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

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#### 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 and Nesi bounds in the region of parameters where they are loose. The bounds by polyconvex envelope are modifies by taking into account the range of fields in optimal structures. The bounds are a solution of a formulated finite-dimensional constrained optimization problem. For three-material composites, bounds for effective conductivity are found in an explicit form. Three-material isotropic microstructures of extremal conductivity are found. It is shown that they realize the bounds for all values of conductivities and volume fractions. 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 more than 40,000 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

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

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

 $k_1 < k_2 < \ldots k_N$  are conductivities of the materials (materials), and  $m_1 \ge 0, \ldots, m_N \ge 0$   $(m_1 + \ldots + m_N = 1)$  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] expanded 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  $\kappa_1$  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 threematerial laminates for two-dimensional conductivity, [4, 3]. New optimal threematerial 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 derive new bounds of isotropic effective conductivity that complement Hashin-Shtrikman bounds. In order to establish them, we analyze assumptions on admissible microstructures and introduce a constrain on fields in them, called *rank-one connectedness*. Section 2.3 describes the set of admissible microstructures and explains the rational of choosing it. We also find structures that explicitly 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, a corresponding variational problem, and assumptions. 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  $k_3 = \infty$ .

### 2 Periodic conducting composites

#### 2.1 Equations

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

The variable conductivity k(x) within the cell is

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

where  $x = (x_1, x_2)$  and  $\chi_i$  is the characteristic function of subdomain  $\Omega_i$ :

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

The area of subdomain  $\Omega_i$  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.

$$m_i > 0, \quad \sum_{i=1}^N m_i = 1.$$
 (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  $\Omega_i$ , because  $k(x) = k_i$  is constant there.

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

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

$$\arg\left(\sup_{x\in\Omega_{i}}|\nabla u_{a}(x)|\right)\in\partial\Omega_{i},\quad i=1,\ldots,N. \tag{2.6}$$

(ii) Gradient  $\nabla u_a(x)$  is  $\Omega$ -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  $\partial_{pm}$  between domains  $\Omega_p$  and  $\Omega_m$ ,  $p, m = 1, \ldots N, p \neq m$ , are satisfied

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

and

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

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

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

and n and  $\tau$  are the normal and tangent to  $\partial_{pm}$ . 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  $\tau$  are defined almost everywhere on  $\partial_{pm}$ .

**Energy** The energy  $\Pi_a$  of the periodicity unit cell  $\Omega$  in an external field  $E_a$  is equal to

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

where

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

### 2.2 Effective Properties

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

$$\Pi_a = \frac{1}{2} k_*(\chi)_{11} E_a^T E_a.$$
(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  $\chi = (\chi_1, \ldots, \chi_N)$  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  $\Pi_b$  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

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

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

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

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

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

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

Because  $e_0$  is arbitrary and  $K_*(\chi)$  that depends only on layout (structure)  $\chi$ , (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))

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

At the dividing curve  $\partial_{mp}$  between the domains  $\Omega_m$  and  $\Omega_p$ , 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  $J(e_0, \chi)$ 

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

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

rank 
$$[\nabla u]_p^m = 1$$
, rank  $[k\nabla u]_p^m = 1$ . (2.20)

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

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

Condition (2.20) implies that sets  $\Psi_m$  and  $\Psi_p$  are rank-one connected:

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

**Optimal composites** A layout  $\chi$  (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]).

$$\inf_{\chi_i \text{ as in } (2.3), (2.4)} J(e_0, \chi) = \frac{1}{2} \operatorname{Tr} \left( K_L e_0 e_0^T \right).$$
(2.23)

It is assumed that  $\chi$  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

$$e_0^T(K_*(\chi) - K_L)e_0 \ge 0 \quad \forall \chi \text{ as in } (2.3), (2.4), \ \forall e_0.$$
 (2.24)

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

$$\det(K_*(\chi) - K_L) \ge 0 \quad \forall \chi \text{ as in } (2.3), (2.4), \ \forall e_0.$$
(2.25)

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

$$K_L = k_L I \quad \text{if } e_0 = sI. \tag{2.26}$$

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

$$k_L = \frac{1}{s^2} \inf_{\chi_i} J(sI, \chi).$$
 (2.27)

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],

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

$$(2.28)$$

#### 2.3 Relaxed rank-one connectedness

Our goal is to describe optimal composites or optimal subdomains  $\Omega_i$  that minimize  $J(e_0, \chi)$ , (2.16). A minimizing sequence may contain domains  $\Omega_i$  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  $\Omega_i$  neighbors a fine-scale mixture of other materials, and the scales are separated. Namely, we assume that field  $e_i$  at the boundary of  $\Omega_i$  must be in rank-one connection with a convex combination of the fields in the remaining part of  $\Omega$  that represent an averaged field at the other side of the boundary. Therefore,  $\Psi_i$  sets must satisfy the conditions

$$\exists e_i \in \Psi_i, \ \exists e_c = \mathcal{C}\left(\bigcup_{k \neq i} \Psi_k\right): \ \det(e_i - e_c) = 0$$
(2.29)

of relaxed rank-one connectedness. Here,  $\mathcal{C}(X)$  means the convex envelope of X.

