

# Necessary conditions and optimality of multiphase structures

by Andrej Cherkaev  
Department of Mathematics  
University of Utah  
Salt Lake City, Utah 84112

November 24, 1999

**Keywords:** microstructures, multiphase composites, quasiconvexity, structural optimization, variational calculus.

## Abstract

The paper is concerned with variational technique for non-quasiconvex multiwell Lagrangians. Specifically, it deals with the problem of optimal structures of multiphase conducting composites. This problem is formulated as a multivariable extremal problem with a non-quasiconvex Lagrangian. A variational technique is developed for such problems: Special strong local variations are introduced and the necessary conditions of stability to these variations are derived. The minimal extension of the Lagrangian is introduced based on these necessary conditions. The extended problem preserves the cost of the original unstable problem and is stable against the class of the perturbations. Specifically, optimal structures of multiphase conducting composites in 2D are investigated. Two examples are analysed. It is shown that the suggested necessary conditions are equivalent to the known sufficient conditions (the translation bounds) for the problem of optimal two-component mixture. For three component mixtures, new structures are found that show the best conductivity; their properties are discussed.

## 1 Introduction.

This paper is concerned with the variational technique for non-convex variational problems. This technique is developed for the specific problem of optimal effective properties of multiphase composites.

**Two-material and multi-material optimal composites.** We consider the problem of determination of a structure of multiphase composites with extremal effective properties. The case of two-component optimal mixtures is well investigated: the bounds of effective properties and the matching parameters microstructures that realize these bounds are described for a number of cases. The list of solved problems includes numerous examples of conducting, elastic, electromagnetic and other materials and is continuing to grow (see for the references Cherkaev and Kohn [7]). Optimal multiphase mixtures are investigated much less. Several approaches to the problem and some examples of optimal structures have been suggested in the papers by Milton [25], Kohn & Milton [16], Lurie & Cherkaev [22], Cherkaev & Gibiansky [5], Golden [12], by using different methods. However the total picture is still obscure due to the lack of a systematic approach.

From a physical viewpoint, many optimal mixtures of two materials have an intuitively expected topology. The best periodic mixture from a “good” and a “bad” materials with prescribed volume fractions contains the “bad” material in compact nuclei surrounded by continuum of the “good” material which forms the connected structure. This topology increases the influence of the good material and reduces the disadvantage of the bad one. Of course, it is a long way from this intuitive idea to a mathematically rigorous description of optimal microstructures, but their topology is clear from a beginning. The known optimal solutions: high-rank laminates, coated spheres or ellipsoids, “truly periodic structures” (see Hashin and Shtrikman [15], Lurie & Cherkaev [21, 23], Kohn and Strang [17], Milton [26], Vigdergauz [36]) demonstrate different realizations of this intuitive idea. On the contrary, multi-material optimal mixtures can hardly be treated using similar intuitive ideas. The question where to place the material with intermediate properties is more delicate, and intuitive answer is not so clear. As we demonstrate below, an optimal topology depends not only on ordering of the material’s properties, but also on the concentrations of the materials in the composite.

The optimal multiphase mixtures are worth to study. The majority of natural and artificial composites involves more than two materials, especially those which show unusual properties. In structural optimization, knowledge of the geometry of two-component optimal mixtures has allowed to the solutions of the problems of topology optimization (see the book by Bendsoe [1] for details). Here, one of the given “materials” is void and the problem of optimal structures reduces to the problem of optimal topology of the solid phase. Therefore, a meaningful consideration of optimal design of even two-component mixtures requires knowledge of the geometry of optimal three-component mixtures, since void is an

additional “material” that could be always added. One also deals with multiphase mixtures in problems of the phase equilibrium in solids, where differently oriented anisotropic materials participate in optimal mixtures (see, for example, the paper by Bhattacharya and Kohn [2]).

**Methods for optimization of effective properties.** The problem of optimal composite is formulated as a variational problem of minimization of the sum of stored energies in the composite. It is assumed that an unknown periodic structure is exposed to several uniform orthogonal external fields. To find the optimal composite, we compute the sum  $I$  of stored in the composite energies caused by these fields; then we minimize  $I$  upon all structures of the same volume fractions of the materials (see the next section for mathematical formulation). The obtained variational problems are irregular (ill-posed, non-lower-weakly semicontinuous, or non-*quasiconvex*), since the minimizers include the characteristic function of materials which indicates what material is placed in a point of the structure.

**Sufficient conditions and optimal structures for two-phase composites.** The technique that is widely used for solving the problems of optimal mixtures includes two mutual supplementary elements. On one hand, one establishes *sufficient optimality conditions*. They have the form of classical Wiener bounds, Hashin-Shtrikman bounds [15], translation bounds (Lurie & Cherkaev [21], Tartar and Murat [35], Milton [28], Gibiansky and Torquato [11], and other), or similar bounds by Zhikov [39]), by Kohn and Milton [16], bounds by Nesi [32], etc. Bounds for composites of non-linear materials have been found by Willis [37], Talbot and Willis [34], Ponte-Castaniedo [33], et al. These bounds constrain the stored in a fixture energy by establishing inequalities between it and an explicit function of the mean field, properties, and volume fractions of mixed materials. These inequalities are valid for all mixtures regardless of their geometry. It is possible to obtain information about the fields in them using the sufficient conditions (see Milton [29], Grabovsky [13]) assuming that these conditions are attainable.

This technique (at least in its present form) is mainly restricted to two-component mixtures and does not provide a guide for non-trivial generalization to multiphase case. Although the methods lead to sufficient conditions also for multicomponent mixtures, there are no guarantee that the bounds are exact. For instance, the sufficient conditions based on the translation method fail to be exact for a whole range of volume fractions of phases (see the discussion in the papers by Kohn and Milton [16], Cherkaev and Gibiansky [5], Nesi [32]). These conditions are too rigid: They *a priori* specify an algebraic form of bounds.

**Laminates.** On the other hand, one finds (essentially by guessing) specific structures of *optimal geometry* by considering special class of structures. For two-phase composites, a number of structures has been suggested that realize the bound so that the corresponding inequalities in the sufficient conditions become equalities. This match allows one to prove

simultaneously the optimality of the structures (which represent minimizing sequences of the variational problem) and the sharpness of the bounds.

However, it is hard to speculate on an optimal structure in an arbitrary chosen class in the absence of reliable sufficient conditions. Besides, the problem of an optimal multicomponent mixture depends on large number of prescribed parameters: properties of materials and their fractions. This makes the straightforward optimization in a class of arbitrary chosen structures ineffective because it requires an *a priori* hint of optimal topology and a corresponding factorization of the class of suspicious structures.

Some optimality conditions can be established by the consideration of the so-called “stability under lamination” approach by Francfort and Milton [9, 30] and Grabovsky and Milton [14]. In principle, this approach allows to derive effective properties of a large class of arbitrarily high-rank laminate mixtures, which could include the optimal structures. In this method, a set of laminates with varying volume fractions is viewed as a curve in the space of characteristics of effective tensors; this curve joins the points that represent the mixing materials. The set of effective properties of all laminates corresponds to a subset of this space. To find this subset, one uses an iterative procedure. Although this scheme is geometrically clear, its implementation for specific problems is far from trivial. The difficulties correspond to the necessity to describe a rather complicated surface of the final extension.

Recently, an interesting approach was developed by Gibiansky and Sigmund [10] that combines the laminates and computational approach.

**Necessary conditions of Weierstrass type and an extension.** The purpose of this paper is to enlarge the arsenal of available tools for structural optimization problems. We turn to the classical variational technique. Namely, we develop a technique of *strong necessary conditions of optimality* for these variational problems. These conditions detect instabilities of solutions. Based on the same necessary conditions, we also suggest *a minimal extension* of unstable variational problems that make it stable with respect to these variations and preserves its cost.

The considered optimality condition (strong variations of the material’s properties) have been introduced by Lurie in a series of pioneering papers in the seventeens [18, 19, 20], where he considered the optimization problem for a conducting medium. The method is a multidimensional analog of the Weierstrass variations in classical calculus of variations and of Pontriagian’s maximum principle in one variable control problems. This technique has been used by Lurie [18, 20], and by Lurie, Cherkhaev and Fedorov [24] for analysis of several problems of optimal design of conducting and elastic media. Here we consider a more complicated problems. For them, we introduce a class of variations and analyse the fields in optimal structures. Besides, we introduce the minimal extension of a non-quasiconvex Lagrangian.

**Structure of the paper.** The structure of the paper is the following. In Section 2 we formulate the problem and sketch a procedure of Weierstrass type necessary conditions and of the corresponding minimal extension. In Section 3 we derive formulae for a Weierstrass type variation, in Section 4 we apply this technique to the problem of two-component mixtures and show that the derived necessary conditions are also sufficient for this problem, in Section 5 we derive the necessary conditions for three component mixtures, and in Section 6 we analyse them and demonstrate new optimal structures.

## 2 Variational technique for unstable variational problems.

### 2.1 Formulation of the problem.

Here we formulate the problem of optimizing the structure of conducting materials in a two-dimensional domain, clearly the simplest problem of structural optimization. We develop the necessary conditions of optimality for this problem.

**Conductivity problem.** Consider a unit square  $\mathcal{O} = \{\mathbf{x} = (x_1, x_2) : 0 \leq x_i \leq 1, i = 1, 2\}$  divided into  $N$  subdomains  $\mathcal{O}_i, i = 1, 2, \dots, N$ :  $\mathcal{O} = \cup \mathcal{O}_i$  and repeated periodically in a plane. Suppose that the subdomains  $\mathcal{O}_i$  are filled with isotropic materials with conductivities  $\sigma_1, \sigma_2, \dots, \sigma_N$  so that a material  $\sigma_i$  occupies the domain  $\mathcal{O}_i$ . The conductivities are ordered as following:

$$0 \leq \sigma_1 < \sigma_2 < \dots < \sigma_N \leq \infty$$

The variable conductivity  $\sigma(\mathbf{x})$  in  $\mathcal{O}$  is equal to :

$$\sigma(\mathbf{x}) = \sum_{i=1}^N \sigma_i \chi_i(\mathbf{x}) \quad (2.1)$$

where  $\mathbf{x}$  the point in  $\mathcal{O}$  and  $\chi_i$  is the characteristic function of  $\mathcal{O}_i$ :

$$\chi_i = \begin{cases} 1 & \text{if } \mathbf{x} \in \mathcal{O}_i, \\ 0 & \text{elsewhere,} \end{cases} \quad \sum_i^N \chi_i(\mathbf{x}) = 0 \quad \forall \mathbf{x} \in \mathcal{O}. \quad (2.2)$$

Suppose that the periodic structure is exposed to a uniform external electrical field  $\mathbf{P}_1$  which causes the variable field  $\tilde{\mathbf{E}}_1(\mathbf{x})$  in each point of  $\mathcal{O}$ . The field  $\tilde{\mathbf{E}}_1(\mathbf{x})$  is a solution of the variational problem

$$\Pi(\mathbf{P}_1, \chi_i) = \min_{\tilde{\mathbf{E}}_1 \in \tilde{\mathcal{E}}_1} \int_{\mathcal{O}} \tilde{\mathbf{E}}_1 \cdot \sigma(\mathbf{x}) \tilde{\mathbf{E}}_1, \quad \tilde{\mathcal{E}}_1 = \left\{ \tilde{\mathbf{E}}_1 : \nabla \times \tilde{\mathbf{E}}_1 = \mathbf{0}, \int_{\mathcal{O}} \tilde{\mathbf{E}}_1 = \mathbf{P}_1 \right\}. \quad (2.3)$$

The Euler-Lagrange equations of this problem

$$\nabla \cdot \sigma \tilde{\mathbf{E}}_1 = 0, \quad \nabla \times \tilde{\mathbf{E}}_1 = \mathbf{0}, \quad \int_{\mathcal{O}} \tilde{\mathbf{E}}_1 = \mathbf{P}_1, \quad \tilde{\mathbf{E}}_1 \text{ is periodic in } \mathcal{O} \quad (2.4)$$

coincide with the equations of the steady state conductivity.

**Optimization problem.** Suppose that composite cells are exposed sequentially to two different external fields  $\mathbf{P}_1$  and  $\mathbf{P}_2$  which produce two interior fields  $\tilde{\mathbf{E}}_1$  and  $\tilde{\mathbf{E}}_2$ , respectively. Consider the following optimization problem: Minimize the sum of energies stored in the cell by choosing the best shape of domains  $\mathcal{O}_i$  (or the functions  $\chi_i(\mathbf{x})$ )

$$\min_{\chi_i \text{ as in (2.2)}} \Pi(\mathbf{P}_1, \chi_i) + \Pi(\mathbf{P}_2, \chi_i)$$

subject to constrains

$$\int_{\mathcal{O}} \chi_i - m_i = 0, \quad m_i \geq 0, \quad \sum_i^N m_i = 1, \quad i = 1, \dots, N \quad (2.5)$$

which fix the amounts (volume fractions)  $m_i$  of the materials. We add the constrains (2.5) with the Lagrange multipliers  $\gamma_i$  to the minimizing functional and formulate the minimization problem:

$$I' = \min_{\chi_i \text{ as in (2.2)}} \left\{ \Pi(\mathbf{P}_1, \chi_i) + \Pi(\mathbf{P}_2, \chi_i) + \sum_i^N \gamma_i \left( \int_{\mathcal{O}} \chi_i - m_i \right) \right\} \quad (2.6)$$

It is convenient to use the following notations. First, we introduce a  $2 \times 2$  not symmetric matrix  $\tilde{\mathbf{E}}$  of the fields:

$$\tilde{\mathbf{E}} = \begin{pmatrix} \tilde{\mathbf{E}}_1 & \tilde{\mathbf{E}}_2 \end{pmatrix}. \quad (2.7)$$

The sum of energies in an isotropic material  $\sigma$  is equal to  $\sigma \text{Tr}(\tilde{\mathbf{E}}^T \cdot \tilde{\mathbf{E}})$ . Also, we introduce a symmetric positively defined matrix  $\mathbf{E}$ :

$$\mathbf{E} = \left( \tilde{\mathbf{E}}^T \cdot \tilde{\mathbf{E}} \right)^{1/2} \quad (2.8)$$

with non-negative eigenvalues  $E_a \geq 0$ ,  $E_b \geq 0$ . The matrix  $\mathbf{E}$  allows a convenient representation of the sum of energies  $\Pi(\mathbf{P}_1, \chi_i) + \Pi(\mathbf{P}_2, \chi_i)$ :

$$\sum_{i=1}^2 \left( \tilde{\mathbf{E}}_i \cdot \sigma \tilde{\mathbf{E}}_i \right) = \text{Tr} \left( \sigma \mathbf{E}^2 \right). \quad (2.9)$$

Notice that if the fields  $\tilde{\mathbf{E}}_1$  and  $\tilde{\mathbf{E}}_2$  are mutually orthogonal ( the matrix  $\tilde{\mathbf{E}}$  is symmetric) then  $\mathbf{E} = \tilde{\mathbf{E}}$  and the eigenvalues  $E_a$  and  $E_b$  become magnitudes of these fields.

Similarly, we introduce the matrix  $\mathbf{P} = (\mathbf{P}_1, \mathbf{P}_2)$  of the external loadings. We consider orthogonal loadings ( $\mathbf{P}_1 \cdot \mathbf{P}_2 = 0$ ) which corresponds to the orthogonal matrix  $\mathbf{P}$ . Obviously:

$$\mathbf{P} = \int_{\mathcal{O}} \mathbf{E} \quad (2.10)$$

Finally, we rewrite problem (2.6) using the introduced matrix  $\mathbf{E}$  (2.1) and omitting the constant term  $(-\sum_i^N \gamma_i m_i)$ :

$$I(\mathbf{P}; \gamma_1, \dots, \gamma_N : \sigma_1, \dots, \sigma_N) = \min_{\chi_i \text{ as in (2.2)}} \left\{ \min_{\mathbf{E} \text{ as in (2.10)}} \int_{\mathcal{O}} W \right\}, \quad (2.11)$$

where the Lagrangian  $W$  is

$$W = \sum_i^N (\sigma_i \text{Tr} (\mathbf{E}^2(\mathbf{x})) + \gamma_i) \chi_i(\mathbf{x}).$$

The functional depends on external fields  $\mathbf{P}$ , on the Lagrange multipliers  $\gamma_1, \dots, \gamma_N$  (interpreted as the costs of the materials), and on the conductivities  $\sigma_1, \dots, \sigma_N$ .

An alternative formulation is provided by straight minimization of  $W$  over  $\chi_i$ . The variational problem becomes

$$I(\mathbf{P}; \gamma_1, \dots, \gamma_N : \sigma_1, \dots, \sigma_N) = \min_{\mathbf{E} \text{ as in (2.10)}} \int_{\mathcal{O}} W_{well},$$

where  $W_{well}$  is a multiwell Lagrangian

$$W_{well} = \min_i \left\{ \sigma_i \text{Tr} (\mathbf{E}^2(\mathbf{x})) + \gamma_i \right\}.$$

**Bounds for effective tensors.** The considered sum of energies indirectly defines the effective (homogenized) properties of an optimal structure. Namely, effective properties tensor  $\sigma_*$  of a structure is defined as a constant conductivity tensor that corresponds to the same energy as an inhomogeneous medium. Therefore

$$\Pi(\mathbf{P}_1, \chi_i) + \Pi(\mathbf{P}_2, \chi_i) = \sigma_*(\chi_i) \text{Tr} (\mathbf{P}^2)$$

Clearly, effective tensors depend on the structure of the composite cell. The set of all possible effective tensors correspond to all microstructures with fixed fractions  $m_1, \dots, m_N$  of components is called [21] the  $G_m$ -closure of the set of tensors  $\sigma_1, \dots, \sigma_N$ .

