R. Kohn and G. Strang. Optimal design and relaxation of variational problems. III. Comm. Pure Appl. Math. 39 (1986), no. 3, 353–377. 39 (1986), no. 1, 113–137. 39 (1986), no. 2, 139–182.

[21] K. A. Lurie. Optimal control in problems of mathematical physics, Nauka, 1975. In Russian.

[22] K. A. Lurie. Applied optimal control: Theory of distributed systems New York: Plenum Press, 1993.

[23] K.Lurie, A. Cherkaev. G-closure of a set of conducting media (two-dimensional problem). - Doklady Akademii Nauk SSSR, 1981, 259, N.2, pp. 238-241.

K. A. Lurie and A. V. Cherkaev G-closure of a set of anisotropic conducting media in the case of two dimensions", Doklady, 259, No 2, pp.328–331 (in Russian).

[24] K.Lurie, A. Cherkaev. Exact estimates of conductivity of mixtures composed of two isotropic media taken in prescribed proportion. Report 783, Physical Technical. Inst. Acad. Sci. USSR, 1982, 32p. (in Russian). Proceed. Roy. Soc. Edinburgh, sect. A, 1984, 99 (P1-2), pp. 71-87.

[25] K.Lurie, A. Cherkaev. Exact estimates of conductivity of a binary mixture of isotropic compounds. Report N.894, Physical Technical. Inst. Acad. Sci. USSR, 1984 (in Russian) Proceedings R. Soc. Edinburgh, sect. A, 1986, 104 (P1-2), pp. 21-38.

[26] K. Lurie and A. Cherkaev. Optimization of properties of multicomponent isotropic composites. Report No. 895, Physical Technical. Inst. Acad. Sci. USSR, 1984. (in Russian)- J. Optimization. Theory and Applications., 1985, 46, N.4, pp. 571-580.

[27] K. A. Lurie and A. V. Cherkaev. Effective characteristics of composite materials and the optimal design of structural elements. (Russian). Uspehi Mechaniki, 1985. English translation in [12].

[28] G. W. Milton. The theory of composites. Cambridge Monographs on Applied and Computational Mathematics, 6. Cambridge University Press, Cambridge, 2002.

[29] G. W. Milton. Concerning bounds on the transport and optical properties of a multi-component composite material. J.Appl. Physics, 52, 5294-5304.

[30] G. W. Milton. A brief review of the translation method for bounding effective elastic tensors of composites. Continuum models and discrete systems, Vol. 1 (Dijon, 1989), 60–74, Interact. Mech. Math. Ser., Longman Sci. Tech., Harlow, 1990.

[31] G. W. Milton and R. Kohn. Variational bounds on the effective moduli of anisotropic composites. J. Mech. Phys. Solids 36 (1988), no. 6, 597–629.

[32] F. Murat. Contre-examples pour divers problèmes où le contrôle intervient dans les coefficients, Annali di Matematica Pura ed Applicata. Serie Quarta, 1977, pp.49–68.

[33] V. Nesi. Bounds on the effective conductivity of 2d composites made of $n \geq 3$ isotropic phases in prescribed proportion. Proc. Roy. Soc. Edinburgh Sect. A, 1995

[34] V. Smyshlyaev, J. R. Willis. On the relaxation of a three-well energy. Proc Royal Soc London, A, V455, Number 1983 / March 8, 1999, pp. 779 - 814

[35] K. Schulgasser. Sphere assemblage model for polycrystal and symmetric materials. J. Appl. Phys. 54 (1982) 1380–1382.

[36] D. R. S. Talbot, J. R. Willis, and V. Nesi. On improving the Hashin-Shtrikman bounds for the effective properties of three-phase composite media, IMA J. Appl. Math. 54 (1995), 97-107.

[37] L. Tartar. Estimations fines des coefficients homogénéisés. (French) [Fine estimates of homogenized coefficients] Ennio De Giorgi colloquium (Paris, 1983), 168–187, Res. Notes in Math., 125, Pitman, Boston, MA, 1985.

[38] S. Vigdergauz. Regular structures with extremal elastic properties. Mechanika Tverdogo tela, 24, 3, (1989), 57-63 (in Russian)