Admissible microstructures Condition (2.29) states that there exist an almost everywhere differentiable boundary  $\Gamma$  which separates domain  $\Omega_i$  filled with  $k_i$ from an external domain  $\Omega_{\text{ext}}$  that does not contain  $k_i$ . This condition follows from continuity of potential u and the assumed local differentiability of  $\Gamma$ . It excludes some fractal microstructures that contain  $k_i$  in infinitely many scales. To the author's opinion, such constraints on microgeometry are necessary to avoid ambiguity in the basic definitions. For instance, a fractal minimizing sequence of microstructures (like laminates of infinite rank) requires consideration of Laplace equation (2.5) and continuity of u in domains separated by a generalized curve which may densely cover the whole periodicity cell. Boundary condition (2.8) that follows from the continuity of u should be redefined on such fractals and checked for consistency with major physical assumptions. 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. On a larger scale boundary between slices of "smaller scale" laminates, the conditions are satisfied for the averaged in smaller scales fields in accordance to (2.29). This scheme implies an assumption that the ratio of the scales tends to zero.

Notice that (2.29) assumes that domain  $\Omega_{\text{ext}}$  does not contains material  $k_i$  in a smaller scale but it does not requires that all microstructural boundaries are of this type. This condition is valid on the boundary of a laminates which contain a material  $k_i$  in the smallest scale. Any sequential laminate satisfies (2.29) if the rank of lamination is arbitrarily large but finite. Still, (2.29) excludes some fractal sequences of self-repeated layouts. If these sequences are the limits of sequential laminates, (2.29) could be relaxed. For instance, the functional may be adjusted by adding penalization for its violation.

#### Remark 2.1 (Underlying finite-difference equation could be ambiguous)

The necessity of some constraints on admissible microstructures is clear from examining the underlying finite-difference equation. Partial differential equation (2.5) in  $\Omega_i$  is conventionally viewed as a limit of a finite differences equation in which the potential is defined at knots of a simple lattice. This consideration implies an assumption that the characteristic scale of  $\Omega_i$  is much larger than the distance between the knots in the difference equation. However, there is no means to keep the scales separated when the functional is minimized unless and additional assumptions (like additional terms in the energy) are introduced.

Alternatively, one may allow to assign conductivity  $k_i$  at every knot of lattice, thereby introducing one scale for both the structure and potentials. Then, there exist checkerboard-type structures without clear boundaries and domains  $\Omega_i$  without interiors. The corresponding difference equations do not tend to (2.5), (2.8) and an additional convention is required for interpreting of the limiting equations.

In order to avoid these ambiguities in definitions, some constraint about the boundary  $\Gamma$  must be imposed. The used here condition (2.29) is an example of such constraint.

#### 2.4 Notations

For the next consideration, it is convenient to introduce a matrix basis for  $2 \times 2$  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  $\delta_{ij}$  is the Kronecker symbol. Any  $2 \times 2$  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

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

One can immediately verify that

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

where

$$D^2 = D_*^2 + D_{**}^2. (2.32)$$

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  $\nabla u$  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

$$S(\nabla u) = \frac{1}{\sqrt{2}} \left( \frac{\partial u_a}{\partial x_1} + \frac{\partial u_b}{\partial x_2} \right); \quad D_*(\nabla u) = \frac{1}{\sqrt{2}} \left( \frac{\partial u_a}{\partial x_1} - \frac{\partial u_b}{\partial x_2} \right), D_{**}(\nabla u) = \frac{1}{\sqrt{2}} \left( \frac{\partial u_a}{\partial x_2} + \frac{\partial u_b}{\partial x_1} \right), \quad V(\nabla u) = \frac{1}{\sqrt{2}} \left( \frac{\partial u_a}{\partial x_2} - \frac{\partial u_b}{\partial x_1} \right).$$
(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

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

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

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

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

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

where

$$S_{i} = \frac{1}{\|\Omega_{i}\|} \int_{\Omega_{i}} S(x) \, dx, \ D_{i} = \frac{1}{\|\Omega_{i}\|} \int_{\Omega_{i}} D(x) \, dx, V_{i} = \frac{1}{\|\Omega_{i}\|} \int_{\Omega_{i}} V(x) \, dx, \ (3.4)$$