The formulated optimization problem (2.11) defines a point of the boundary of the  $G_m$ -closure:

$$I = \min_{\sigma_* \in G_m \text{ closure}} \left( \text{Tr} (\sigma_* \cdot \mathbf{P}^2) + \sum_i^N \gamma_i m_i \right) \quad (2.12)$$

After the variational problem (2.11) is solved, we could use its solution to find the boundary of the  $G_m$ -closure.

We use (2.5) to determine the costs  $\gamma_i$ . This way we find optimal volume fractions  $m_i$  and an optimal tensor  $\sigma_*$  as a function of the mean field  $\mathbf{P}$ . Different values of parameters

$\mathbf{P}$  correspond to different effective tensors  $\boldsymbol{\sigma}_*$  that lie on the boundary of the  $G_m$  - closure. The set of this tensors could be found by exclusion of parameters  $\mathbf{P}$  and  $\gamma_i$  from the solution. The remaining relation

$$\Psi(\lambda_1, \lambda_2, m_1..m_N, \sigma_1, \dots, \sigma_N) = 0 \quad (2.13)$$

(where  $\lambda_1, \lambda_2$  are the eigenvalues of  $\boldsymbol{\sigma}_*$ ) describes the component of the  $G_m$ -closure of three materials structure.

Technically, it is easier to fix  $\mathbf{P}$  and  $\gamma_i$  and to find an optimal structure for these parameters. However, we should be aware that the optimal structure does not necessary contain all available materials, but it may degenerate into a solid phase or into a mixture of a part of available materials, which corresponds to vanishing of some of fractions  $m_i$ .

## 2.2 Variation of properties.

The optimality of a structure is checked by a variational technique which requires the comparing of two proximate configurations rather than the comparing all configurations as sufficient methods do. Let us introduce a structural variation. To perform this variation we may implant an infinitesimal inclusion of an admissible material  $\sigma'$  in a point  $\mathbf{x}$  in the domain  $\mathcal{O}$  occupied by a different host material  $\sigma$ , and compute the difference in energies and in the cost. If the examined structure is optimal, the increment of the cost is positive.

The increment in energy depends on a shape of the implant; this shape must be adjusted to the field so that the increment reaches its minimal value (which, however, remains non-negative). If we priori restrict ourselves with elliptical inclusions, then we need to solve the problem of an single elliptical inclusion in an infinite plane (the Eshelby problem) to compute the increment of the energy.

Here we prefer to use a slightly different but equivalent procedure: we compute the increment caused by the replacement of the material  $\sigma$  in a neighborhood of a point  $\mathbf{x}$  by a quasiperiodic dilute composite of orthogonal second-rank laminates, figure 1. In this composite, the envelope is made of the host material  $\sigma$  and the inclusions are made of implant  $\sigma'$ . Doing this, we consider an array of infinitesimal and dilute inclusions instead of one elliptical inclusion. The advantage of this is the possibility to use the explicit formulae for homogenized properties  $\boldsymbol{\sigma}_* = \sigma + \delta\boldsymbol{\sigma}$  of the composite (see figure 1) and the smallness of  $\delta\boldsymbol{\sigma}$  for dilute composites.

Namely, a matrix laminate composite of second rank is characterized by its effective tensor [4]:

$$\boldsymbol{\sigma}_* = \sigma\mathbf{I} + m \left( (\sigma'\mathbf{I} - \sigma\mathbf{I})^{-1} + (1 - m)Q(\sigma) \right)^{-1}, \quad (2.14)$$

where the matrix  $Q$  determines the degree of anisotropy:

$$Q = \frac{1}{\sigma} \begin{pmatrix} \alpha_a & 0 \\ 0 & \alpha_b \end{pmatrix}, \quad \alpha_a + \alpha_b = 1, \quad \alpha_i \geq 0, \quad (2.15)$$

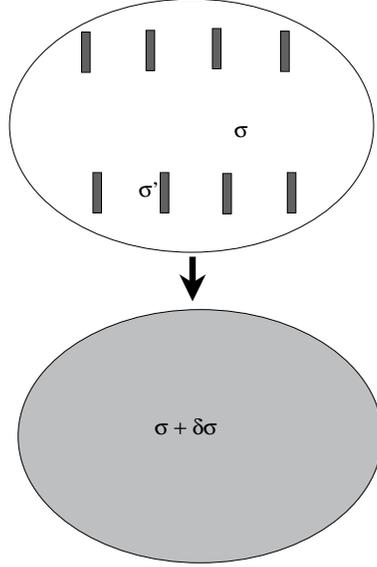


Figure 1: A dilute array of inclusions (above) and an equivalent homogenized inclusion.

the basis of of  $Q$  coincides with normals to lamination of the first and the second rank,  $\alpha_a$  and  $\alpha_b = 1 - \alpha_a$  are inner parameters of the structure that determine a relative elongation (densities in the orthogonal directions) of the inclusions,  $m$  is the volume fraction of material in the inclusions, and  $\mathbf{I}$  is the unit matrix.

To compute the variation  $\delta\sigma$  of the conductivity tensor caused by the array of infinitely dilute nuclei with infinitesimal volume fraction  $dm$ , we replace  $m$  by  $\delta m \ll 1$ , and  $\sigma_*$  by  $\sigma + \delta\sigma$ . Then (2.14) becomes

$$\delta\sigma = \delta m \left( (\sigma' - \sigma)^{-1} \mathbf{I} + Q(\sigma) \right)^{-1} + o(\delta m) = \delta m \begin{pmatrix} \lambda_a & 0 \\ 0 & \lambda_b \end{pmatrix} + o(\delta m). \quad (2.16)$$

where

$$\lambda_i = \frac{\sigma(\sigma' - \sigma)}{\sigma + \alpha_i(\sigma' - \sigma)}, \quad i = a, b. \quad (2.17)$$

The increment depends on  $\alpha_i$  and on the orientation of the directions of laminates. One can check by a direct calculation that the form of the increment (2.16) coincides with the increment caused by an single elliptical inclusion of the equal area. <sup>1</sup>

<sup>1</sup>However, in the corresponding elasticity problem, the array of inclusions leads to more sensitive variation than a single inclusion of the same area, see the paper by Cherkaev, Grabovsky, Movchan, and Serkov [6]

**Increment of the functional.** Let us compute the variation  $\delta I$  of energy caused by the variation (2.17) of properties  $\delta\sigma$ . For simplicity, we assume that the main axes of  $\delta\sigma$  are codirected with the principle axes of the matrix  $\mathbf{E}$  (later we demonstrate that the obtained necessary conditions are the strongest ones, which justify this assumption). The cost consists of the increment in energy due to the variation of conductivity  $\delta\sigma$  and of the “direct cost” of the variation: The change in the total cost due to change of quantities of the used materials. The direct cost of the variation is determined by its type: we replace the material  $\sigma$  (with the specific cost  $\gamma$ ) with the material  $\sigma'$  (with the specific cost  $\gamma'$ ); the change of the total cost is

$$(\gamma' - \gamma) \delta m. \quad (2.18)$$

The energy increment  $\delta\Pi\delta m$  is equal to

$$\delta\Pi\delta m = \text{Tr}(\mathbf{E}^2 \cdot \delta\sigma)\delta m = (\lambda_a E_a^2 + \lambda_b E_b^2) \delta m \quad (2.19)$$

where  $E_a$  and  $E_b$  are defined by (2.44). Using (2.17) and (2.15) we transform the increment to the form

$$\delta\Pi(\alpha) = \sigma(\sigma' - \sigma) \left( \frac{E_a^2}{\sigma + \alpha(\sigma' - \sigma)} + \frac{E_b^2}{\sigma + (1 - \alpha)(\sigma' - \sigma)} \right). \quad (2.20)$$

where we use the notation  $\alpha_a = \alpha$ . The variation of the Lagrangian  $W$  is denoted by  $\delta W\delta m$  where

$$\delta W(\alpha) = (\gamma' - \gamma + \delta\Pi(\alpha)); \quad (2.21)$$

it depends on the shape of the domain of variation, specifically, on the parameter  $\alpha$  of anisotropy (elongation) of the inclusions.

Note that the computed variation of the cost does not take into account the variation of the fields  $\mathbf{E}$  due to the variation of the structure. One can see that this variation is of the order  $o(\epsilon)$ . Of course, the fields inside the inclusion are significantly different than the outside fields, but this is accounted in the formula (2.14) for the effective properties of laminates.

**The Weierstrass test.** If the structure is optimal, then all variations, including the most sensitive one, lead to non-negative increment  $\Delta W$  of the Lagrangian:

$$\delta W \geq \Delta W, \quad \Delta W = \gamma' - \gamma + \min_{\alpha} \delta\Pi(\alpha) \geq 0. \quad (2.22)$$

because otherwise the cost can be reduced by this variation, and the structure fails the test.

**The most sensitive variations,  $\sigma' < \sigma$ .** Let us compute the most sensitive variation  $\Delta W$ . Note, that the second derivative of  $v$  with respect to  $\alpha$  has the sign of  $(\sigma' - \sigma)$ :

$$\frac{\partial^2}{\partial^2 \alpha_1} \delta W(\alpha) = (\sigma' - \sigma) \psi^2, \quad (2.23)$$

where  $\psi$  is real, therefore  $\alpha$  belongs to the boundary of the interval  $[0, 1]$ :

$$\alpha = 0 \quad \text{or} \quad \alpha = 1 \quad \text{if} \quad (2.24)$$

$$\sigma' - \sigma < 0. \quad (2.25)$$

In this case,  $\Delta W$  is equal to

$$\Delta W = \min_{\alpha} \delta W(\alpha) = \gamma' - \gamma + \sigma(\sigma' - \sigma) F_2(\sigma, \sigma', E) \quad (2.26)$$

where

$$F_2(\sigma', \sigma, E) = \begin{cases} \frac{E_a^2}{\sigma'^2} + \frac{E_b^2}{\sigma^2} & \text{if } \frac{E_a}{E_b} \geq 1, \\ \frac{E_a^2}{\sigma^2} + \frac{E_b^2}{\sigma'^2} & \text{if } \frac{E_a}{E_b} \leq 1. \end{cases} \quad (2.27)$$

For a physical interpretation, it is convenient to imagine an equivalent elliptic trial inclusion instead of the array of inclusions. As we mentioned before, the formula for the corresponding increment stays the same, and  $\alpha$  is interpreted as the parameter of elongation of the trial ellipse. If an inclusion is less conducting than the host material, then the best shape of the inclusion is a strip (an extremely elongated ellipse), elongated along the direction of the maximal field. The less conducting material tries to expose itself by creating an elongated obstacle across the direction of the maximal current to maximally reduce the conductivity of the structure.

**Permitted region** The formulae (2.22), (2.26), and (2.27) show that that the material  $\sigma$  can be optimal if the intensities  $(E_a, E_b)$  lie in a domain called the “permitted region”. In the plane of parameters  $E_a, E_b$ , the permitted region is the interior of the intersection of two mutually orthogonal ellipses. The elongation of these ellipses is determined by the ratio  $\sigma'/\sigma$  and their scale is defined by the difference in costs  $\gamma' - \gamma$ . Note that the boundary of the permitted set possesses the corner point  $E_a = E_b = (\gamma - \gamma') \frac{\sigma'}{\sigma^2 - \sigma'^2}$ .

**The most sensitive variations,  $\sigma' > \sigma$ .** In the opposite case

$$\sigma' - \sigma > 0, \quad (2.28)$$

the optimal value  $\alpha_0$  of  $\alpha$  varies in  $[0, 1]$  depending on the field  $\mathbf{E}$ . We find the stationary value  $\alpha'$  of  $\alpha$  from the equation  $\frac{\partial v}{\partial \alpha} = 0$  as:

$$\alpha' = \frac{E_b \sigma' - E_a \sigma}{(E_a + E_b)(\sigma' - \sigma)}. \quad (2.29)$$

Optimal  $\alpha_0$  is

$$\alpha_0 = \begin{cases} \alpha' & \text{if } \alpha' \in (0, 1), \\ 1 & \text{if } \alpha' > 1, \\ 0 & \text{if } \alpha' < 0. \end{cases} \quad (2.30)$$

We substitute this value of  $\alpha$  in (2.20) and find:

$$\Delta W = \gamma' - \gamma + \sigma(\sigma' - \sigma)F_1(\sigma, \sigma', E), \quad (2.31)$$

where

$$F_1(\sigma', \sigma, E) = \begin{cases} \frac{E_a^2}{\sigma'} + \frac{E_b^2}{\sigma} & \text{if } \frac{E_a}{E_b} \leq \frac{\sigma}{\sigma'}, \\ \frac{(E_a + E_b)^2}{\sigma + \sigma'} & \text{if } \frac{E_a}{E_b} \in \left[ \frac{\sigma}{\sigma'}, \frac{\sigma'}{\sigma} \right], \\ \frac{E_a^2}{\sigma} + \frac{E_b^2}{\sigma'} & \text{if } \frac{E_a}{E_b} \geq \frac{\sigma'}{\sigma}, \end{cases} \quad (2.32)$$

Physically, we interpret the result in terms of "trial ellipses": If the inclusion has a higher conductivity  $\sigma'$  than the host medium, its best shape is either a circle (if the field  $\mathbf{E}$  is isotropic), an ellipse (if the eigenvalues of the field  $\mathbf{E}$  are close to each other), or a strip elongated across the direction of minimal field (if the ratio of the eigenvalues of the field  $\mathbf{E}$  is large enough). The highly conducting inclusions try to hide in the domain to minimize the decrease of the total conductivity.

**Permitted region** In the plane of the parameters  $E_a, E_b$ , the permitted region is the convex envelope supported by two mutually orthogonal ellipses; note that the boundary of the set possesses a straight component. The elliptical parts of the boundary of the permitted region correspond to the strip-like inclusions (the case when  $\alpha_0 = 0$  or  $\alpha_0 = 1$ ), the straight part corresponds to the elliptical inclusions (the case when  $\alpha_0 \in (0, 1)$ ).

**Remark 2.1** *One can check by the direct calculation that the assumption of the orientation of the optimal trial ellipse along principle axes of  $\mathbf{E}$  was correct.*

**Necessary conditions. Forbidden region.** The obtained inequalities (2.26) and (2.31) can be viewed as inequalities for the field  $\mathbf{E}$  in different material within an optimal structure. Suppose that we want to determine the range of the field  $\mathbf{E}_i$  in the material  $\sigma_i$ . Put an inclusion of any admissible material  $\sigma_j$  into the host material  $\sigma_i$ . The resulting increment  $\delta\Pi(\sigma_j, \sigma_i, \mathbf{E}_i)$  must be non-negative. This provides constraints on the admissible field  $\mathbf{E}_i$ . The field  $\mathbf{E}_i$  is optimal if it corresponds to non-negative increments for all trial inclusions:

$$\mathcal{V}_i = \{\mathbf{E}_i : \Delta W(\sigma_j, \sigma_i, \mathbf{E}_i) \geq 0, \quad \forall j = 1, \dots, N\}. \quad (2.33)$$

The region of optimality is denoted by  $\mathcal{V}_i$

Computing the regions  $\mathcal{V}_i$ , we meet the following possibilities

- If the regions  $\mathcal{V}_i$  overlap each other, we conclude that the used variations are not sensitive enough to distinguish materials.
- If the union  $\mathcal{V} = \cup \mathcal{V}_i$  of all region  $\mathcal{V}_i$  coincides with the whole space  $\mathcal{E}$  of  $\mathbf{E}$ , the problem is regular: each external field correspond to optimality of a given material.
- If the union  $\mathcal{V} = \cup \mathcal{V}_i$  of all region  $\mathcal{V}_i$  does not coincides with the whole space  $\mathcal{E}$  of  $\mathbf{E}$ , the problem is unstable. A region of fields is forbidden: the fields never take values in the region  $\mathcal{V}_f = \mathcal{E} - \mathcal{V}$ . This implies that an external field  $\mathbf{P} \in \mathcal{V}_f$  correspond to discontinuous solution  $\mathbf{E}(\mathbf{x})$  which takes values in more than one region  $\mathcal{V}_i$ , so that its mean value is equal to  $\mathbf{P} \in \mathcal{V}_f$ .

### 2.3 Minimal extension.

**Definition.** The necessary conditions allow to extent the Lagrangian, that is to determine a new Lagrangian in the forbidden region. The extended Lagrangian corresponds to minimal energy achievable by a fast oscillating minimizing sequence. Physically, the extended Lagrangian defines minimal energy stored in a composite medium, assembled from the given materials. The extended Lagrangian  $SW(\mathbf{E})$

i) preserves the cost of the variational problem (2.11)

$$I(W(\mathbf{E})) = I(SW(\mathbf{E})), \quad \forall \mathbf{E};$$

ii) has a solution for all fields  $\mathbf{E}$  (including those in the forbidden region), that cannot be improved by considered class of variations:

$$\Delta(W(S\mathbf{E})) \geq 0, \quad \forall \mathbf{E}.$$

We define the minimal extension of a Lagrangian  $W(\mathbf{E})$  as

$$SW(\mathbf{E}) = \max\{\mathcal{R}W(\mathbf{E})\}, \quad (2.34)$$

where the functions  $\mathcal{R}W$  satisfies the inequalities:

$$W(\mathbf{E}) \geq \mathcal{R}W(\mathbf{E}), \quad \forall \mathbf{E} \quad (2.35)$$

and

$$\Delta(\mathcal{R}W(\mathbf{E})) \geq 0, \quad \forall \mathbf{E}. \quad (2.36)$$

The last inequality states that the new Lagrangian is stable against the considered variations.