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

$$\mathcal{N}_{i} = k_{i} \int_{\Omega_{i}} \left[ (S(x) - S_{i})^{2} + (D_{i} - D(x))^{2} + (V_{i} - V(x))^{2} \right] dx.$$
(3.6)

The mean values are subject to integral constraints

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

$$S(x) = S_i, \quad D(x) = D_i \quad V(x) = V_i \quad \forall x \in \Omega_i, \quad i = 1, \dots, N,$$
(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:

$$V_i = 0, \quad D_i = 0, \quad i = 1, \dots, N.$$
 (3.9)

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

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

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

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

Notice that fields (3.8)-(3.9) are not compatible. Since e is constant in  $\Omega_i$  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 (2.29). 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  $\Omega_i$  by their averages. However, the differential constraints are indirectly accounted for via quasiaffinity of det $(\nabla u)$ ,

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

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

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

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

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

recalling that the applied field  $e_0 = \frac{1}{\sqrt{2}}S_0I$  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

$$\frac{1}{2}(k_* + t)S_0^2 \ge \frac{1}{2}W_t^{\text{poly}}(e_0)$$
(3.15)

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

$$W_t^{\text{poly}} = \inf_{e \in \mathcal{E}} \sum_{i=1}^N \int_{\Omega_i} \left[ (k_i + t) \left( S^2(x) + V^2(x) \right) + (k_i - t) D^2(x) \right] dx.$$
(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

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

 $W_t^{\text{poly}}$  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

$$k_* \ge k_L = \frac{W_t^{\text{poly}}}{S_0^2} - t \quad \forall t \in R_1.$$
 (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  $W_t^{\text{poly}}$  (3.16) are bounded as

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

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

$$G_i^{poly} = \begin{cases} (k_i + t)(S_i^2 + V_i^2) + (k_i - t)D_i^2 & \text{if } 0 < t \le k_i \\ -\infty & \text{if } t > k_i \end{cases}$$
(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  $\Omega_i$  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  $\Omega_i$  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  $W_t^{\text{poly}}$  becomes

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

where

$$S: \left\{ S_1, \dots, S_N : \sum_{i}^N m_i S_i = S_0 \right\}.$$
(3.21)

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

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

where

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

Then we compute  $\Gamma$ ,

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

and arrive at a lower bound (3.17)

$$k_* \ge B(t) \quad \forall t \in [0, k_1]; \quad B(t) = (-t + H_0(t)).$$
 (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.

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

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

Optimal *D*-components are

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

$$D(x) = 0, \ \forall x \in \Omega - \Omega_1.$$
(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,

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

Notice that the polyconvex bound admits a minimizer with nonzero D-component in  $\Omega_1$ , 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, ..., 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  $\Omega_1$  is placed between the other domains which have mutually incompatible fields.

In other terms, sets  $\Psi_i$ , i > 1 of ranges of  $\nabla u$  in  $\Omega_i$  are rank-one connected to  $\Psi_1$  set, see (2.22), (2.29). 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  $\Psi_1$  consists of all symmetric (V=0) matrices with a fixed trace and arbitrary *D*-component,  $\Psi_1 = \{\nabla u : S = S_1, D = 0\}$ . The equality (2.18) of the tangent components of  $\nabla u$  in  $\Omega_1$  and a neighboring subdomain  $\Omega_i$  is expressed as  $S_i = S_1 + D_1$  in notations (2.33). By choosing a proper value of D in  $\Psi_1$ , one can make sets  $\Psi_1$  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  $K_*$ 

$$2\frac{\det K_* - k_1^2}{\operatorname{Tr} K_* - 2k_1} \ge H_0(k_1) \quad \forall K_* \text{ in } G\text{-closure}$$
(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  $\Omega_1$  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  $\Omega_1$  is bounded,

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

In  $\Omega_m$ , 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  $\partial_{im}$ , the continuity conditions (2.18), (2.19) are satisfied. Since the field in  $\Omega_m$  is constant and isotropic, the field component S, D, V at  $\Omega_i$ -side of the boundary satisfies the conditions

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

$$D^{2} = (S - S_{m})^{2}, \quad S = \frac{k_{i} + k_{m}}{2k_{i}}S_{m}, \quad V = 0 \text{ on } \partial_{im}$$
 (3.31)

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

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

$$\frac{\partial u_a}{\partial x_1} + \frac{\partial u_b}{\partial x_2} = 2\beta_i, \quad \frac{\partial u_a}{\partial x_2} - \frac{\partial u_b}{\partial x_1} = 0 \quad \forall x \in \Omega_1.$$
(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  $\Omega_i$  function  $\hat{u}$  of  $x_1 + ix_2$ , respectively,

$$u_a = \beta_i x_1 + \Re(\hat{u}), \quad u_a = \beta_i x_2 + \Im(\hat{u}).$$
 (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  $\Omega_i$ . Using (3.32), we exclude derivatives of  $u_b$  and express det  $\nabla u$ through gradient  $\nabla u_a$  of a harmonic in  $\Omega_i$  function  $u_a$ ,

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

The right-hand side of (3.34) reaches its minimum at the boundary  $\partial_{im}$  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,  $S(x) = S_i = \text{constant}$ ,  $x \in \Omega_i$ , therefore

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

Correspondingly, D(x) reaches its maximum at  $\partial_{im}$  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  $\Omega_i$  and  $\Omega_m$  is nonnegative defined:

$$e(x) - e(y) \ge 0 \Rightarrow \det(e(x) - e(y)) \ge 0 \quad \forall x \in \Omega_i, \ \forall y \in \Omega_m.$$
(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.

or

**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  $e \ge 0$  (see [33, 5]) or

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

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  $\Psi_i$  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  $\Omega_j$  and  $\Omega_i$ , 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  $\Omega_i$  and  $\Omega_j$ , respectively. It uniformly restricts the fields in  $\Omega_i$  and  $\Omega_j$ .

**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  $\alpha_i$  are ordered constants,  $0 \leq \alpha_N \leq \ldots \leq \alpha_1 < \infty$ . These inequalities can be proven if the variational problem (2.23) is rewritten as a multiwell problem (see, for example [9]) with the Lagrangian

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

that depends only on e. Here  $\gamma_i$  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  $\Omega_1$  is bounded as well. Indeed, potential  $u_a$  in domain  $\Omega_1$  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,  $\nabla u_a$  is bounded, see (4.2). The jump conditions (2.18) requires that  $\nabla u_a$  at  $\partial \Omega_1$  is bounded too; therefore it is bounded everywhere in  $\Omega_1$ . The same is true for  $\nabla u_b$ . Therefore,  $\|e(x)\|^2 = S^2 + D^2 + V^2$  is bounded everywhere in  $\Omega$ .

**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  $\Psi_i$ -sets improves the bounds on effective properties. To derive the bound, we explore a simple lemma.

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

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

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

v

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

Then

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

Indeed, if  $\alpha \geq 0$ , integrant  $\alpha v^2$  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  $v_{\text{max}}$ . If  $\alpha \leq 0$ , integrant  $\alpha v^2$  is a concave function of v, therefore the minimum corresponds to piece-wise constant v(x) that alternates its extreme values

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

Measures of the subdomains where and  $v_{\text{opt}} = -v_{\text{max}}$  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  $v_{\text{opt}} = v_{\text{max}}$  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,  $m_A = \frac{v_0 + v_{\text{max}}}{2v_{\text{max}}}$  Then (4.3) is satisfied.

#### 4.2 Optimal Constrained Fields and Bounds

Assume that ranges  $\Psi_i$  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

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

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

We return to the scheme of polyconvex envelope for a multiphase composite,  $N \geq 3$  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

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

$$G_i = (k_i + t)S_1^2, \quad i = 2, \dots, N.$$
 (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):

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

$$S(x) = S_i, \ D(x) = 0 \qquad \forall x \in \Omega_i, \ i > 2, S(x) = S_1, \ D(x) = \pm \Theta_1^{\frac{1}{2}} \quad \forall x \in \Omega_1.$$
(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  $\Omega_2$ , and  $\Omega_2$  plays the same role as  $\Omega_1$  plays in the translation bound. The optimal fields are

$$S(x) = S_i, \ D(x) = 0, \qquad \forall x \in \Omega_i, \ i > 2,$$
  

$$S(x) = S_1, \ D(x) = \pm \Theta_1^{\frac{1}{2}}, \qquad \forall x \in \Omega_1,$$
  

$$S(x) = S_2, \ D(x)^2 \le \Theta_2, \ D_2(x) \text{ is not defined } \forall x \in \Omega_2.$$

$$(4.11)$$

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  $k_r < t \leq k_{r+1}$ , r constraints are active:

$$G_{i} = \begin{cases} (k_{i} + t)S_{i}^{2} - (t - k_{i})\Theta_{i}(S_{i}) & \text{if } i < r\\ (k_{i} + t)S_{1}^{2} & \text{if } r \leq i \leq N \end{cases}$$
(4.12)