The equality (2.34) allows us to present the minimal extension  $SW$  by the variational inequality:

$$\begin{aligned} SW(\mathbf{e}) &= W_i(\mathbf{e}), & \Delta_*(\mathbf{e}) &\geq 0, & (\mathbf{e} \in \mathcal{V}_i), \\ SW(\mathbf{e}) &\leq W_i(\mathbf{e}), & \Delta_*(\mathbf{e}) &= 0, & (\mathbf{e} \notin \cup \mathcal{V}_i) \end{aligned}$$

**Remark 2.2** *In the one-dimensional setting,*

$$I = \min_u \int_0^1 W(x, u, u_x).$$

*the extension leads to replacing the Lagrangian with its convex envelope. Indeed, here the Weierstrass condition requires the convexity of  $W(x, u, u_x)$  with respect to  $u_x$ . The extension is the maximal function that is not greater than  $W$ , and satisfies the Weierstrass test; it obviously coincides with the definition of the convex envelope of  $W$ . In the considered multidimensional problem the Weierstrass type condition requires a less obvious property than convexity; however the scheme of the extension stays the same.*

The obtained extension is the upper bound of the quasiconvex envelope of the energy, that is the infimum of the energy stores in an arbitrary structure. Indeed, there may exist a different necessary conditions that further constrict  $\mathcal{V}_i$ . These potential restrictions lead to lower the value of  $SW(\mathbf{E})$ . Therefore we obtain the inequality

$$QW(\mathbf{E}) \leq SW(\mathbf{E}) \leq W(\mathbf{E}), \quad \forall \mathbf{E}. \quad (2.37)$$

where  $QW$  is the quasiconvex envelope of  $W$ .

**The fields separation.** The optimality requires “phase separation”:  $\mathbf{E}(\mathbf{x})$  belongs to allowed regions  $\cup \mathcal{V}_i$  in any point of the periodic structure,

$$\mathbf{E}(\mathbf{x}) = \chi_i(x)\mathbf{E}_i(\mathbf{x}), \quad \mathbf{E}_i \in \mathcal{V}_i \quad (2.38)$$

and its mean value is equal to  $\mathbf{P} \in \mathcal{V}_f$ . We have

$$\mathbf{P} = \int_{\mathcal{V}} \mathbf{E}(\mathbf{x}) = \sum_{i=1}^N m_i \langle \mathbf{E}_i(\mathbf{x}) \rangle_{\mathcal{O}_i}, \quad m_i = \int_{\mathcal{V}} \chi_i(\mathbf{x}). \quad (2.39)$$

where the average is:

$$\langle z \rangle_{\mathcal{O}_i} = \frac{1}{|\mathcal{O}_i|} \int_{\mathcal{O}_i} z$$

Note that the field  $\mathbf{E}_i$  in  $i$ -th material is not necessary constant.

If a structure satisfies necessary conditions, its energy  $SW(\mathbf{E})$  is

$$SW(\mathbf{E}) = \sum_{i=1}^N m_i \sigma_i \langle \text{Tr } \mathbf{E}_i^2 \rangle_{\mathcal{O}_i}, \quad (2.40)$$

where the parameters  $m_i$  and  $\langle \mathbf{E}_i^2 \rangle_{\mathcal{O}_i}$  are determined from the condition (2.34). It requires in particular, that the fields  $\langle \mathbf{E}_i^2 \rangle_{\mathcal{O}_i}$  belong to the boundaries of  $\mathcal{V}_i$ . We have

$$SW(\mathbf{E}) = \min_{m_i} \min_{\mathbf{E}_i \in \partial \mathcal{V}_i} \sum_{i=1}^N m_i \sigma_i \text{Tr } \mathbf{E}_i^2, \quad \mathbf{E} = \sum_{i=1}^N m_i \mathbf{E}_i. \quad (2.41)$$

**Effective properties.** For a composite of linear materials, the extension leads to an optimal effective properties tensor  $\boldsymbol{\sigma}_*$ . The extended Lagrangian  $SW(\mathbf{E})$  has the form:

$$SW(\mathbf{E}) = \text{Tr}(\boldsymbol{\sigma}_* \mathbf{E}^2) + \gamma_* \quad (2.42)$$

where  $\boldsymbol{\sigma}_*$  is an anisotropic effective tensor of composite. It depends on the field  $\mathbf{E}$  since the structure of optimal composite varies together with the field; therefore the form (2.42) does not diminish the generality.

The cost  $\gamma_*$  of the composite is defined by the quantities  $m_i$  of the used materials and their costs  $\gamma_i$ :

$$\gamma_* = \sum_j^N m_j \gamma_j. \quad (2.43)$$

To find  $\boldsymbol{\sigma}_*$ , we suppose that the field  $\mathbf{E} \in \mathcal{V}_f$  corresponds to an optimal material  $\boldsymbol{\sigma}_*$ . We insert an inclusion of  $\sigma_i$  in the anisotropic material  $\boldsymbol{\sigma}_*$ , optimize its shape, and compute the increment, using (2.43)

$$\Delta(SW) = \Delta\Pi(\sigma_i, \boldsymbol{\sigma}_*, \mathbf{E}) - \gamma_i + \gamma_* = \Delta\Pi(\sigma_i, \boldsymbol{\sigma}_*, \mathbf{E}) + \sum_j^N m_j (\gamma_j - \gamma_i).$$

Then we repeat the procedure for all materials  $\sigma_i$ .

The minimal extension corresponds to the equality

$$\Delta_* = \min_i \left\{ \Delta\Pi(\sigma_i, \boldsymbol{\sigma}_*, \mathbf{E}) + \sum_j^N m_j (\gamma_j - \gamma_i) \right\} = 0, \quad (2.44)$$

which states that minimal of increments is equal to zero. This equality determines the unknown tensor  $\boldsymbol{\sigma}_*(\mathbf{E})$  and, further, the extended Lagrangian (see (2.42)).

**An alternative variation.** It may be convenient to use another variation to determine the extended Lagrangian. We could replace the material  $\sigma_i$  in a point of the allowed region  $\mathbf{E}_i \in \mathcal{V}_i$  with the composite material  $\boldsymbol{\sigma}_*$  and choose the best geometry of that inclusion. The resulting variation has the form

$$\delta W(\boldsymbol{\sigma}_*, \sigma_i, \mathbf{E}_i) - \gamma_* + \gamma_i \quad (2.45)$$

The minimal extension corresponds to the equality

$$\min_i \min_{\mathbf{E}_i \in \mathcal{V}_i} \delta W(\boldsymbol{\sigma}_*, \sigma_i, \mathbf{E}_i) - \gamma_* + \gamma_i = 0 \quad (2.46)$$

which determines the extended Lagrangian or the tensor  $\boldsymbol{\sigma}_*$ . To find the most dangerous variation, we should vary the shape of the inclusion and the field  $\mathbf{E}_i \in \mathcal{V}_i$  in the phase  $\sigma_i$ , and we examine all regions  $\mathcal{V}_i$ .

**Generalization: Other Variations** These results depend on the type of variations one uses. For multicomponent composites, one can introduce more sophisticated variations. For instance, one can consider the inclusions in the dilute matrix composites that are filled not with a given materials, but with a composite of several available materials. The requirement is that the effective properties of this composite must be an explicitly computable function, as in laminates. Accordingly, one optimizes the variations by choosing the most suitable composite in the inclusion together with the shape of inclusions. The example of such variation is discussed below.

### 3 Necessary conditions for two-phase structures

First, we apply the technique to find the optimal two-phase structures. This problem has been independently solved i by Lurie and Cherkaev [21] and by Murat and Tartar [35] by means of sufficient conditions (a version of the translation method). Here, we use this problem as a test ground for the suggested technique.

#### 3.1 Optimality of the fields. Forbidden region.

Consider an optimal structure made of two materials  $\sigma_1$  and  $\sigma_2 > \sigma_1$  and find the range of fields permitted by the described variations. Applying formulae (2.27) and (2.32) where the material constants  $\sigma$  and  $\sigma'$  are properly chosen, we obtain the following inequalities.

The increment  $\delta_{12}$  caused by inserting an inclusion of the material  $\sigma_2$  into the domain  $\mathcal{O}_1$  filled with  $\sigma_1$  is:

$$\delta_{12} = (\sigma_2 - \sigma_1)\sigma_1 F_1(\sigma_1, \sigma_2, \mathbf{E}_1(x)) + \gamma_2 - \gamma_1 \geq 0; \quad (3.1)$$

where  $\mathbf{E}_1$  is the field in  $\mathcal{O}_1$ . The increment  $\delta_{21}$  caused by inserting an inclusion of the material  $\sigma_1$  into the domain  $\mathcal{O}_2$  filled with  $\sigma_2$  is

$$\delta_{21} = (\sigma_1 - \sigma_2)\sigma_2 F_2(\sigma_2, \sigma_1, \mathbf{E}_2(x)) - \gamma_2 + \gamma_1 \geq 0; \quad (3.2)$$

where  $\mathbf{E}_2$  is the field in  $\mathcal{O}_2$ .

Let the set of permitted values of the field in the first material be  $\mathcal{V}_1$  and the set of permitted values of the field in the second material be  $\mathcal{V}_2$ . Assume that the eigenvalues of  $\mathbf{E}$  are ordered as

$$0 \leq E_a \leq E_b. \quad (3.3)$$

Using (2.27) and (2.32), we have:

$$\left. \begin{aligned} \sigma_1(\sigma_2 - \sigma_1) \left( \frac{E_A^2}{\sigma_2} + \frac{E_B^2}{\sigma_1} \right) + \gamma_2 - \gamma_1 \geq 0 & \text{ if } \frac{E_A}{E_B} \leq \frac{\sigma_1}{\sigma_2} \\ \frac{\sigma_1(\sigma_2 - \sigma_1)}{\sigma_1 + \sigma_2} (|E_A| + |E_B|)^2 + \gamma_2 - \gamma_1 \geq 0 & \text{ if } \frac{E_A}{E_B} \geq \frac{\sigma_1}{\sigma_2} \end{aligned} \right\} \text{ in } \mathcal{V}_1 \quad (3.4)$$

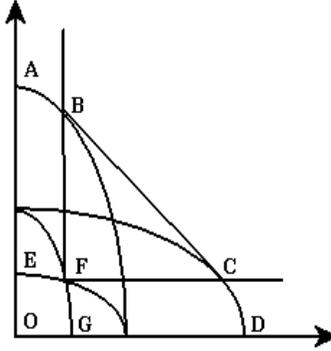


Figure 2: The permitted regions.

The region  $\mathcal{V}_1$  lies outside ABCD, the region  $\mathcal{V}_2$  lies inside EFG , and the forbidden region  $\mathcal{V}_f$  lies in between.

and

$$\frac{E_A^2}{\sigma_1} + \frac{E_B^2}{\sigma_2} \leq (\gamma_1 - \gamma_2) \frac{1}{\sigma_2(\sigma_2 - \sigma_1)} \quad \text{in } \mathcal{V}_2 \quad (3.5)$$

The corresponding graph of the permitted fields is presented in Figure 2 (the ordering of eigenvalues of  $\mathbf{E}$  is not assumed).

Let us analyse the fields in an optimal structure. Assume that an external field  $\mathbf{P}$  is given. If  $\mathbf{P} \in \mathcal{V}_1$  or  $\mathbf{P} \in \mathcal{V}_2$ , the optimal “structure” consists of one material  $\sigma_1$  or  $\sigma_2$  , respectively. In this case, the volume fractions are zero and one, respectively, and the field is constant everywhere.

The non-trivial case occurs when the mean field belongs to the forbidden region  $\mathcal{V}_f$ . The field  $\mathbf{E}$  cannot belong to this region, therefore  $\mathbf{E}$  must belong to  $\mathcal{V}_1$  or to  $\mathcal{V}_2$ . In this situation we are dealing with a true mixture and the solution of the variational problem is given by a non-smooth minimizer, since the field  $\mathbf{E}$  jumps on the boundary between the regions.

### 3.2 Minimal extension.

Let us perform the minimal extension of the Lagrangian in the forbidden region. Notice, that the minimal extension leads to determination of effective properties of optimal composites without the guessing optimal microstructures.

To find the extension, we use the scheme (2.45). We compute the increment caused by

replacing an isotropic material  $\sigma_1$  by an anisotropic inclusion made of material  $\sigma_*$

$$\boldsymbol{\sigma}_* = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \quad (3.6)$$

with eigenvalues  $\lambda_1$  and  $\lambda_2$ . The procedure of calculating of the increment  $\delta_{*1}$  caused by an array of inclusions made of  $\boldsymbol{\sigma}_*$  was described above. In this case, however, the inclusion is anisotropic. Following that procedure, we find the increment caused by the inserting a material  $\boldsymbol{\sigma}_*$  into the domain  $\mathcal{O}_1$ , where  $\mathbf{E} \in \mathcal{V}_1$ . The increment is

$$\delta_{*1}(\mathbf{E}, \alpha) = \sigma_1 E_A^2 \frac{\lambda_1 - \sigma_1}{\alpha \lambda_1 + (1 - \alpha) \sigma_1} + \sigma_1 E_B^2 \frac{\lambda_2 - \sigma_1}{\alpha \sigma_1 + (1 - \alpha) \lambda_2} + \gamma_* - \gamma_1. \quad (3.7)$$

The difference  $\gamma_* - \gamma_1$  of the cost of materials  $\sigma_*$  and  $\sigma_1$  is proportional to the amount of the second material used in the formation of  $\sigma_*$ :

$$\gamma_* - \gamma_1 = (\gamma_2 - \gamma_1) m_2. \quad (3.8)$$

The increment depends on the parameter  $\alpha \in (0, 1)$ . As before, we find the minimal increment by calculating an optimal value of  $\alpha$  and substituting it into (3.7):

$$\Delta_{*1}(\mathbf{E}) = \sigma_1 (E_A + E_B)^2 \frac{(\lambda_1 - \sigma_1)(\lambda_2 - \sigma_1)}{\lambda_1 \lambda_2 - \sigma_1^2} + (\gamma_2 - \gamma_1) m_2. \quad (3.9)$$

It is assumed in this calculation that the optimal value of  $\alpha$  lies in  $(0, 1)$  which correspond to the external field in the triangle BFC, see Figure 2. The increment (3.9) is equal to zero, if the tensor  $\boldsymbol{\sigma}_*$  (the minimal extension) is stable under the considered variations:

$$\Delta_{*1}(\mathbf{E}) = 0, \quad \text{if } \boldsymbol{\sigma}_* \text{ is stable for the variation.} \quad (3.10)$$

This equality must be fulfilled for all fields  $E_A$  and  $E_B$  in the region  $\mathcal{V}_1$ .

Finally, we recall that the fields  $E_A$  and  $E_B$  on the boundary of  $\mathcal{V}_1$  (see (2.32)) satisfy the equality

$$(E_A + E_B)^2 = (\gamma_1 - \gamma_2) \frac{\sigma_1 + \sigma_2}{\sigma_1(\sigma_2 - \sigma_1)} \quad \text{if } \frac{E_A}{E_B} \geq \frac{\sigma_1}{\sigma_2}. \quad (3.11)$$

We substitute this value into (3.9) and obtain an equality for  $\lambda_1, \lambda_2$ :

$$\frac{(\lambda_1 - \sigma_1)(\lambda_2 - \sigma_1)}{\lambda_1 \lambda_2 - \sigma_1^2} = m_2 \frac{\sigma_2 - \sigma_1}{\sigma_2 + \sigma_1}. \quad (3.12)$$

After obvious manipulations, this equality is transferred to the familiar form

$$\frac{1}{\lambda_1 - \sigma_1} + \frac{1}{\lambda_2 - \sigma_1} = \frac{1}{m_2} \left( \frac{2}{\sigma_2 - \sigma_1} + \frac{m_1}{\sigma_1} \right), \quad (3.13)$$

that represent the boundary of  $G_m$ -closure (see Lurie and Cherkaev[21]) obtained by translation method.

In a similar way, one can obtain the minimal extension for the case when  $\mathbf{P} \in \mathcal{V}_f$ ,  $\mathbf{P} \notin BFC$ , see Figure 2. In this case, the optimal value of  $\alpha$  in (3.9) is either zero or one. One can check, that the extension corresponds to the effective tensor with eigenvalues

$$\begin{aligned}\lambda_1 &= m_1/\sigma_1 + m_2/\sigma_2 \\ \lambda_2 &= m_1\sigma_1 + m_2\sigma_2.\end{aligned}$$

This extension matches the other sufficient condition, the Wiener bounds.

**Remark 3.1** *The other variations that consist of inserting an isotropic inclusion of  $\sigma_1$  or of  $\sigma_2$  into an anisotropic material  $\sigma_*$  lead to the same results, as one can check by a straight calculation.*

The obtained necessary conditions lead to an extension that coincide with an extension provided by sufficient conditions. This means that these necessary conditions are the strongest ones for the considered problem.

### 3.3 Optimality conditions and the structures.

**Compatibility.** Let us obtain information about the structures of optimal composites by analysis of necessary conditions. Firstly, we find a form for these conditions that does not depend on  $\gamma_1$  and  $\gamma_2$ . Consider the sum of the variations (2.27) and (2.32): we interchange two small inclusions of equal volume, putting the inclusion of  $\sigma_1$  into the domain  $\mathcal{O}_2$  occupied by  $\sigma_2$  and vice versa. Note that inclusions may be of different shapes, only their volume are equal. Clearly, this variation does not change the total amounts of materials  $\sigma_1$  and  $\sigma_2$ . Therefore the values of Lagrange multipliers  $\gamma_1$  and  $\gamma_2$  are irrelevant.

The total increment in the functional due to the interchange of the materials is found from (3.1) and (3.2) :

$$\delta_{12} + \delta_{21} = (\sigma_2 - \sigma_1)(\sigma_2 F_1(\sigma_1, \sigma_2, \mathbf{E}_1(x)) - \sigma_1 F_2(\sigma_2, \sigma_1, \mathbf{E}_2(x))). \quad (3.14)$$

The variation cannot decrease the energy of the optimal structure (which possesses the minimal energy), therefore the inequality holds

$$\delta_{12} + \delta_{21} \geq 0, \quad \forall \mathbf{E}_1 \in \mathcal{V}_1, \quad \forall \mathbf{E}_2 \in \mathcal{V}_2, \quad (3.15)$$

or

$$\sigma_2 F_1(\sigma_1, \sigma_2, \mathbf{E}_1(x)) - \sigma_1 F_2(\sigma_2, \sigma_1, \mathbf{E}_2(x)) \geq 0 \quad \forall \mathbf{E}_1 \in \mathcal{V}_1, \quad \forall \mathbf{E}_2 \in \mathcal{V}_2. \quad (3.16)$$

This inequality restricts the gap between the fields in different materials.

**The jump conditions.** Let us consider how these optimality conditions match the jump conditions on the phase boundaries. We compute the jump of the matrix  $\mathbf{E}$  on the boundary line between zones  $\mathcal{O}_1$  and  $\mathcal{O}_2$ . The normal to the boundary is denoted as  $\mathbf{n} = (\cos \theta, \sin \theta)$ . The elements of the matrix  $\tilde{\mathbf{E}} : \nabla \times \tilde{\mathbf{E}} = 0$  are discontinuous along the boundary due to the differential constraint (2.7). The continuity conditions that follow from the curl free nature of the fields  $\tilde{\mathbf{E}}_i$  and the natural variational boundary conditions are

$$\left[ \sigma \tilde{\mathbf{E}}_i \cdot \mathbf{n} \right]_{-}^{+} = 0, \quad \text{and} \quad \left[ \tilde{\mathbf{E}}_i \cdot \mathbf{t} \right]_{-}^{+} = 0, \quad i = 1, 2. \quad (3.17)$$

where  $[\cdot]_{-}^{+}$  denotes the jump:  $[z]_{-}^{+} = z_{+} - z_{-}$ .

**Remark 3.2** *The last condition indicates that  $\text{rank}(\tilde{\mathbf{E}}_2 - \tilde{\mathbf{E}}_1) = 1$ , it is called the rank-one connection between the fields matrices  $\tilde{\mathbf{E}}_2$  and  $\tilde{\mathbf{E}}_1$ .*

The rank-one conditions (3.17) can be rewritten as

$$\left[ \begin{pmatrix} \sigma & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \tilde{\mathbf{E}} \right]_{-}^{+} = 0. \quad (3.18)$$

where  $\phi$  is the angle of the decline of the normal to the boundary.

We want to compare the jump conditions with the necessary optimality conditions. The technical difficulty is that the jump conditions are expressed in terms of the matrix  $\tilde{\mathbf{E}}_i$  while the optimality condition is written in terms of the symmetric matrix  $\mathbf{E} = \left( \tilde{\mathbf{E}} \tilde{\mathbf{E}}^T \right)^{1/2}$ . Therefore we need to express the jump conditions in terms of the matrix  $\mathbf{E}$ .

The conditions (3.18) imply in particular that the determinants of the matrices  $\tilde{\mathbf{E}}$  and  $\mathbf{E}$  on the opposite sides of the boundary are connected by an equality

$$\left[ \sigma \det \tilde{\mathbf{E}}_i \right]_{-}^{+} = \left[ \sigma \det \mathbf{E} \right]_{-}^{+} = 0. \quad (3.19)$$

applied to both matrices  $\tilde{\mathbf{E}}$  and  $\mathbf{E}$ .

More complicated is the calculation of the jump of the trace of the matrix  $\tilde{\mathbf{E}}$ . It depends on the normal  $\mathbf{n}$  to the boundary. Using (3.17), we compute the jump of the trace of  $\tilde{\mathbf{E}}$  and compute the jump of the trace of the matrix  $\mathbf{E}$  which depends, as on parameters, on the angle between the normal and an eigenvector of  $\mathbf{E}$  and on the antisymmetric part of  $\tilde{\mathbf{E}}$ . Finally, we compute the bounds of the jump of  $\text{Tr} \mathbf{E}$  by optimization with respect to those parameters. We do not show here the details of this rather technical calculation performed by using Maple, but only review the results.

The minimization with respect to the mentioned parameters leads to the inequality

$$\text{Tr} (\mathbf{E}_1) \leq \frac{\sigma_1}{\sigma_2} \min\{(E_2)_a, (E_2)_b\} + \max\{(E_2)_a, (E_2)_b\} \quad (3.20)$$

This inequality is satisfied as an equality, if the jump is consistent with the optimality conditions. The equality in (3.20) corresponds to the following conditions

1. The matrices  $\tilde{\mathbf{E}}_1$  and  $\tilde{\mathbf{E}}_2$  are symmetric, so that  $\tilde{\mathbf{E}} = \mathbf{E}$  at both sides the boundary.
2. The normal  $\mathbf{n}$  is codirected with the eigenvector of  $\tilde{\mathbf{E}}$  that corresponds to its minimal eigenvalue.
3. The field in phase  $\sigma_1$  belongs to the boundary of the set of permitted fields  $\mathcal{V}_1$  and the field on the other side belongs to the boundary of  $\mathcal{V}_2$ .

Only if all these conditions are satisfied, it is possible to jump over the forbidden region. Hence, the derived necessary conditions are the strongest possible for the considered problem. Indeed, if there were a variation which would lead to larger forbidden region, then it would be impossible to jump across this region. The system of such hypothetical necessary conditions would be inconsistent with the jump on the dividing line.<sup>2</sup>

We also conclude that  $\mathbf{n}$  is not uniquely determined only if the field  $\mathbf{E}_2$  in  $\mathcal{V}_2$  is isotropic:  $\mathbf{E}_2 = \beta \mathbf{I}$ . This implies that either the field in the second phase is isotropic, or the optimal structure is a simple laminate. In the first case,  $\mathbf{E}_1$  satisfies the equality

$$\frac{E_a}{E_b} = \frac{\sigma_1}{\sigma_2}.$$

The field belongs to that point B of the boundary of  $\mathcal{V}_1$  (Figure 2) where its elliptical component meets the straight component .

### 3.4 Necessary conditions and the known optimal geometries.

To illustrate the obtained system of necessary conditions, two examples of the known optimal structures are studied.

**Coated spheres.** First, consider the construction of coated spheres (Hashin and Shtrikman, [15]), Figure 3. This geometry provides the best isotropic effective modulus [15]. If  $\mathbf{E} = I$ , it corresponds to minimum of the sum of stored energies.

The two coated spheres, placed in the homogeneous medium with effective isotropic conductivity  $\sigma_*$ , leave the outside field uniform and equal to the unit matrix everywhere. The effective conductivity of this structure found by Hashin and Shtrikman bound [15], is

$$\sigma_* = \sigma_{HS} = \sigma_1 + \left( \frac{m_1}{2\sigma_1} + \frac{m_2}{\sigma_1 + \sigma_2} \right)^{-1}. \quad (3.21)$$

The potentials  $u_1$  and  $u_2$ , ( $\mathbf{E}_i = \nabla u_i$ ) for this geometry are

$$u_1 = R(r) \cos \theta, \quad u_2 = R(r) \sin \theta; \quad (3.22)$$

---

<sup>2</sup>Notice, that this conclusion does not refers to any sufficient conditions.

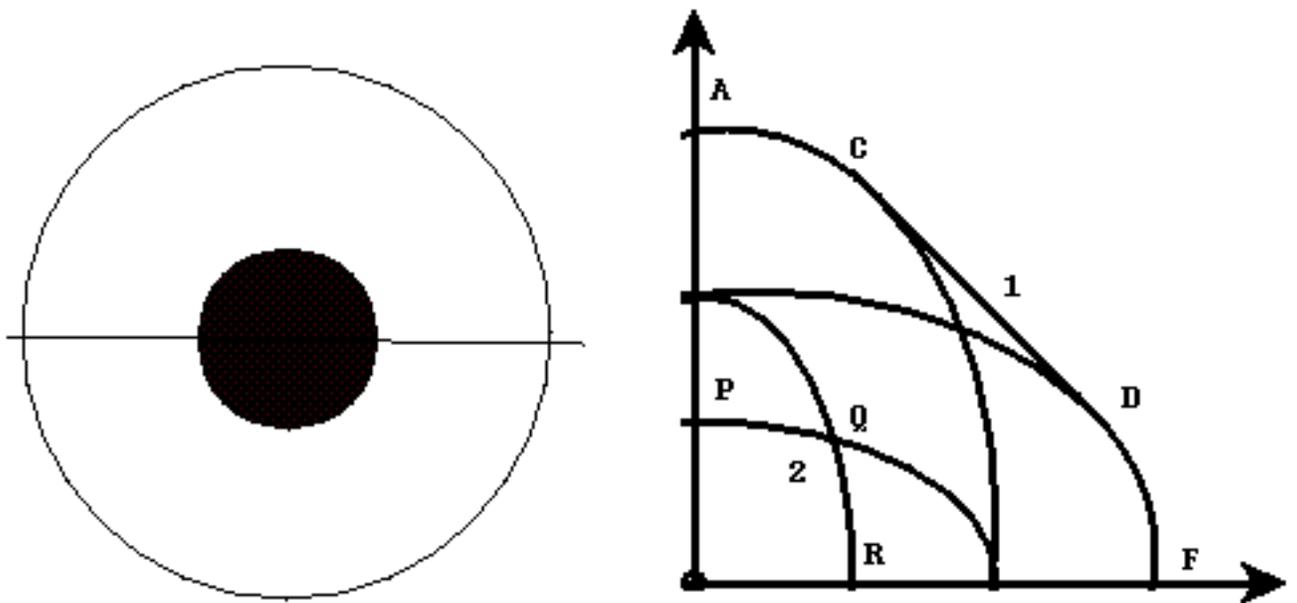


Figure 3: The structure of coated spheres.

The field inside the second material is isotropic (point Q), the field in the core varies along the interval  $CD$ , the boundary between regions corresponds to the point C.

where  $r$  is the polar radius,  $\theta$  is a polar angle, and

$$R(r) = \begin{cases} a_0 r & \text{if } 0 \leq r \leq r_0, \\ a_1 r + b_1/r & \text{if } r_0 \leq r \leq 1, \dots \\ 1r & \text{if } 1 \leq r \end{cases} \quad (3.23)$$

Here

$$\begin{aligned} a_0 &= \frac{2\sigma_2}{m_2\sigma_1 + (1+m_1)\sigma_2}, \\ a_1 &= \frac{\sigma_1 + \sigma_2}{m_2\sigma_1 + (1+m_1)\sigma_2}, \\ b_1 &= \frac{m_1(-\sigma_1 + \sigma_2)}{m_2\sigma_1 + (1+m_1)\sigma_2}. \end{aligned} \quad (3.24)$$

The matrix  $\mathbf{E}(r, \theta)$  has the eigenvectors directed along the polar axes  $\theta = \text{constant}$  and  $r = \text{constant}$ , and the eigenvalues of  $\mathbf{E}$  are:

$$E_r = R', \quad E_\theta = R/r. \quad (3.25)$$

From the solution (3.22), (3.23), one sees that the field in the nucleus is isotropic:

$$\mathbf{E}_r^1 = \mathbf{E}_\theta^1 = a_0, \quad \text{if } r \leq r_0; \quad (3.26)$$

therefore  $\mathbf{n}$  is not uniquely defined.

The jump conditions on the boundary between the nucleus and the envelope are satisfied:

$$\mathbf{E}_r = a_1 - b_1/r^2 = (\sigma_2/\sigma_1) a_0 \quad \mathbf{E}_\theta = a_1 + b_1/r^2 = a_0. \quad (3.27)$$

These conditions are in accord with the optimality conditions for the fields, since the field  $\mathbf{E}_2 = a_0 \mathbf{I}$  on one side of the boundary is isotropic, on the other side the matrix  $\tilde{\mathbf{E}}$  is symmetric, the eigenvectors are codirected in each point with the radial direction, that is with the normal to the dividing line.

The field in the envelope has the constant trace:

$$\mathbf{E}_r^1(r) + \mathbf{E}_\theta^1(r) = 2a_1; \quad (3.28)$$

meaning that it belongs to the straight component of the boundary of  $\mathcal{V}_1$  everywhere.

Let us also check the optimality conditions at the boundary point  $r = 1$  where the materials  $\sigma_1$  and  $\sigma_{HS}$  meet. We have

$$\begin{aligned} \mathbf{E}_r &= a_1 - b_1 = \frac{(1+m_1)\sigma_1 + m_2\sigma_2}{m_2\sigma_1 + (1+m_1)\sigma_2} = \frac{\sigma_{HS}}{\sigma_1} \\ \mathbf{E}_\theta &= a_1 + b_1 = 1 \end{aligned} \quad (3.29)$$

which indicates that the necessary conditions are again satisfied on the boundary between the material  $\sigma_1$  and the effective medium  $\sigma_* = \sigma_{HS}$ . Therefore the necessary conditions are satisfied as equalities everywhere.

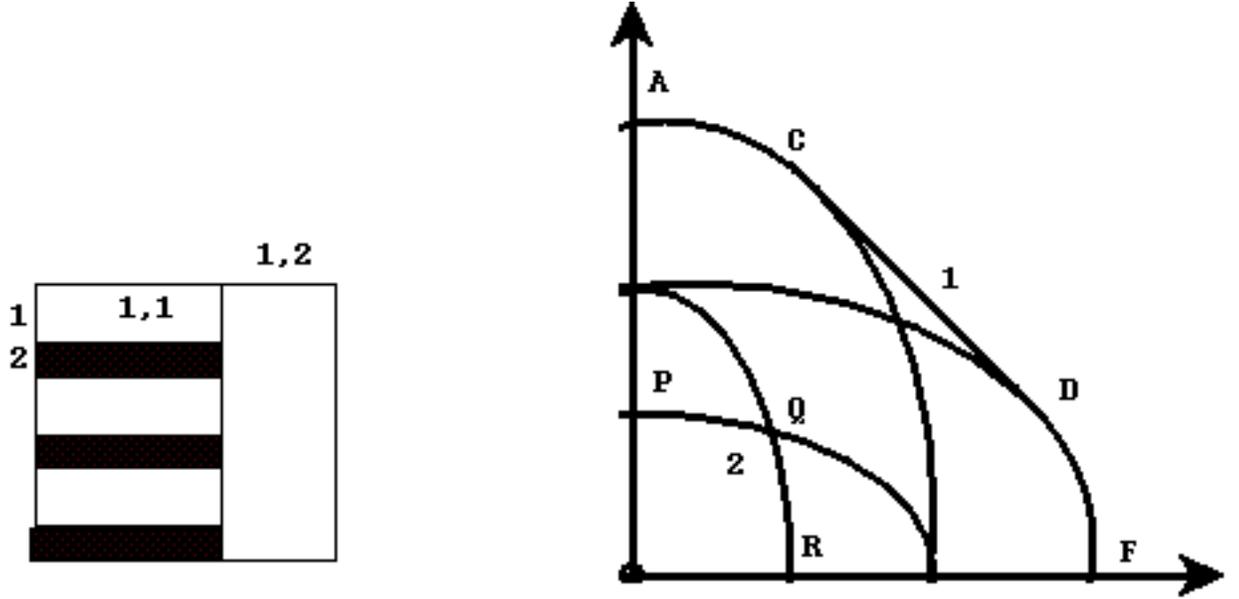


Figure 4: Matrix laminate structures.

The field on the second material is isotropic (point  $Q$  in  $\mathcal{V}_2$ ). The field on the region (1.1) is in rank-one connection with the field in  $\mathcal{V}_2$  (point  $C$ ). The field on the region (1.2) varies with the external field, and it belongs to interval  $CD$ .

**Matrix laminates.** Consider the other known optimal two-phase geometry: the second rank matrix laminates (see 4). These structures are known (Lurie and Cherkhaev [21]) to be optimal in anisotropic external fields. They are built as the laminate composite of the layers of the first material and the layer made of laminates of the first and second materials, mixed in smaller scale and oriented orthogonal to the larger layers. The calculation of the fields can be done using the technique described in Appendix. One can check that optimization of the sum of the energies leads to following results:

1. The field in the nucleus is isotropic and belongs to the corner point of  $\mathcal{V}_2$
2. The contact conditions between the fields  $\mathbf{E}_2$  and  $\mathbf{E}_{1,1}$  in neighboring layers are satisfied.
3. Both fields  $\mathbf{E}_{1,1}$  and  $\mathbf{E}_{1,2}$  belong to the boundary of  $\mathcal{V}_1$ :  $\text{Tr } \mathbf{E}_{1,1} = \text{Tr } \mathbf{E}_{1,2} = \sigma_2/\sigma_2 \text{Tr } \mathbf{E}_2$ . The mean field  $\langle \mathbf{E} \rangle_{\mathcal{O}_1}$  belongs to that boundary as well.

When the degree of anisotropy of  $\mathbf{P}$ , the field in the nucleus of an optimal matrix structure remains isotropic, unless the structure degenerates into a simple laminate. In the optimal laminate both fields  $\mathbf{E}_1$  and  $\mathbf{E}_2$  are constant. They belong to the elliptical parts of the boundaries of  $\mathcal{V}_1$  and  $\mathcal{V}_2$ . Again, all necessary conditions are satisfied as equality in every point.

**Remark 3.3** *Note that necessary conditions are satisfied as equality everywhere in both laminates and optimal matrix laminates. They describe the optimality of both types of structures. On the contrary, the sufficient conditions require separate consideration of these cases.*

**The linearity of the components of  $\partial\mathcal{V}_i$  and non-uniqueness of solution.** The two above examples demonstrate that the fields are different in the structures of coated spheres and of matrix laminates. However, both structures possess the same extremal effective properties that also can be obtained by the formal procedure minimal extension. Why does this happen?