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

and

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

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

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

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

$$S(x) = S_i, \ D(x) = 0, \qquad x \in \Omega_i, \ i = r + 1, \dots, N$$
  

$$S(x) = S_i, \ D(x)^2 = \Theta_i, \qquad x \in \Omega_i \ i = 1, \dots, r - 1$$
  

$$S(x) = S_i, \ \begin{cases} D(x)^2 = 0 & \text{if } t < k_r \\ D(x)^2 < \Theta_2 & \text{if } t = k_r \end{cases}, \ x \in \Omega_r$$
(4.17)



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,  $k_2 < t < k_3$ 

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  $\Theta_i$  on the optimal fields in  $\Omega_i$  become active everywhere in these sets when  $t > k_i$ . The points of  $\Omega_i$  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

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

$$(4.18)$$

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  $\Gamma$  (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

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

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  $\Omega_1$ . This condition implies that  $det(\nabla u) = 0$  or that  $\nabla u_a$  and  $\nabla u_b$  are collinear almost everywhere in  $\Omega_1$ . 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  $\Omega_i$  can be arbitrary, therefore the constraints on  $\Psi_i$  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  $\Omega_i$ , etc, since these can be arbitrary chosen to minimize the energy; the points in optimal  $\Omega_i$  domains are undistinguishable. Constraints on  $\Psi_i$  are expressed only through the values of e in  $\Omega_i$ .

Sets  $\Psi_i$  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  $\Psi_i$  are described by inequalities  $\bar{\theta}_i(e) \geq 0$ . The constraints have the forms

$$\bar{\theta}_i(S, D, V, M) \ge 0 \text{ or } D^2 \le \bar{\Theta}_i(S, V, M) \quad \text{ in } \Omega_i$$

$$(4.19)$$

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

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

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

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

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

$$\frac{\partial k_L}{\partial \Theta_i} \le 0, \quad i = 1, \dots, N.$$
(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  $(k_N \to \infty)$  exact, see Section 8.2. This bound could be further improved if  $\Theta_i$  are smaller, see Remark 4.4. The toughest bound corresponds to the smallest  $\Theta_i \ge 0$ . 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 (2.29) should be satisfied for all  $\Psi_i$ . For continuity of the potentials at the interfaces, it is *sufficient* to require that the sets  $\Psi_i$  contain relaxed rank-one connected matrices.

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

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

This assumption does not decreases  $\Psi_i$ -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, ..., 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  $\Psi_p$  contains the point  $[S_p, D_i = 0, V = 0]$ , and  $\Psi_i$  contains the point  $[S_i, D_i = S_i - S_p, V = 0]$ , or

$$\theta_p(S_p, 0, 0) \ge 0, \quad \theta_i(S_i, \pm (S_i - S_p), 0) \ge 0, \ 1 \le i (4.23)$$

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),

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

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

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

3. The smallest  $\Psi_i$ -set, rank-one connected with  $\Psi_N$  (4.25) contains a field e such that  $\det(e - \beta_N I) = 0$  or

$$(S - \beta_N)^2 - D^2 = 0, \quad S = S(x), D = D(x), \ x \in \Omega_i$$

The smallest function  $\Theta_i(S)$  that allows this connection is as follows

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

Notice that (4.26) is stronger than (4.18) and coincides with it when  $\beta_N = 0$  or  $k_N = \infty$ . Condition (4.26) is derived from the optimality requirements of minimization of  $\Theta_i$  coupled with the rank-one connectedness requirements. It is valid for optimal structures, while (4.18) – for all structures.

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

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

In terms of microstructures, the constrains do not prevent any two subregions  $\Omega_i$ and  $\Omega_j$  from being neighbors in the structure. Sets  $\Psi_i$  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  $\Psi_1$  and  $\Psi_N$  are independent of properties  $k_i$  of intermediate materials. Notice also that the ranges of intermediate materials belong to the convex envelope of  $\Psi_1$  and  $\Psi_N$ ,

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

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



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

**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).

### 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  $k_1 < t \leq k_2$  and substitute  $\Theta_1 = (S_1 - S_N)^2$  into inequalities (4.7), (4.8). We have

$$G_1 = (k_1 + t)S_1^2 + (k_1 - t)(S_1 - S_N)^2$$
  
= 2 k<sub>1</sub>S<sub>1</sub><sup>2</sup> + (k<sub>1</sub> - t) (-2S<sub>1</sub> + S<sub>N</sub>) S<sub>N</sub>,  
$$G_i = (k_i + t)S_i^2, \quad i = 2, ..., N.$$

The value of  $\Gamma$  (see (4.13)) in the interval  $k_1 < t \leq k_2$  is denoted as  $\Gamma_1$  where index 1 points to left end of the interval  $(k_1, k_2]$  of variation of t. It is equal to

$$\Gamma_{1} = \Gamma|_{t \in (k_{1}, k_{2}]} = 2m_{1}k_{1}S_{1}^{2} + \sum_{i=2}^{N-1} m_{i}(k_{i}+t)S_{i}^{2}$$
$$- 2m_{1}(k_{1}-t)S_{1}S_{N} + (m_{N}(k_{N}+t) + m_{1}(k_{1}-t))S_{N}^{2}$$
(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

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

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

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

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

A rank-one nonsymmetric matrix  $Y_1 P^T$  has only one nonzero entry  $(Y_1 P^T)_{1N} = -2m_1(k_1 - t)$  that corresponds to term  $-2m_1(k_1 - t)S_1S_N$  in right-hand side of (5.1).