The minimal extension procedure treats the fields in each phase as single tensors not as functions of the point of the domain; these fields are in fact the mean fields within the correspondent subdomains  $\mathcal{O}_i$ . The minimization among the fields  $\mathbf{E}_i \in \mathcal{V}_i$  in the minimal extension procedure requires that the mean fields belong to the boundary  $\partial\mathcal{V}_i$ .

$$\mathbf{E}_i = \int_{\mathcal{O}_1} \mathbf{E}(\mathbf{x}) \chi_i(\mathbf{x}) \quad \in \partial\mathcal{V}_i \quad (3.30)$$

On the other hand, the field  $\mathbf{E}(\mathbf{x})$  belongs to  $\mathcal{V}_i$  in each point  $\mathbf{x}$ . This happens since  $\mathbf{E}(\mathbf{x})$  varies among a component  $\partial_1\mathcal{V}_i$  of the boundary of  $\mathcal{V}_i$   $\partial_1\mathcal{V}_i \subset \partial\mathcal{V}_i$ .

$$\mathbf{E}(\mathbf{x}) \in \partial_1\mathcal{V}_1, \quad \forall \mathbf{x} \in \mathcal{O}_1 \quad (3.31)$$

and since his component is linear

$$\mathbf{E} = \sum c_k \mathbf{E}_k \in \partial_1\mathcal{V}_i, \quad \text{if } \mathbf{E}_k \in \partial_1\mathcal{V}_i, \quad c_k \geq 0, \quad \sum c_k = 1. \quad (3.32)$$

In both checked structures, the trace of the field in the first phase is constant. The mean field  $\langle \mathbf{E} \rangle_{\mathcal{O}_1}$  obviously has the same trace. The necessary conditions are satisfied for  $\mathbf{E}_1(\mathbf{x})$  in every point  $\mathbf{x}$  and also for the mean field.

One could expect non-unique microstructures of optimal structure if a permitted region  $\mathcal{V}_i$  has a linear component of the boundary; in this case one could also expect that the field in the  $i$ -th material varies along this component. On the contrary, the strongly convex region  $\mathcal{V}_i$  (like the region  $\mathcal{V}_2$  in the checked examples) suggests that the field in the  $i$ -th material is constant in every point of  $\mathcal{O}_i$  and it may correspond to a compact inclusion like the nucleus in the checked geometries.

## 4 Three-materials structures.

### 4.1 Single variations.

We apply the developed technique of necessary conditions to an open problem of optimal three-material mixtures. In this section, we discuss appropriate variations and we obtain the domains  $\mathcal{V}_i$  and the forbidden domain  $\mathcal{V}_f$ . In the next section, we use them to find some optimal structures of three-materials composites.

**Setting.** Consider again a composite with minimal conductivity, that is made of three materials with conductivities

$$\sigma_1 < \sigma_2 < \sigma_3. \quad (4.1)$$

To simplify calculations, assume that

$$\sigma_3 = \infty, \quad (4.2)$$

i.e. the third material is an ideal conductor.

We normalize cost of the materials and assign the cost  $\gamma_2$  of the intermediate material to be between the costs of the extremal materials

$$\gamma_1 = 1, \quad \gamma_3 = 0, \quad 0 < \gamma_2 < 1. \quad (4.3)$$

**The variations.** To begin, we compute the necessary conditions for the fields in each of the materials, using the described above variations. Namely, we place each of three materials into regions occupied by the other two materials, and calculate the corresponding inequalities.

The trial inclusion of the material  $\sigma_3$  with infinite conductivity in the regions  $\mathcal{V}_1$  and  $\mathcal{V}_2$  occupied with materials  $\sigma_1$  and  $\sigma_2$  respectively leads to the inequalities:

$$F_1(\infty, \sigma_1, \mathbf{E}_1) \geq 0 \quad \Longrightarrow \quad E_a + E_b \geq \sqrt{\frac{1}{\sigma_1}} \quad \text{in } \mathcal{V}_1 \quad (4.4)$$

$$F_1(\infty, \sigma_2, \mathbf{E}_2) \geq 0 \quad \Longrightarrow \quad E_a + E_b \geq \sqrt{\frac{\gamma}{\sigma_2}} \quad \text{in } \mathcal{V}_2. \quad (4.5)$$

These inequalities follow from (2.27) (2.32) if the materials are properly specified.

The trial inclusion of the material  $\sigma_2$  in  $\mathcal{V}_1$  produces the inequalities:

$$F_1(\sigma_2, \sigma_1, \mathbf{E}_1) \geq 0 \quad \Longrightarrow \quad \left. \begin{array}{l} \sigma_1(\sigma_2 - \sigma_1) \left( \frac{E_a^2}{\sigma_2} + \frac{E_b^2}{\sigma_1} \right) + \gamma - 1 \geq 0 \quad \text{if } \frac{E_a}{E_b} \leq \frac{\sigma_1}{\sigma_2}, \\ \frac{\sigma_1(\sigma_2 - \sigma_1)}{\sigma_1 + \sigma_2} (E_a + E_b)^2 + \gamma - 1 \geq 0 \quad \text{if } \frac{E_a}{E_b} \geq \frac{\sigma_1}{\sigma_2} \end{array} \right\} \text{ in } \mathcal{V}_1 \quad (4.6)$$

(remind that  $E_a \leq E_b$ , see (3.3)).

The trial inclusion of materials  $\sigma_1$  in  $\mathcal{V}_2$  produces the inequality:

$$F_2(\sigma_1, \sigma_2, \mathbf{E}_2) \geq 0 \implies \sigma_2(\sigma_1 - \sigma_2) \left( \frac{E_a^2}{\sigma_2} + \frac{E_b^2}{\sigma_1} \right) + 1 - \gamma \geq 0 \quad \text{in } \mathcal{V}_2 \quad (4.7)$$

Finally, placing the inclusions of the material  $\sigma_1$  into  $\mathcal{V}_3$  leads to conditions

$$F_2(\sigma_1, \sigma_3, \mathbf{E}_3) \geq 0 \implies E_a = E_b = 0 \quad \text{in } \mathcal{V}_3. \quad (4.8)$$

They show that the field in the third superconducting phase is always zero, as it should be.

The topology of the obtained permitted regions  $\mathcal{V}_i$  is described as follows. The region  $\mathcal{V}_1$  is permitted for fields of great magnitudes, region  $\mathcal{V}_3$  is permitted for zero fields only. The forbidden region  $\mathcal{V}_f$  lies between these two regions, which makes the picture similar to that of the problem for two materials. The region  $\mathcal{V}_2$  is located inside the forbidden region. Here the second (intermediate) material is optimal. If this region is not empty, it either divides  $\mathcal{V}_f$  into two disconnected parts – forms a “belt” in  $\mathcal{V}_f$ , or it leaves  $\mathcal{V}_f$  connected – forms an “island” in  $\mathcal{V}_f$ , see Figure 5.

## 4.2 Composite variations.

Before further analysing the system of necessary conditions, let us discuss if these conditions are the strongest ones. The analysis of the Section 3.3 is applicable to a boundary between domains of any two materials. It shows, that the considered variation leads to the maximally broad forbidden region that is consistent with the assumption that the pair of the materials have a common boundary. One could conclude that no other variations are needed. Such conclusion, however, would be inaccurate.

Indeed, it is possible that the geometry of multi-materials composites includes zones where all three materials are densely mixed together. The dividing curves contains a dense set of points where  $\mathcal{O}_1$ ,  $\mathcal{O}_2$ , and  $\mathcal{O}_3$  meet. Our previous analysis is not applicable to the proximity of these points.

To examine the optimality of multicomponent boundaries, one need to consider more complicated types of local variations. Here, we consider a “composite variation”. The variation is performed as following: A composite of two available materials is placed into a domain of the third one. A mixture inside the inclusion is described by its tensor of effective properties  $\sigma_{inc}$ . We use the bounds for effective properties of any two-component mixture (the  $G_m$ -closure problem) to find optimal composition of the “stuffed” inclusions.

### 4.2.1 Improving of $\mathcal{V}_2$

**Scheme.** Here we introduce new variations and improve the bounds for the permitted region  $\mathcal{V}_2$ . The scheme is the following. We form a composite with the conductivity  $\sigma_*(c)$

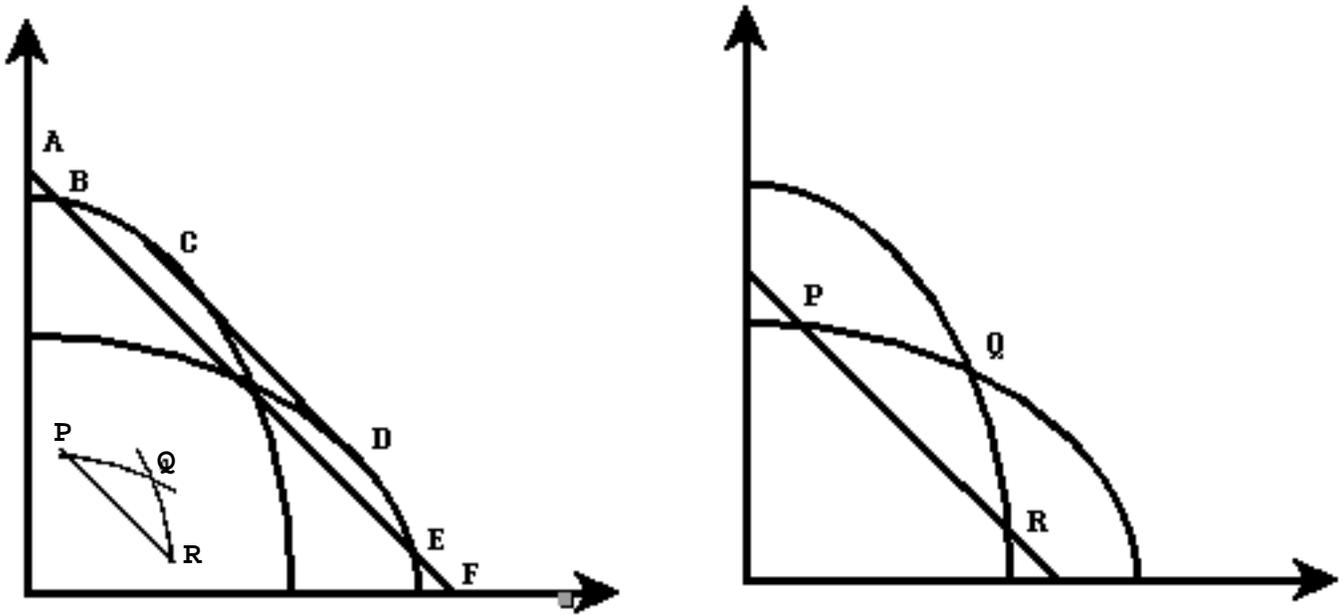


Figure 5: The permitted regions, based on single variations.

Left field - The regions  $\mathcal{V}_1$  and  $\mathcal{V}_2$ , right field: magnified picture of the region  $\mathcal{V}_2$ .

The boundary curve  $B C D E$  comes from the inclusions of  $\sigma_2$  into  $\mathcal{V}_1$ , the boundary straight line  $A F$  comes from the inclusions of  $\sigma_3$  into  $\mathcal{V}_1$ , the boundary due to intersection of two ellipses comes from the inclusions of  $\sigma_1$  into  $\mathcal{V}_2$ , the boundary straight line  $P R$  comes from the inclusions of  $\sigma_3$  into  $\mathcal{V}_2$ .

The mutual positions of the boundary curves depends on  $\gamma$ .

from the materials  $\sigma_1$  and  $\sigma_3$  and place it as an inclusion in the domain  $\mathcal{O}_2$  of second material, see figure 6. Here  $c$  is the volume fraction of material  $\sigma_1$  (obviously, the fraction of  $\sigma_3$  is  $1 - c$ ). The change of materials' cost due to the variation is computed as the difference between the cost of the taken material  $\sigma_2$  and the cost of the inserted materials:

$$\delta W = -\gamma_2 + c\gamma_1 + (1 - c)\gamma_3. \quad (4.9)$$

In our setting (4.3), the cost is  $\delta W = \gamma + c\delta\gamma$ . The increment has the form

$$\delta W(\boldsymbol{\sigma}_*(c), \sigma_2, \mathbf{E}) = \delta\Pi + \delta\gamma, \quad (4.10)$$

where  $\delta\Pi$  is the increment of the energy caused by an anisotropic composite inclusion  $\boldsymbol{\sigma}_*(c)$  inserted into the domain of  $\mathcal{O}_2$ . This time, the increment depends on the shape of the inclusion, and on the properties of the composite in the inclusion  $\boldsymbol{\sigma}_*(c)$ .

Let us compute the increment  $\delta\Pi(\boldsymbol{\sigma}_*(c), \sigma_2, \mathbf{E})$  of the energy. We denote the eigenvalues of  $\boldsymbol{\sigma}_*(c)$  as  $l_1(c), l_2(c)$  and use (3.7). The increment  $\delta\Pi$  is

$$\delta\Pi = \sigma_2 E_a^2 \frac{l_1(c) - \sigma_2}{\alpha l_1(c) + (1 - \alpha)\sigma_2} + \sigma_2 E_b^2 \frac{l_2(c) - \sigma_2}{\alpha\sigma_2 + (1 - \alpha)l_2(c)}; \quad (4.11)$$

as before, the parameter  $\alpha \in [0, 1]$  defines the rate of anisotropy of the second-rank laminate structure or the elongation (eccentricity) of the equivalent elliptical inclusion.

In order to obtain a maximally sensitive variation,  $\boldsymbol{\sigma}_*(c)$  must be chosen as a composite of extremal conductivity: it belongs to the boundary of  $G_c$ -closure for two materials.<sup>3</sup> However,  $\boldsymbol{\sigma}_*(c)$  can be anisotropic.

The boundary of the  $G_c$ -closure is realized by second rank laminates, where  $\sigma_1$  plays the role of envelope, and  $\sigma_3$  forms inclusions [21]. The eigenvalues of these second rank laminates (see (2.14)) are equal to:

$$\begin{aligned} l_1(c, \beta) &= \sigma_1 + (1 - c) \left( \frac{1}{\sigma_3 - \sigma_1} + \frac{c\beta}{\sigma_1} \right)^{-1} \\ l_2(c, \beta) &= \sigma_1 + (1 - c) \left( \frac{1}{\sigma_3 - \sigma_1} + \frac{c(1-\beta)}{\sigma_1} \right)^{-1}, \end{aligned} \quad (4.12)$$

where the parameter  $\beta \in [0, 1]$  defines the degree of anisotropy of a composite – the rate of the elongation of the inclusions inside  $\boldsymbol{\sigma}_*(c)$ , and  $c$  is the fraction of material  $\sigma_1$ . Equations (4.12) show that each eigenvalue  $l_i$  varies in the interval

$$\left[ \frac{\sigma_1\sigma_3}{c\sigma_3 + (1 - c)\sigma_1}, \quad c\sigma_1 + (1 - c)\sigma_3 \right]$$

---

<sup>3</sup>Recall, that  $G_c$ -closure is the set of effective properties of all composites assembled from given materials mixed in the proportions  $c$  and  $1 - c$ .

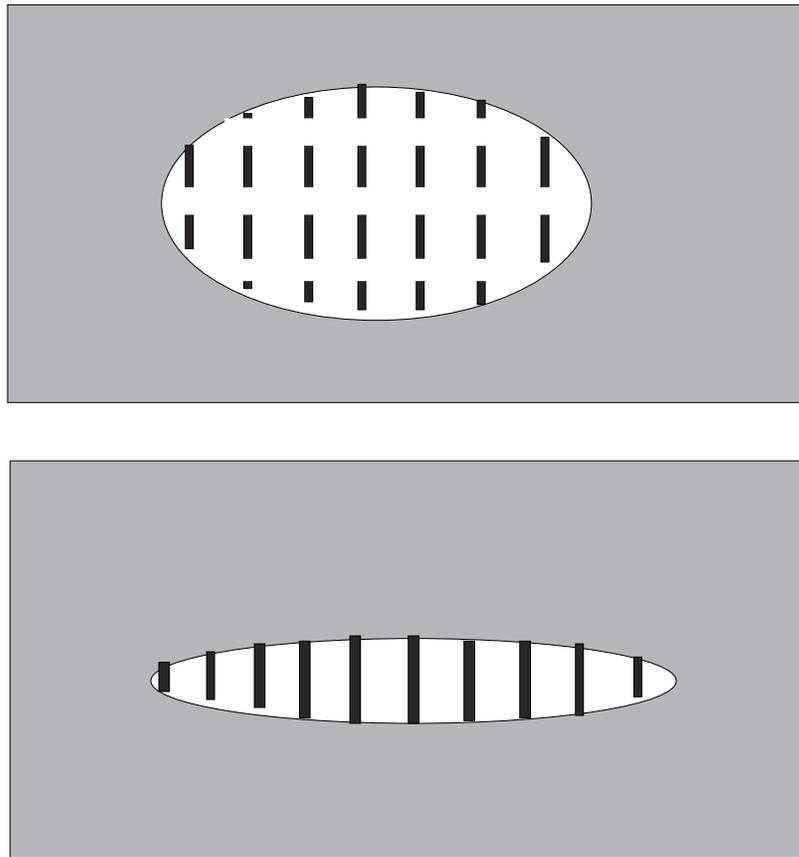


Figure 6: An admissible(above) and an optimal complex variation.

when  $\beta$  varies in the interval  $[0, 1]$ . If  $\sigma_3 = \infty$ , the formulae become

$$\begin{aligned} l_1(c, \beta) &= \sigma_1 \left(1 + \frac{1-c}{c\beta}\right) \\ l_2(c, \beta) &= \sigma_1 \left(1 + \frac{1-c}{c(1-\beta)}\right); \end{aligned} \quad (4.13)$$

each eigenvalue  $l_i$  varies in the interval  $[\sigma_1/c, \infty]$ .

The increment  $\delta W$  depends on three parameters: (i) the volume fraction  $c$  of material that form the composite in the inclusion, (ii) the degree of anisotropy of that composite  $\beta$ , and (iii) the relative elongation (eccentricity)  $\alpha$  of the inclusions, Each parameter varies in the interval  $[0, 1]$ . To find an extremal variation, we solve the optimization problem

$$\delta_0 = \min_{c \in [0, 1]} \min_{\alpha \in [0, 1]} \min_{\beta \in [0, 1]} \delta \Pi(\alpha, \beta, c) + , (c). \quad (4.14)$$

where  $\delta \Pi(\alpha, \beta, c)$  is defined by (4.10)

**Laminate variation.** Minimization of (4.14) with respect to  $\alpha$  and  $\beta$  is independent of the costs ,  $i$  since the variation affects only geometrical structure of an inclusion but not the quantities of materials. Each parameter  $\beta$  and  $\alpha$ , varies in the interval  $[0, 1]$ . Therefore the optimal point corresponds either to an inner point of the square in the plane of the parameters  $\beta \in (0, 1)$ ,  $\alpha \in (0, 1)$  or to its side ( $\beta = 0$  or ,  $\beta = 1$ ,  $\alpha \in (0, 1)$ ) or ( $\beta \in (0, 1)$ ,  $\alpha = 0$  or ,  $\alpha = 1$ ).

First, let us check the case  $\beta = 1$ . The inclusion is a laminate composite with the eigenvalues (see (4.13))

$$l_1(c) = \sigma_1/c, \quad l_2 = \infty. \quad (4.15)$$

The increment (4.11) becomes

$$\delta W = \sigma_2 E_a^2 \frac{\sigma_1 - c\sigma_2}{\alpha\sigma_1 + c(1-\alpha)\sigma_2} + \sigma_2 E_b^2 \frac{1}{(1-\alpha)} + \gamma + c, \quad \alpha \in [0, 1]. \quad (4.16)$$

Let us show, that the optimal parameter  $\alpha$  is equal either to one or to zero. Indeed, suppose that  $\alpha \in (0, 1)$ . We find the stationary  $\alpha$  from the equation ( $\frac{\partial \delta W}{\partial \alpha} = 0$ ) and exclude it from the (4.16). The increment  $\delta W$  becomes a linear function of  $c$ . Therefore the optimal values of  $c$  are either zero or one, which reduces the complex variations to the already investigated case of single variations.

The two remaining cases are  $\alpha = 0$ ,  $Gb = 1$  and  $\alpha = 1$ ,  $\beta = 1$ . We are dealing with a laminate inclusion filled with a laminate composite. The value  $\alpha = 1$  leads to infinite increment and is obviously not optimal. The case  $\alpha = 0$  corresponds to the strips in the inclusion are orthogonal to its long sides. This case corresponds to the increment:

$$\delta_{c,2}(\mathbf{E}) = \Delta - \gamma + c = (\sigma_1/c - \sigma_2)E_a^2 + \sigma_2 E_b^2 - \gamma + c \geq 0 \quad \forall c \in [0, 1] \quad (4.17)$$

that depends only on volume fraction  $c$ .

The optimal value  $c_0$  is found from the condition

$$\frac{\partial}{\partial c} \delta W_{c,2} = 1 - \frac{\sigma_1}{c^2} E_a^2 \quad (4.18)$$

and is equal to

$$c_0 = \begin{cases} \sqrt{\sigma_1} E_a & \text{if } E_a \leq \frac{1}{\sqrt{\sigma_1}} \\ 1 & \text{if } E_a \geq \frac{1}{\sqrt{\sigma_1}} \end{cases} \quad (4.19)$$

The case  $c_0 = 1$  corresponds to two-materials variation. The inequality  $E_a \leq \frac{1}{\sqrt{\sigma_1}}$  is surely satisfied for all fields  $\mathbf{E} \in \mathcal{V}_2$ , that are optimal from the viewpoint of single variations (see (4.7))

The case  $c_0 \in (0, 1)$  leads to the new necessary condition

$$\Delta_0 = 2\sqrt{\sigma_1} E_a - \sigma_2 E_a^2 + \sigma_2 E_b^2 - \gamma \geq 0, \quad (4.20)$$

or

$$\left( \sqrt{\sigma_2} E_a - \sqrt{\frac{\sigma_1}{\sigma_2}} \right)^2 - \sigma_2 E_b^2 \leq -\frac{\sigma_1}{\sigma_2} + \gamma. \quad (4.21)$$

**Remark 4.1** *This inequality provides an additional constraint on the set  $\mathcal{V}_2$ . The condition checks the optimality of a boundary between the phase  $\sigma_2$  and the pack of orthogonal to the boundary laminates of  $\sigma_1$  and  $\sigma_3$ . This boundary is not a dividing line between any two of available phases, and the jump conditions on it involves all three phases. Clearly, the variation that involves only two materials is not enough selective to judge about the optimality of such boundary.*

The conditions (4.20) and (4.21) are supplemented by the twin conditions in which the eigenvalues  $E_a$  and  $E_b$  are interchanged. Finally we obtain the inequalities (see Figure 7)

$$\max \left\{ \left( \sqrt{\sigma_2} E_a - \sqrt{\frac{\sigma_1}{\sigma_2}} \right)^2 - \sigma_2 E_b^2, \left( \sqrt{\sigma_2} E_b - \sqrt{\frac{\sigma_1}{\sigma_2}} \right)^2 - \sigma_2 E_a^2 \right\} \leq -\frac{\sigma_1}{\sigma_2} + \gamma \quad (4.22)$$

The obtained inequalities restrict the set  $\mathcal{V}_2$  by two symmetric hyperbolas with asymptotes:

$$(\pm E_a \pm E_b) = \frac{\sqrt{\sigma_1}}{\sigma_2} \quad (4.23)$$

These inequalities must be added to the restrictions obtained by single variations (4.5), (4.7). The graph of  $\mathcal{V}_2$  is represented in Figure 7.

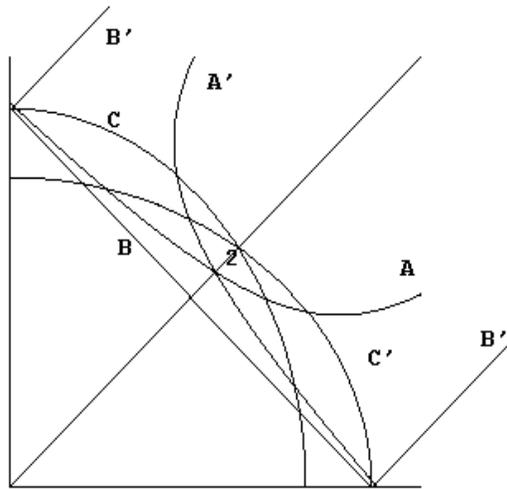


Figure 7: Permitted region  $\mathcal{V}_2$ , based on complex variations.

A, A' - Hyperbolic bounds, obtained from composite variations. B, B' - The asymptotes of the hyperbolas. B - The (improved) bound, obtained from single variation. C, C' - The bound, obtained from single variation.

**Other variations.** It can be shown that no other choice of parameters  $\beta$ ,  $\alpha$ , and  $c$  improves the bound given by the obtained inequality (4.20) and the single permutations. The formal investigation is routine but a long one, and Maple is a real help. Formally, one can check that the stationary points of the increment  $\delta_{c,2}$  inside the square in the variables  $\beta$ ,  $\alpha$  corresponds to saddles and therefore are not optimal.

Instead of presenting here the details of corresponding calculations, let us discuss physical reasons of why the other variations fail to improve the bounds. The case  $\beta \in (0, 1)$  corresponds to the following situation. The micro-inclusions material  $\sigma_3$  are placed inside the material  $\sigma_1$  and the resulting composite is placed into the domain  $\mathcal{O}_2$  occupied  $\sigma_2$ . This construction corresponds to contacts between pairs materials  $\sigma_2$  and  $\sigma_1$  (on the boundary of the inclusion) and between  $\sigma_1$  and  $\sigma_3$  (inside the inclusions). But the optimality of these boundaries has been investigated by the trial inclusions of solid materials, therefore these more complicated variations do not produce more restricted inequalities.

#### 4.2.2 Improving of $\mathcal{V}_1$

To complete the investigation we need to consider two other schemes: the mixture of materials  $\sigma_2$  and  $\sigma_3$  placed into domain of  $\sigma_1$  and the mixture of materials  $\sigma_1$  and  $\sigma_2$  placed into domain of  $\sigma_3$ . In our setting, the last case is trivial.

The complex variations also shrink the domain  $\mathcal{V}_1$ . The scheme of the variations is the same as in the previous case. Note that we can a priori restrict ourself to the case  $\beta = 0$  because we look for inclusions that produce a common boundary between all three materials. The new inequality can be algebraically obtained from (4.10), (4.11), (4.13) where one interchange  $\sigma_1$  and  $\sigma_2$  and put  $\gamma = 1 - c\gamma$ . The optimal variation corresponds to a strip-like inclusion assembled with perpendicular layers of  $\sigma_2$  and  $\sigma_3$ ; the fraction  $c$  of  $\sigma_2$  is optimally chosen.

The corresponding graph is shown in Figure 8. The new boundary component  $ABC$  of the boundary of  $\mathcal{V}_1$  corresponds to a hyperbola that joins the corner point  $A$  (where  $c = 0$  and strip-like inclusions of  $\sigma_3$  are optimal) and the elliptical boundary component  $C$  where  $c = 1$  and strip-like inclusions of  $\sigma_2$  are optimal.

## 5 Some optimal structures for three-materials mixtures.

### 5.1 Range of values of the Lagrange multiplier.

The problem of the best composite structure is characterized by three parameters: the volume fractions  $m_1$  and  $m_2$  of the first and second materials in the mixture, and the degree of anisotropy of resulting composite. The volume fractions are subject to obvious constrains

$$m_1 \geq 0, m_2 \geq 0, m_1 + m_2 \leq 1. \quad (5.1)$$

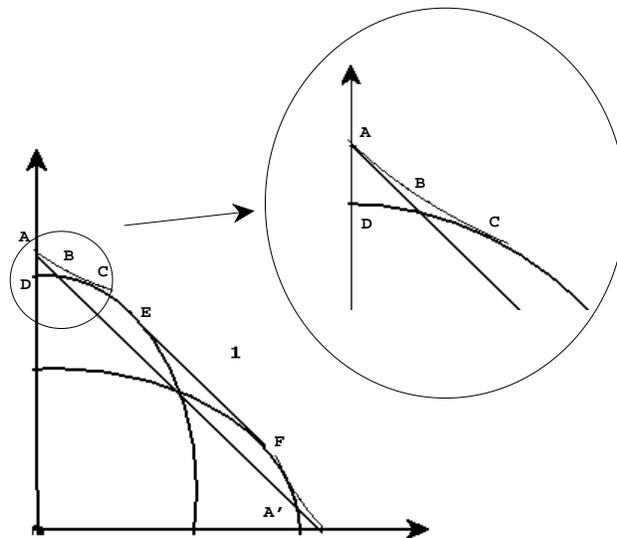


Figure 8: Permitted region  $\mathcal{V}_1$ , based on complex variations.  
 A B C - Hyperbolic bounds, obtained from composite variations. A A' - The bound, obtained from variation with inclusions of  $\sigma_3$ . D C E F - The bound, obtained from variation with inclusions of  $\sigma_2$ .

In the variational procedure, these parameters are replaced by three other parameters: the magnitude of the external field  $\mathbf{P}$ , the ratio of eigenvalues of  $\mathbf{P}$ , and the relative cost of the second material  $\gamma$ . Not all values of these three new parameters correspond to optimal volume fractions  $m_i \in (0, 1)$ . For some values, an optimal solution corresponds either to two component mixture:  $m_i = 0$ ,  $i = 1, 2, 3$  or even to a solid material.

Let us find the range of parameters  $\mathbf{P}$  and  $\gamma$  that lead to three component mixture. Firstly, the mean field  $\mathbf{P}$  must belong to the forbidden region

$$\mathbf{P} \in \mathcal{V}_f, \quad (5.2)$$

otherwise the solution is trivial: The field is constant everywhere and the structure is filled with one of initially given materials. Two volume fractions out of three are zero.

Secondly, the range of  $\gamma$  should correspond to three (not two) materials in optimal mixture. We show that the range

$$\gamma_2 \leq \gamma \leq \gamma_1, \quad \gamma_1 = \frac{2\sigma_1}{\sigma_1 + \sigma_2}, \quad \gamma_2 = \frac{\sigma_1}{\sigma_2} \quad (5.3)$$

corresponds to all three-materials optimal mixtures.

**Remark 5.1** *The question of the materials costs which require a three-component mixture as the optimal solution is non-trivial. In the paper [3] by Burns and Cherkaev, the problem was considered of three materials mixture, similar to the present one. In that paper, the energy of a mixture  $\sigma_*(\nabla u)^2$  was optimized and not the sum of energies. The considered case corresponds to singular matrix  $\mathbf{E}$ . The problem was reduced to the problem of the convex envelope of three wells  $\sigma_i(\nabla u)^2 + \gamma_i$ . It was shown, that all three-component mixtures correspond to a unique value of the cost  $\gamma$  of  $\sigma_2$ . Indeed, all three materials can coexist in an optimal composite only if the convex envelope possesses a straight component supported by all these three wells simultaneously. Geometrically, this indicates that three parabolas (wells) touch the same tangent. That requirement uniquely determines  $\gamma_2$ . In that case, the optimal volume fractions are not defined uniquely.. Contrary to this result, we show that non-trivial three-component mixtures correspond to a range of  $\gamma$  in the considered problem for the sum of energies.*

The range of  $\gamma$  is determined by the shape of the region  $\mathcal{V}_2$ . The field in the second region  $\mathcal{V}_2$  satisfies the inequalities:

$$F_1(\sigma_2, \sigma_1, \mathbf{E}_2) \leq \frac{1 - \gamma}{\sigma_2(\sigma_2 - \sigma_1)} \quad (5.4)$$

$$F_2(\sigma_2, \infty; \mathbf{E}_2) = E_a + E_b \geq \sqrt{\frac{\gamma}{\sigma_2}} \quad (5.5)$$

$$F_3(\sigma_2, \sigma_1, \infty; \mathbf{E}) \geq (\gamma\sigma_2 - \sigma_1)/\sigma_2^2 \quad (5.6)$$

Inequality (5.4) shows that the set  $\mathcal{V}_2$  belongs to an intersection of two ellipses, obtained by the consideration of inclusions of the first material. Inequality (5.5) shows that the set  $\mathcal{V}_2$  lies above the straight line, obtained from the consideration of inclusions of the third material. The inequality (5.6) shows that the set  $\mathcal{V}_2$  lies above the intersection of two hyperbolas, obtained by the consideration of inclusions of composite type.

- If  $\gamma > \gamma_1$ , then the set  $\mathcal{V}_2$  is empty and the second material is never optimal. We interpret it this as material  $\sigma_2$  being too expensive to use in an optimal composition: It is always cheaper to mimic material  $\sigma_2$  by a mixture of the first and the third materials.

- If  $\gamma = \gamma_1$ , then the set  $\mathcal{V}_2$  degenerates to a point

$$\mathbf{E}_2 = \sqrt{\frac{\sigma_1}{2\sigma_2(\sigma_1 + \sigma_2)}} \mathbf{I}; \quad (5.7)$$

and the optimal structure keeps the field in the second phase constant and isotropic (see Figure 9).

- If  $\gamma \in [\gamma_1, \gamma_2]$ , then the set  $\mathcal{V}_2$  is strongly convex:

$$F_1(\sigma_2, \sigma_1, \mathbf{E}_2) \leq \frac{1 - \gamma}{\sigma_2(\sigma_2 - \sigma_1)} \quad (5.8)$$

$$F_3(\sigma_2, \sigma_1, \infty; \mathbf{E}) \geq (\gamma\sigma_2 - \sigma_1)/\sigma_2^2 \quad (5.9)$$

$\sigma_2$  is restricted by ellipses and hyperbolas, the straight component corresponds to a strong (inactive) inequality. This indicates, that the field in the second phase stays constant. In this case, the domain  $\mathcal{V}_2$  forms an “island” in the forbidden region which leaves the possibility of optimal three-component mixtures. (see Figure 10)

- If  $\gamma = \gamma_2$ , then region  $\mathcal{V}_2$  possesses a straight component:

$$\begin{aligned} F_2(\sigma_2, \sigma_1; \mathbf{E}_2) &\leq 1/\sigma_2^2 \\ F_1(\sigma_2, \infty; \mathbf{E}_2) &= E_a + E_b \geq \frac{\sqrt{\sigma_1}}{\sigma_2}. \end{aligned} \quad (5.10)$$

Both hyperbolas degenerate into their straight asymptotes. The degenerated hyperbolic component of  $\partial\mathcal{V}_2$  coincides with the straight line described by the inequality (5.5) that becomes active. The straight component of the  $\partial\mathcal{V}_2$  shows that the field in the second phase could vary (see Figure 11).