Quadratic form  $\Gamma_1$  is assumed to be nonnegative. This assumption corresponds to symmetric part of matrix  $R_1 + Y_1 P^T$  being nonnegative defined. Solving the last condition for  $m_N$  we arrive at a condition

$$m_N \ge m_1 \frac{2t(t-k_1)}{(k_1+t)(k_N+t)} \quad \forall t \in (k_1, k_2].$$
 (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,  $S_0 = m_1 S_1 + \ldots + m_N S_N = 1$  or, in the vector form,

$$M^T S = 1, \quad M^T = (m_1, \dots m_N).$$
 (5.6)

and minimize  $\Gamma_1$  over vector  $S = (S_1, \ldots, S_N)$ . Performing minimization, we find vector  $S_{\text{opt}}$  of optimal fields

$$S_{\text{opt}}(t) = H_1 (R_1 + Y_1 P^T)^{-1} M$$
 and  $\min_S \Gamma_1 = \frac{1}{H_1}$  (5.7)

where

$$H_1 = \frac{1}{M^T (R_1 + Y_1 P^T)^{-1} M}.$$
(5.8)

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

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

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

$$\frac{1}{H_1} = \sum_{i=2}^{N-1} \frac{m_i}{k_i + t} + \frac{(k_1 - t)m_1^2 + (k_N + 2k_1 - t)m_1m_N + 2k_1m_N^2}{(k_1^2 - t^2)m_1 + 2k_1(k_N + t)m_N}.$$
(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

$$\Psi_{1} = \{S_{1}, \pm (S_{1} - S_{N})\}$$

$$\Psi_{2} = \begin{cases} \{S_{2}, 0\} & \text{if } t \in (k_{1}, k_{2}) \\ \{S_{2}, D\}, D \leq S_{1} - S_{N} \text{ if } t = k_{2} \end{cases}$$

$$\Psi_{i} = \{S_{i}, 0\}, i = 3, \dots, N$$
(5.11)

where  $S_i$  are as in (5.7).

Formulas (5.11) imply that field e in  $\Omega_1$  is always in the rank-one contact with  $e_N = S_N I$  in an optimal structure. In  $\Omega_1$ , 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

$$\int_{\Omega_1} D(e_1) dx = D_0 = 0.$$
 (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  $\Omega_2$  becomes undefined. Its mean value satisfies the constraint

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

**Remark 5.1** Nonzero values of D(x) in  $\Omega_2$  provide the continuity of potential u at the interfaces when the uniformly bounded field  $\nabla u$  in  $\Omega_1$  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  $\Omega_2$  becomes non-zero.



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:  $k_2 < t_0 < k_3$ 

#### 5.2 Next bounds

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

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

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

We compute as in (4.12)

$$G_{ri} = \begin{cases} (k_i + t)S_i^2 + (k_i - t)(S_i - S_i)^2 & \text{if } i = 1, \dots, r\\ (k_i + t)S_i^2 & \text{if } i = r + 1, \dots, N \end{cases}$$
(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  $\Gamma$  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  $(R_r)_{ii}$ 

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

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

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

$$(Y_r)_i = \begin{cases} 2m_i(k_i - t) & \text{if } i = 1, \dots, r\\ 0 & \text{if } i = r + 1, \dots, N \end{cases}$$
(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  $(R_r + Y_r P^T)$ ,

$$(R_r + Y_r P^T) > 0. (5.18)$$

**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  $S_{\text{opt}}$  of optimal fields in the materials is

j

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

where

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

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

where  $k_0 = 0$ .