- If  $\gamma < \sigma_2$ , then the region  $\mathcal{V}_2$  forms a “belt” which divides the forbidden region into the two disconnected parts  $\mathcal{V}_f^{12}$  and  $\mathcal{V}_f^{23}$ . If the mean field belongs to the inner part  $\mathcal{V}_f^{23}$  of the forbidden region, then only connections between materials  $\sigma_3$  and  $\sigma_2$  are optimal. If the mean field belongs to the exterior part  $\mathcal{V}_f^{12}$  of the forbidden region, then the only connections between materials  $\sigma_1$  and  $\sigma_2$  are optimal.

This range of  $\gamma$  corresponds to two-component composites. The type of optimal composites is determined by the mean field  $\mathbf{P}$ . When the mean field  $\mathbf{P}$  belongs to the region  $\mathcal{V}_f^{23}$  (the proximity of the origin), optimal composites consist of  $\sigma_3$  and  $\sigma_2$ . When the magnitude

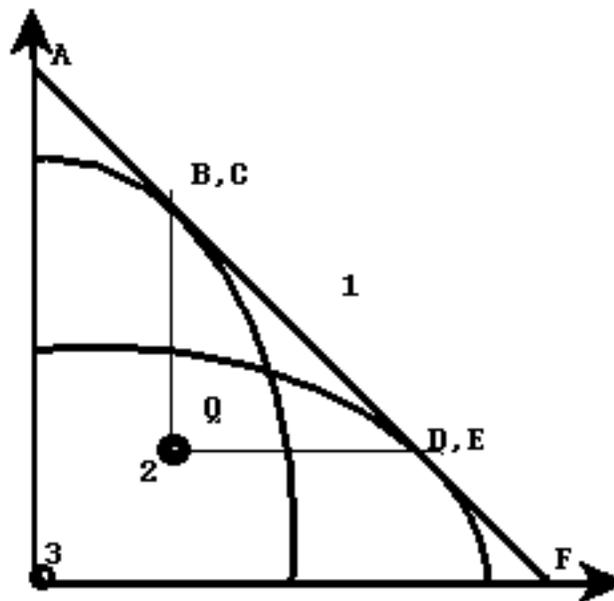


Figure 9:  
 The permitted regions,  $\gamma = \gamma_1$ .  
 In this case, the sets  $\mathcal{V}_2$  and  $\mathcal{V}_3$  degenerate into single points, and the boundary  $\partial\mathcal{V}_1$  becomes straight line.

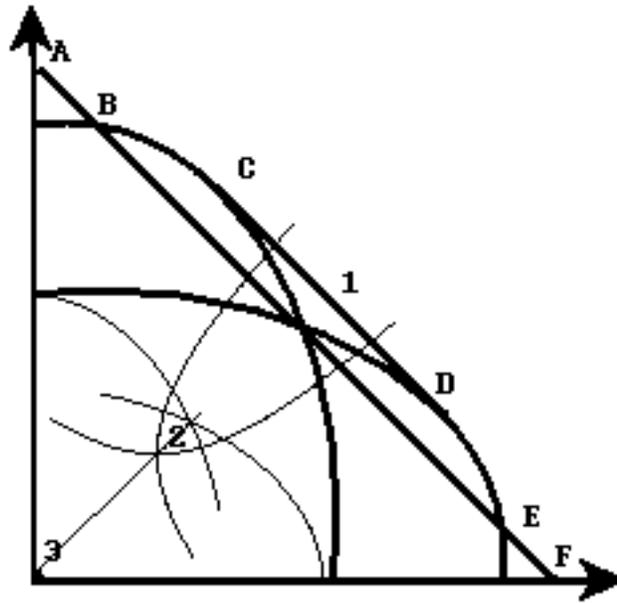


Figure 10: Permitted regions. Intermediate values of  $\gamma$ .  
 $\partial\mathcal{V}_1$  is represented by the curve  $ABCDEF$ . The set  $\mathcal{V}_2$  is strictly convex.

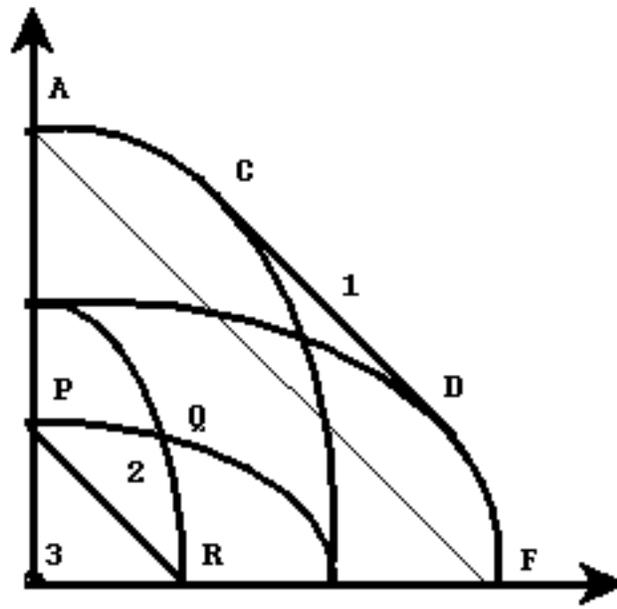


Figure 11: Permitted regions,  $\gamma = \gamma_2$ .  
 The boundary of  $\mathcal{V}_2$  has a straight component. Both hyperbolas degenerate and coincide with their asymptotic.

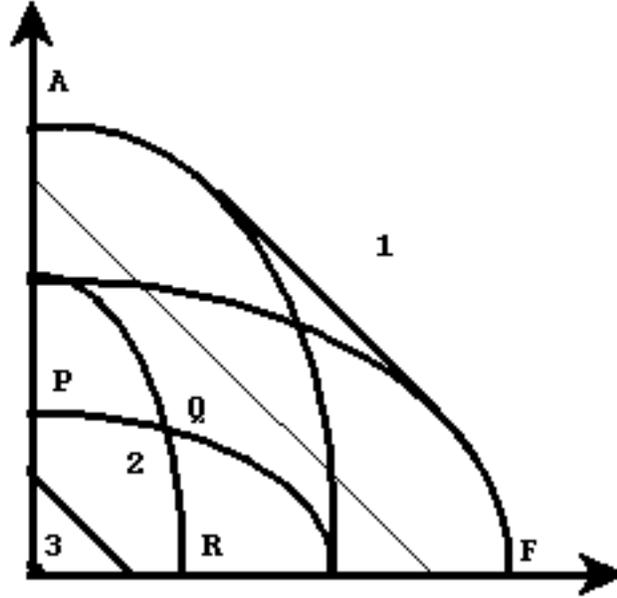


Figure 12: The permitted regions.  $\gamma$  is outside of  $[\gamma_1, \gamma_2]$ . Three component mixtures are not optimal.

of the mean field increases, the fraction of  $\sigma_3$  decreases and the fraction of  $\sigma_2$  increases. When  $\mathbf{P}$  reaches the belt-like region  $\mathcal{V}_2$ , the optimal mixture degenerates into pure material  $\sigma_2$ . Further increase of the magnitude of  $\mathbf{P}$  ( $\mathbf{P} \in \mathcal{V}_f^{12}$ ) brings the field into the region  $\mathcal{V}_f^{12}$ , Optimal mixtures are made of  $\sigma_2$  and  $\sigma_1$ . The fraction of  $\sigma_2$  in the mixture decreases with the increase of the magnitude of  $\mathbf{P}$ . When  $\mathbf{P}$  reaches the exterior region  $\mathcal{V}_1$ , it becomes zero.

Note, that three-composite mixtures never appear in that process. We interpret this as the second material being too “cheap”. It is always better to use this material then a mixture of materials  $\sigma_1$  and  $\sigma_3$ . (see Figure 12).

**Remark 5.2** *The described range of parameters  $\mathbf{P} \in \mathcal{V}_f$ ,  $\gamma \in [\gamma_1, \gamma_2]$  is sufficient to produce optimal solutions that involves all three materials. More detailed consideration could further shrink this set. The answer to the question: what is better to use,  $\sigma_2$  or the mixture of  $\sigma_1$  and  $\sigma_3$  depends on the degree of anisotropy of  $\mathbf{P}$ . This feature is illustrated in Figures 9 - 12. The closer to the isotropy is  $\mathbf{P}$ , the more useful is  $\sigma_2$  comparing with the mixture of other two materials. The dependence on the degree of anisotropy leads to*

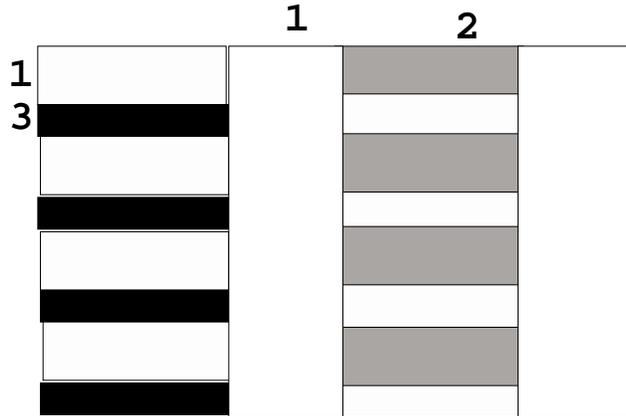


Figure 13: Optimal structures (Kohn, Milton); large volume fractions of  $\sigma_1$ .

*the optimality of three component mixtures in a range of  $\gamma$ , contrary to optimization of one energy [3] which corresponds to the trajectory along the axis  $E_B = 0$*

## 6 Examples of optimal microstructures.

Let us now determine some optimal structures that satisfy the necessary conditions as equality everywhere. Our search is guided by the derived conditions. We demonstrate how they are satisfied on the already known structures (see Milton [25], Lurie and Cherkaev [22], and Kohn and Milton [16]). Also we demonstrate a new type of optimal structures. These structures are optimal for a range of small volume fraction of  $\sigma_1$ , they realize the bounds by Nesi [32].

**Large volume fractions of  $\sigma_1$ .** Consider the case  $\gamma = \gamma_1$ , Figure 9. Suppose that the mean field  $\mathbf{P}$  belongs to the triangle  $CDQ$ . The optimal structures possess isotropic fields  $\mathbf{E}_2$  and  $\mathbf{E}_3$  in the second and in the third materials, and varying field  $\mathbf{E}_1$  in the first material; and the trace of  $\mathbf{E}_1$  is constant. One also easily sees from the necessary conditions that the following rank-one contacts are allowed:  $\sigma_2$  with  $\sigma_1$ ,  $\sigma_3$  with  $\sigma_1$ , but the contact between  $\sigma_2$  and  $\sigma_3$  is not allowed.

The structures that satisfy all these requirements are known: they have been suggested by Kohn and Milton [16], following the earlier work by Milton [25]. Note, that these structures realize the sufficient (translation) conditions and therefore are surely optimal.

The topology of the structures is the following. The materials  $\sigma_2$  and  $\sigma_3$  are placed in separated inclusions in the domain  $\mathcal{O}_1$ . (see Figure 13). The first material is divided into two parts with the fractions  $cm_1$  and  $(1 - c)m_1$ , where  $c \in (0, 1)$  is a parameter. The first part of  $\sigma_1$  is mixed with the all the amount of  $\sigma_2$  and it forms a matrix layered composite with effective tensor  $\boldsymbol{\sigma}_{12}$  and with eigenvalues  $\lambda_1(12)$  and  $\lambda_2(12)$ . The second part of  $\sigma_1$  is mixed with all the amount of  $\sigma_3$  and it forms a matrix layered composite with effective tensor  $\boldsymbol{\sigma}_{13}$  and with eigenvalues  $\lambda_1(13)$  and  $\lambda_2(13)$ . Next, the fraction  $c$  of the partition is so chosen that the composites  $\boldsymbol{\sigma}_{12}$  and  $\boldsymbol{\sigma}_{13}$  have the same eigenvalues

$$\lambda_1(12) = \lambda_1(13) \quad \text{and} \quad \lambda_2(12) = \lambda_2(13) \quad (6.11)$$

and are equivalent to each other. Clearly, that a mixture of  $\boldsymbol{\sigma}_{12}$  and  $\boldsymbol{\sigma}_{13}$  has the same effective properties, independently of the geometry of that mixture. The effective properties of these structures satisfy the translation bounds; (see [16]); for isotropic composites, conductivity satisfies Hashin -Shtrikman bounds which in the discussing case  $\sigma_3 = \infty$  becomes

$$\frac{1}{\sigma_* + \sigma_1} = \frac{m_1}{2\sigma_1} + \frac{m_2}{\sigma_1 + \sigma_2}. \quad (6.12)$$

The limitations of this construction come from the requirements (6.11). Clearly, that  $\boldsymbol{\sigma}_{12}$  has the eigenvalues smaller that  $\sigma_2$ . One need to put a significant amount of  $\sigma_1$  into  $\boldsymbol{\sigma}_{13}$  to obtain the mixtures with such conductivities. (see the discussion in [16]) In particular, isotropic mixtures have the effective conductivity  $\sigma_*$  in the interval  $[\sigma_1, \sigma_2]$ . The requirement  $\sigma_* \in [\sigma_1, \sigma_2]$ , combined with (6.12) leads to the condition

$$m_1 \geq 2(1 - m_2) \frac{\sigma_1}{\sigma_1 + \sigma_2} \quad (6.13)$$

of attainability of the described isotropic mixtures (for more detailed discussion see [16])

The necessary conditions (the Figure 13) show the optimality of the fields in that structures. Note that  $\boldsymbol{E}_2$  and  $\boldsymbol{E}_3$  are in rank-one contact with  $\boldsymbol{E}_1$ , but with each other. This contacts correspond to laminates of the pair  $\sigma_2$  and  $\sigma_1$ , and the pair  $\sigma_2$  and  $\sigma_1$ . These laminates are in rank-one contact if the volume fraction of  $\sigma_1$  is properly chosen. The outside layer of  $\boldsymbol{E}_1$  is in rank-one contact with the laminates.

The fields in three parts of the structure in the Figure 13 belong to the following points of the boundary (see Figure 9): F, D, and a point on the line  $[C, D]$ , their relative fractions are chosen to preserve the trace of the field  $\boldsymbol{E}_1$  in these parts. The effective property  $\sigma_*$ , (6.12), is easily obtained from these fields.

**Remark 6.1** *There are several geometrically different realizations of these structures. The first is the mentioned combination of matrix laminates. Other known realizations correspond to isotropic composites. First of such constructions has been suggested by Milton in [25]; the structure uses the constructions of coated spheres of materials  $\sigma_1$  and  $\sigma_2$  and of materials*

$\sigma_1$  and  $\sigma_3$ , these two composites are mixed together. A topologically different realization was suggested by Lurie and Cherkaev [22]. In this scheme, we first form a coated spheres construction from all amount of  $\sigma_3$  that forms the nucleus, and a part of  $\sigma_1$  that forms the core. The coated spheres have the effective conductivity equal to  $\sigma_2$  due to the choice of the amount of  $\sigma_1$ . The obtained nucleus is wrapped by a ring of  $\sigma_2$ . Further, the whole construction is placed inside the remaining part of  $\sigma_1$  as in coated spheres. One can check, that the fields  $\mathbf{E}_2$  and  $\mathbf{E}_3$  are constant, and the field  $\mathbf{E}_1$  continuously varies along  $\partial\mathcal{V}_1$  and its trace is constant everywhere (the proof is similar to the presented above example of two-phase coated spheres).

### 6.0.1 Small volume fraction of $\sigma_1$ .

Next, we demonstrate structures which satisfy necessary conditions when  $\gamma = \gamma_2$  and  $\mathbf{P}$  lies between  $\mathcal{V}_2$  and the the origin. These structures correspond to small volume fractions of  $\sigma_1$ . This time, the field  $\mathbf{E}_2$  can vary, and  $\mathbf{E}_1$  stays constant. Material  $\sigma_1$  can be in a rank-one contact with  $\sigma_2$  and with  $\sigma_3$  only if it is in the corner point (one component is zero).

The optimal three-component structures that realize the necessary conditions are matrices of  $\sigma_2$  with inclusions of laminates of  $\sigma_1$  and  $\sigma_3$ . (note that the domains  $\sigma_1$  and  $\sigma_3$  are not separated from each other).

Let us show how the necessary conditions are satisfied. The field in  $\mathbf{E}_1$  is in the contact with  $\mathbf{E}_3$  (the point F on the Figure 11), the field in the  $\mathcal{O}_2$  is piece-wise constant and its trace is constant, because it forms the matrix laminate across the anisotropic inclusion (point R and a point on the line  $[P, R]$  on the Figure 11).  $\mathbf{E}_2$  is either in rank-one contact with the laminates from  $\sigma_1$  and  $\sigma_3$  (point R on the Figure 11), or (the field in an orthogonal layer) in rank-one contact with the laminate of three materials. (see Figure 14).

The effective parameters are found as following: the eigenvalues  $\lambda_1$  and  $\lambda_2$  of a matrix composite ( $\sigma_2$  is in the core) satisfy the equation

$$g(\lambda_1, \lambda_2) = \frac{1}{\lambda_1 - \sigma_2} + \frac{1}{\lambda_2 - \sigma_2} = C. \quad (6.14)$$

where  $C$  is a constant. To determine  $C$  we observe that the structure degenerates into the ‘‘T-structure’’ (see Figure 15) that possesses the following eigenvalues (see Appendix)

$$\lambda_1^T = \frac{\sigma_2}{m_2}, \quad \lambda_2^T = m_2\sigma_2 + \frac{(1 - m_2)^2}{m_1}\sigma_1 \quad (6.15)$$

This gives the final relations in the form  $g(\lambda_1, \lambda_2) = g(\lambda_1^T, \lambda_2^T)$  or

$$\frac{1}{\lambda_1 - \sigma_2} + \frac{1}{\lambda_2 - \sigma_2} = \frac{1}{\lambda_1^T - \sigma_2} + \frac{1}{\lambda_2^T - \sigma_2}. \quad (6.16)$$

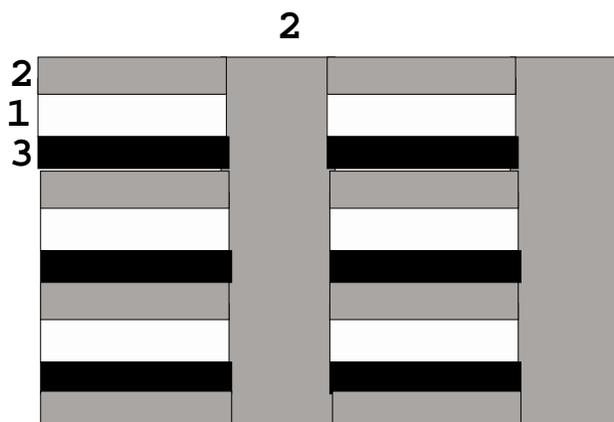


Figure 14: Structures of optimal composites, small volume fractions of  $\sigma_1$ .