When  $m_1 \rightarrow 0$ , 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

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

We compute

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

Using definitions of  $R_r$ , M,  $Y_r$ , we compute

$$M^{T}R_{r}^{-1}M = \sum_{i=1}^{r} \frac{m_{i}}{2k_{i}} + \sum_{i=r+1}^{N-1} \frac{m_{i}}{k_{i}+t} + \frac{m_{N}^{2}}{\rho_{r}},$$
$$M^{T}R_{r}^{-1}Y_{r} = 2\sum_{i=1}^{r} m_{i}\frac{k_{i}-t}{k_{i}}, \quad Y_{r}^{T}R_{r}^{-1}P = 0, \quad P^{T}R_{r}^{-1}M = \frac{m_{N}}{\rho_{r}}.$$

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

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

where  $\rho_r$  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

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

### 6 Generalizations

#### 6.1 Upper (Dual) bound

The dual bound  $k_U \ge k_*$  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 Ris the matrix of 90° rotation, and  $u_{\text{dual}}$  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  $k_* \ge k_L(k_1, \ldots, k_N, m_1, \ldots, m_N, t)$ where  $k_L$  is defined in (5.20), implies the dual bound

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

obtained by the substitution

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

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

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

#### 6.2 Bounds for anisotropic composites

The bound for anisotropic effective conductivity  $K_*$  is derived by a similar procedure, using (2.24), (2.25). 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  $\Psi_i$ , 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  $\Omega_1$  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,  $m_1|D_0| \leq S_1 - S_N$ , the supports  $\Psi_i$  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  $\Psi_i$  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

$$\frac{1}{2}k_1^*(S_0+D_0)^2 + \frac{1}{2}k_2^*(S_0-D_0)^2 + t(S_0^2-D_0^2) - H_r(t)S_0^2 \ge 0,$$
(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 (2.24), (2.25). The nonnegativity is equivalent to the requirement that matrix

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

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

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

Equivalently, it can be rewritten in the form

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

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

where

$$\frac{1}{H_1(t)} = \frac{m_1}{2k_1} + \frac{m_2}{k_2 + t} + \frac{(m_1(k_1 - t) + 2k_1m_3)^2}{2k_1(2k_1m_3(k_3 + t) + m_1(k_1^2 - t^2))}.$$
 (7.2)

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

$$\left. \frac{d}{dt} \left( -t + H_1(t) \right) \right|_{t=t_{\rm St}} = 0 \tag{7.3}$$

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

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

Here,

$$m_{11} = 2\sqrt{m_2}(1 - \sqrt{m_2})\frac{k_1(k_3 - k_2)}{(k_3 - k_1)(k_1 + k_2)}$$
(7.5)

$$m_{12} = \frac{1 - \sqrt{m_2}}{4k_2(k_3 - k_1)} Z_0 \tag{7.6}$$

$$Z_0 = \left(2k_2(k_3 - k_1) + \sqrt{m_2}(k_1 + k_2)(2k_3 - k_1 - k_2) - \sqrt{Z_2}\right)$$
(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)

When  $t_0 = k_1$ , bound (7.2) degenerates into Hashin-Shtrikman bound. This happens when  $m_1 \ge m_{11}$ , 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

$$t_{\rm st}(k_1, k_2, k_3, m_1, m_2) = k_1, \tag{7.12}$$

$$t_{\rm st}(k_1, k_2, k_3, m_1, m_2) = k_2, \tag{7.13}$$

respectively;  $t_{st}$  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  $k_L = B(m_1, m_2)$ :

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

where

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

Here

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

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

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

and

$$Z_5 = m_1 k_1^2 - m_1 k_2^2 + 2m_3 k_1 (k_3 - k_2)$$
  

$$Z_6 = \left[ (1 - \sqrt{m_2})^2 + (1 - m_1 - \sqrt{m_2})^2 \right] k_1 + m_1 (1 - \sqrt{m_2})^2 k_2 + m_1 m_3 k_3$$
  

$$Z_7 = \frac{(k_1 - k_2)m_1^2 + (2k_1 - k_2 + k_3)m_1 m_3 + 2k_1 m_3^2}{(k_1^2 - k_2^2)m_1 + 2k_1 (k_2 + k_3)m_3}.$$

 $B(m_1,m_2)$  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**  $m_1 \rightarrow 1$ . 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  $k_L = B^{\infty}(m_1, m_2)$ :

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



Figure 4: Regions of optimality of  $B_1$ ,  $B_2$ ,  $B_3$ -bounds in the plane  $m_1$ ,  $m_2$ ,  $m_2 \leq 1 - m_1$ , (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  $m_1 + m_2 \leq 1$  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.

where

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

Here,

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

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

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

and

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

Bound  ${B_2}^\infty$  corresponds to an optimal value  $t_0^\infty$  of the translator  $t_{\rm c}$ 

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

### 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,  $m_1 \ge m_{11}$ : 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  $k_1 < k_* \le k_2$  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 = 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



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.

Vigdergauz problems for all pairs  $k_1$  and  $k_i$ , i = 2, ..., 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 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  $\nu_{11}$  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  $\nu_{1p}$ , 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  $\nu_{22}$ . 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  $\nu_{31}$  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  $\nu_4$  - 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  $\Omega_2$  and  $\Omega_3$  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  $(\beta_1, \beta_3)$  in the first material with isotropic field  $(\beta_3, \beta_3)$  in third material. The fields are rank-one connected. The average field in the laminate is  $(e_{\mu}, \beta_3)$  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  $(\beta_2, \beta_2)$ . These fields in the structure are compatible if fraction  $\mu$  is so chosen that field  $(e_{\mu}, \beta_3)$  is in rank-one contact with the field  $(\beta_2, \beta_2)$  in  $k_2$ :  $k_{\mu} = \mu\beta_3 + (1-\mu)\beta_1 = \beta_2$ . Parameters  $\beta_i$  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  $(\beta_3, \beta_1)$  and field in  $k_3$  - to  $(\beta_3, \beta_3)$  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  $m_1 \ge m_{11}$ , see [4]. The described structure realizes Hashin-Shtrikman bound 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  $\Omega$  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  $\nabla u_a$  and  $\nabla u_b$  are orthogonal everywhere in  $\Omega$ , V = 0.
- 2. Field is isotropic and constant everywhere in  $\Omega_3$ , D = 0 and  $S = \beta_3$ .
- 3. S-component of field in  $\Omega_1$  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  $\Omega_2$  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.



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  $\Omega_1$  domain in the left structure is connected, no domains are connected in the structure in the center, and domain  $\Omega_2$  in the right structure is connected. When  $m_1 \rightarrow 0$ , 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  $k_3$ .

**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  $\nu_{11}, \nu_{12}$  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  $\nu_{31}, \nu_{32}$  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  $\nu_4$  – the fraction of the Tstructure, 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

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

$$m_2 = (1 - \nu_4)\nu_{32} + \nu_4(1 - \nu_2)\nu_{12} + \nu_4\nu_2.$$
(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  $\nu_{12}$  and  $\nu_{32}$  are zero,  $\nu_{12} = 0$   $\nu_{32} = 0$  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  $m_1 \rightarrow 0$ , the structure degenerates into an optimal twomaterial 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  $\Omega$ -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  $\Omega_2$  percolates and becomes connected. Domains  $\Omega_1$  and  $\Omega_3$  become inclusions. The field in  $\Omega_3$  remains constant and isotropic.

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## 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  $\mathcal{L}_{123,2,123}$   $(k_3 = \infty)$ 

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

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

$$e_{13} = e_{33} = \begin{pmatrix} 0\\0 \end{pmatrix}.$$
 (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  $\nu_{12}$  and  $\nu_{32}$  are zero,  $\nu_{12} = 0$   $\nu_{32} = 0$  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  $k_2$ 

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

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

- 2. S-component is constant in  $\Omega_1$ , 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  $\Omega_2$ , that is  $e_{22}[1] = e_{22}[2]$  in (9.4), which implies  $\nu_2 = \sqrt{m_2}$   $\nu_4 = \sqrt{m_2}$ , 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  $\nu_{mn}$ , we compute their optimal values denoted as  $v_{mn}$ 

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

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

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

The optimality conditions are

1. S-component is constant in  $\Omega_1$ , 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  $\Omega_2$ , 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  $\nu_p$ , we obtain a family of isotropic structures that have the same optimal effective property  $k_* = B_3^{\infty}$ . Therefore the bound  $B_3^{\infty}$  is exact.

**Nonuniqueness** Optimal structures  $\mathcal{L}_{123,2,123}$  are not unique. There is a freedom in choosing of volume fractions. Namely, fraction  $\nu_{23}$  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

$$v_2 = v_4 = \frac{m_1 k_2 + m_2 k_1}{k_1},\tag{9.12}$$

$$v_{31} = \frac{P}{1+P} \frac{m_1 k_1}{(k_1 - \tilde{k})} + \frac{1-P}{1+P} \frac{\tilde{k}}{2k_2},$$
(9.13)

$$v_{11} = \frac{k_1}{P+1} \left( \frac{m_1 k_1}{k_1 \hat{k} - \hat{k}^2} + \frac{P-1}{2k_2} \right).$$
(9.14)

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

$$P \in \left[P_0, \frac{1}{P_0}\right], \quad P_0 = 1 - \frac{8k_2m_1k_1}{k_1^2 - \hat{k}^2}.$$
 (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  $\Omega_1$  and  $\Omega_2$  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  $\mu_1 = m_{12} - m_1 \ge 0$ , instead of  $m_1$ , and calculate optimal volume fractions  $v_{12}$  and  $v_{32}$ :

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

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

We observe that both fractions  $\nu_{32}$  and  $\nu_{12}$  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  $m_1 \to m_{11} + 0$ .

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