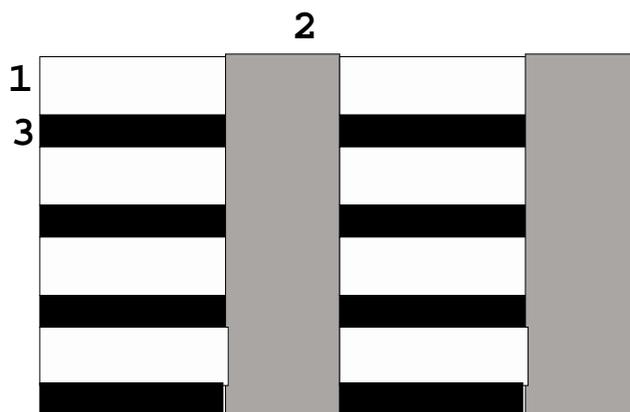


Figure 15: Three materials with conductivities  $\sigma_1$ ,  $\sigma_2$ ,  $\sigma_3$  and the volume fractions  $m_1$ ,  $m_2$ ,  $m_3$  are combined as follows: The first and the third materials form a laminate  $R_{(13)}$ ; then the second material and  $R_{(13)}$  form a laminate of second rank. The normal to the last laminate is orthogonal to the normal of the first-rank laminate.

In particular, the isotropic conductivity  $\sigma_*$  satisfies the relation

$$\frac{1}{\sigma_* + \sigma_2} = \frac{m_1}{2\sigma_1} + \frac{m_2}{2\sigma_2} \quad (6.17)$$

(compare with the Hashin-Shtrikman formula (6.12).

The described structures are optimal in a range of parameters. For isotropic composites, the limiting case correspond to isotropy of T-structures:  $\lambda_1^T \leq \lambda_2^T$  or (use (6.15))

$$0 \leq m_1 \leq \frac{m_2(1 - m_2)}{1 + m_2} \left( \frac{\sigma_1}{\sigma_2} \right) \quad (6.18)$$

Note that these structures have different topology than the previously discussed ones. Namely, (i) the second material forms an matrix and the laminates of the first and the third materials form inclusions. (ii) The first and the third materials are always glued together. (iii) The inclusions are highly anisotropic; for the overall isotropic structures the anisotropy of inclusion is compensated buy an eccentricity of the their shape.

In this case bounds give the rough estimates. Better bounds were suggested recently by Nesi [32]. The described structures exactly satisfy these bounds. The coincidence can be explained by the following: the sufficient condition by Nesi [32] are obtained by estimating the determinant of the field  $\mathbf{E}_1$  by zero. (It was proven that it does not changes its sign everywhere in  $\mathcal{O}$ ). This is exactly the case in the considered geometry: the field in  $\mathcal{V}_3$  is zero due to the infinite conductivity  $\sigma_3$ , therefore the field  $\mathbf{E}_1$  in the neighboring layer of  $\sigma_1$  has one zero component and its determinant is zero.

**Remark 6.2** *One can check by direct calculations, that the described structures have better conductivity than the structures suggested in [16] and in [22] for the considered range of parameters; the last structures do not satisfy the necessary conditions.*

**Postlude.** The discussed examples do not complete the description of optimal structures for three materials. However, we have accomplished our goal which is to demonstrate the applications of the necessary conditions to structural optimization and to show variety of optimal topologies of multicomponent mixtures.

## ACKNOWLEDGMENTS

The author is thankful to Graeme Milton, Leonid Gibiansky, and Elena Cherkaeva for valuable discussions, and to Tom Robbins for improving of the text. The support by the National Science Foundation under Grant No. DM DMS- 9625129. and by U.S.A. - Israel Binational Science Foundation under Grant No. 9400349 is gratefully acknowledged.

## References

- [1] Bendsoe, M. P. (1995) Optimization of structural topology, shape, and material. Springer. Berlin ; NY
- [2] Bhattacharya, K. and Kohn, R.V. (1996) Elastic energy minimization and the recoverable strains of polycrystalline shape-memory materials, Arch. Rat. Mech. Anal., in press.
- [3] Burns T., and Cherkaev A.V. (1997) Optimal distribution of multimaterial composites for torsioned beams. Structural Optimization, 13(1), p. 4-12.
- [4] Cherkaev, A.V. and Gibiansky, L.V. (1992) The exact coupled bounds for effective tensors of electrical and magnetic properties of two-component two-dimensional composites, Proc. of Royal Soc. of Edinburgh **122A** , 93-125.
- [5] Cherkaev, A.V. and Gibiansky, L.V. (1996) External structures of multiphase heat conducting composites. Int. J.Solids Structures, 33, No 18, p. 2609-2623.
- [6] Cherkaev, A., Grabovsky, Y., Movchan, A., and Serkov, S. (1997) An optimal cavity in the elastic plane. Int. J. of Solids and Structures, submitted.
- [7] Cherkaev, A.V. and Kohn, R. (1997). Introduction. in: Topics of mathematical modelling of composite materials. Cherkaev and Kohn - eds. Birkhauser, 1997.
- [8] Ekeland, I. (1990) Convexity methods in Hamiltonian mechanics. Berlin, NY Springer-Verlag.
- [9] Francfort, G. and Milton, G. W. (1994). Sets of conductivity and elasticity tensors stable under lamination. Comm. Pure Appl. Math. 47 , no. 3, 257-279.
- [10] Gibiansky, L.V. and Sigmund, O. (1998) Multiphase composites with extremal bulk modulus. DCAMM Report 600, DTU, Lyngby, Denmark.
- [11] Gibiansky, L.V. and Torquato, S. (1996) Rigorous link between the conductivity and elastic moduli of fiber-reinforced composite materials. Trans. Roy. Soc. London **A 452**, 253-283.
- [12] Golden, K. (1986) Bounds on the complex permittivity of a multicomponent material, *J. Mech. Phys. Solids*, **34(4)**, 333-358.
- [13] Grabovsky, Y. (1996) Bounds and extremal microstructures for two-component composites: a unified treatment based on the translation method. Proc. Roy. Soc. London Ser. A 452 (1996), no. 1947, 919-944.

- [14] Grabovsky Y. and Milton G.W. (1988) Exact relations for composites: towards a complete solution. *Doc. Math. J DMV.* in print.
- [15] Hashin, Z. and Shtrikman, S. (1962) A variational approach to the theory of the effective magnetic permeability of multiphase materials, *J. Appl. Physics* **35**, 3125-3131.
- [16] Kohn, R.V. and Milton, G.W. (1988) Variational bounds on the effective moduli of anisotropic composites, *J. Mech. Phys. Solids* **36(6)**, 597-629.
- [17] Kohn, R. V. and Strang, G. (1986) Optimal design and relaxation of variational problems. *Comm. Pure Appl. Math.* 39 (1986), no. 3, 353–377.
- [18] Lurie, K.A.(1963) The Mayer-Bolza Problem for Multiple Integrals and Optimization of the Behavior of Systems with Distributed Parameters (in Russian), *Prikladnaya Matematika i Mekhanika*, Vol.27, No 5.
- [19] Lurie, K.A. (1970) Optimal distribution of the specific resistance tensor in the canal of magneto-hydrogenerator. *Prikladnaya Matematika i Mekhanika* 34(2) (in Russian).
- [20] Lurie, K. (1993). *Applied Optimal Control*, Plenum, New York.
- [21] Lurie, K.A. and Cherkaev, A.V. (1982) Exact estimates of conductivity of composites formed by two isotropically conducting media taken in prescribed proportion, Preprint No 783, Physico-Technical Institute, Acad. of Sc. of USSR (in Russian). *Proc. Roy. Soc. Edinburgh* , 1984, **99 A**, 71-87.
- [22] Lurie, K.A. and Cherkaev, A.V. (1985) The problem of formation of an optimal isotropic multicomponent composite, *J. Opt. Theory Appl.* **46**, 571.
- [23] Lurie, K.A. and Cherkaev, A.V. (1986) The effective characteristics of composite materials and optimal design of construction, *Advances in Mechanics (Poland)*, 9(2), pp. 3-81. [in Russian]. English translation in: *Topics of mathematical modelling of composite materials*. Cherkaev and Kohn - eds. Birkhauser, 1997.
- [24] Lurie, K., Cherkaev, A., Fedorov, A. (1982) ‘Regularization of optimal problems of design of bars and plates and solving the contradictions in a system of necessary conditions of optimality.’ *J. Opt. Th. Appl.* v. 37, N. 4, pp. 499-542.
- [25] Milton, G.W. (1981) Concerning bounds on transport and mechanical properties of multicomponent composite materials, *Appl. Phys.* **A26**, 123.
- [26] Milton, G.W. (1986) Modeling the properties of composites by laminates, in: *Homogenization and Effective Moduli of Materials and Media*, Ericksen, J.L., Kinderlehrer, D., Kohn, R., and Lions, J.-l. eds., Springer-Verlag, New-York, pp. 150-174.

- [27] Milton, G.W. (1987) Multicomponent composites, impedance networks and new types of continued fraction I,II, *Commun. Math. Phys.* **111**, 281-327, 329-372.
- [28] Milton, G.W. (1990) A brief review of the translation method for bounding effective elastic tensors of composites. In: *Continuum Models and Discrete Systems*, ed. by G. A. Maugin, vol. 1, pp. 60-74.
- [29] Milton G.W. (1991) Private communication.
- [30] Milton, G.W. (1994) A link between sets of tensors stable under lamination and quasiconvexity, *Comm. Pure Appl. Math.* **XLVII**, 959-1003.
- [31] Milton, G.W. and Golden, K. (1990) Representation for the conductivity functions of multicomponent composites, *Comm. Pure Appl. Math.* **18**, 647-671.
- [32] Nesi, V. (1995). Bounds on the effective conductivity of two-dimensional composites made of  $n \geq 3$  isotropic phases in prescribed volume fraction: the weighted translation method. *Proc. Roy. Soc. Edinburgh Sect. A* 125 no. 6, 1219–1239.
- [33] Ponte Castañeda, P. (1996) Exact second-order estimates for the effective mechanical properties of nonlinear composite materials. *J. Mech. Phys. Solids* 44, no. 6, 827–862.
- [34] Talbot, D. R. S.; Willis, J. R. (1992) Some simple explicit bounds for the overall behaviour of nonlinear composites. *Internat. J. Solids Structures* 29, no. 14-15, 1981–1987.
- [35] Tartar, L. (1985) Estimations fines des coefficients homogenises, *Ennio de Giorgi Colloquium, P.Kree,ed., Pitman Research Notes in Math.* **125**, 168 - 187.
- [36] Vigdergauz, S. (1994). Two-dimensional grained composites of extreme rigidity, *Journal of Applied Mechanics. Transactions of the ASME.* **61**(6), 390-394.
- [37] Willis, J. R. Variational and related methods for the overall properties of composites. *Adv. in Appl. Mech.* 21 (1981), 1–78.
- [38] Young, L.C. (1969). *Lectures on the calculus of variations and optimal control theory.* Philadelphia, Saunders.
- [39] Zhikov, V. (1986) On the estimates for the trace of a homogenized matrix, *Math. Notes* **40**, 628-634

## A Appendix. Calculation of the fields inside the laminates

The following is a procedure for calculating the fields in a laminate of a high rank. These structures are combined as laminates from substructures that could also be laminates of substructures of a deeper level, etc. An iterative scheme is needed to compute the fields in the pure materials that form the deepest level of the structure.

The algorithm is as follows: First we calculate the effective properties of a laminate as a function of the known properties of its components. Then we calculate the fields inside the layers of the laminate using the known average field and the effective properties.

Suppose that laminates are assembled from two anisotropic materials with the codirected conductivity tensors  $\mathbf{R}_1$  and  $\mathbf{R}_2$  mixed in proportions  $c_1$  and  $c_2$  ( $c_1 + c_2 = 1$ ). The normal  $\mathbf{n}$  to the laminate and the matrices of materials' properties are

$$\mathbf{n} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{R}_i = \begin{pmatrix} \rho_A^{(i)} & 0 \\ 0 & \rho_B^{(i)} \end{pmatrix}, \quad i = 1, 2. \quad (\text{A.1})$$

The effective properties tensor  $\mathbf{R}_*$  of the laminate is

$$\mathbf{R}_* = \begin{pmatrix} \frac{\rho_A^{(1)} \rho_A^{(2)}}{c_1 \rho_A^{(2)} + c_2 \rho_A^{(1)}} & 0 \\ 0 & c_1 \rho_B^{(1)} + c_2 \rho_B^{(2)} \end{pmatrix}; \quad (\text{A.2})$$

the normal component is given by the harmonic mean of the materials' properties, and the tangent component is given by the arithmetic mean.

Suppose that the laminate is submerged into two mutual orthogonal fields described by the symmetric matrix  $\mathbf{E}$ . that are codirected with the eigenvectors of  $\mathbf{R}_*$ . The field  $\mathbf{E}_1$  in the material  $\mathbf{R}_1$  is computed from the equality  $c_1 \mathbf{E}_1 + c_2 \mathbf{E}_2 = \mathbf{E}$  and from the jump condition. It is equal to

$$\mathbf{E}_1 = \mathbf{K}_1 \mathbf{E}, \quad \mathbf{K}_1 = \begin{pmatrix} \frac{\rho_A^{(2)}}{c_1 \rho_A^{(2)} + c_2 \rho_A^{(1)}} & 0 \\ 0 & 1 \end{pmatrix}. \quad (\text{A.3})$$

The field  $\mathbf{E}_2$  in  $\mathbf{R}_2$  is computed similarly.

To calculate the fields in a laminate of a high rank one must first compute the effective properties of the substructures that form the composite and find the matrices  $\mathbf{K}_i$ . Then one computes the fields using (A.3).

**Example A.1** *As an example let us compute the effective properties of the "T-structure" shown in Figure ???. First, we compute the properties of laminate substructure  $R_{(13)}$  of  $\sigma_1$  and  $\sigma_3$ . The relative fraction of the first and third materials in the substructure are  $\frac{m_1}{m_1+m_3}$  and  $\frac{m_3}{m_1+m_3}$ . Equations (A.1) and (A.2) give*

$$\mathbf{n} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \mathbf{R}_{(13)} = \begin{pmatrix} \rho_A^{(13)} & 0 \\ 0 & \rho_B^{(13)} \end{pmatrix},$$

where (see (A.2))

$$\rho_A^{(13)} = \frac{m_1\sigma_1 + m_3\sigma_3}{m_1 + m_3}, \quad \rho_B^{(13)} = \frac{(m_1 + m_3)\sigma_1\sigma_3}{m_1\sigma_3 + m_3\sigma_1}. \quad (\text{A.4})$$

Now we can compute the fields in the domain  $\mathcal{O}_2$  and the average field in the composed domain  $\mathcal{O}_{13}$

$$\begin{aligned} \mathbf{E}_2 &= \mathbf{K}_2 \mathbf{E}, & \mathbf{K}_2 &= \begin{pmatrix} \frac{\rho_A^{(13)}}{(m_2+m_3)\rho_A^{(13)}+m_2\sigma_2} & 0 \\ 0 & 1 \end{pmatrix}, \\ \mathbf{E}_{(13)} &= \mathbf{K}_{(13)} \mathbf{E}, & \mathbf{K}_{(13)} &= \begin{pmatrix} \frac{\sigma_2}{(m_2+m_3)\rho_A^{(13)}+m_2\sigma_2} & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned} \quad (\text{A.5})$$

Let us compute the fields in the domains  $\mathcal{O}_1$  and  $\mathcal{O}_3$  that compose the first rank laminate  $\mathcal{O}_{13}$ :

$$\mathbf{E}_1 = \mathbf{K}_{(1)} \mathbf{E}_{(13)}, \quad \mathbf{K}_{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{\sigma_3(m_1+m_3)}{m_1\sigma_3+m_3\sigma_1} \end{pmatrix}, \quad (\text{A.6})$$

$$\mathbf{E}_{(3)} = \mathbf{K}_{(3)} \mathbf{E}_{(13)}, \quad \mathbf{K}_{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{\sigma_1(m_1+m_3)}{m_1\sigma_3+m_3\sigma_1} \end{pmatrix}. \quad (\text{A.7})$$

Finally, we obtain the dependence of the fields in the materials on the geometric parameters of the structure (the tensors  $\mathbf{K}_i$ ):

$$\mathbf{E}_1 = \mathbf{K}_{(1)} \mathbf{K}_{(13)} \mathbf{E}, \quad \mathbf{E}_2 = \mathbf{K}_2 \mathbf{E}, \quad \mathbf{E}_3 = \mathbf{K}_{(3)} \mathbf{K}_{(13)} \mathbf{E}. \quad (\text{A.8})$$

Controlling the coefficients  $\mathbf{K}$  one varies the fields  $\mathbf{E}_i$ .