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Bounds on the Effective Moduli of Composite Materials

School on Homogenization
ICTP, Trieste, September 6–17, 1993

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1 Composite materials and their effective properties

1.1 Introduction

The course is devoted to studying the properties of composite materials. Composite-like materials are very common in nature as well as in engineering because they allow to combine the properties of component materials in an optimal way, allow to create media with such unusual and contradictory combination of properties as stiffness and dissipativeness, stiffness in one direction and softness in the other one, high stiffness and low weight etc.

The pore structure of the bonds, trunks of the wood, leafs of the trees provide an examples when mixture of stiff and soft tissues can be treated as a composite and leads to the desired properties. Steel is the other example of the composite. The fine structure of the steel is grain-like mixture of monocrystals.

Engineers use composites for a long time. The well-known examples are given by reinforced concrete, plywood or fiber reinforced carbon composites. Composite materials are important for the optimal design problems because use of composite constructions is often the only way to achieve the desirable combination of properties with the available component materials. For examples, the honeycomb-like structures are light and possess a high bending stiffness due to the special structure that can be treated as a composite of stiff aluminum matrix and air (pores).

The common feature of all these examples is that locally unhomogeneous material behaves as a homogeneous medium when the characteristic size of the inclusions is much smaller then the size of the whole sample and the characteristic wavelength of external fields. In such a situation the properties of the composite can be described by the effective moduli that is some special kind of averaging of the properties of the components. The branch of mathematics that study the behaviour of such materials is called the homogenization theory. In this lecture we

1. formulate mathematical statement of the homogenization problem;
2. give two equivalent definitions of the effective properties of composite material;
3. study the direct problem of homogenization theory, i.e. the problem of calculation of the effective properties for a composite of given structure;
4. find the effective properties of laminate composites and Hashin-Shtrikman assemblages of coated spheres.

The second lecture of the course devoted to the statement of the problem of bounds on the effective properties, in the third one we describe the translation method for deriving such bounds and illustrate this method on the simplest example of the bounds on conducting composite. The fourth lecture devoted to implementation of the translation method to the two-dimensional isotropic elastic composite. We also touch some open questions in this field. The main goal of the course is not only to give an introduction to the problem of bounds on the effective moduli, but also to give rigorous, powerful and simple method to attack the problems of such type.

Remark *The actual course slightly differed from this lecture notes. It also included the description of variational principles for the media with complex moduli with an applications to the problem of bounds on the complex effective conductivity of a composite.*

Last lecture of the course that is not reflected here was devoted to some bounds on conductivity of multiphase materials, description of optimal microstructures (namely, of matrix laminate composite of high rank) that realize some of the bounds. We also discussed the statement of optimal design problem and use of homogenization theory in optimal design. Most of these results can be found in the mentioned at the references original papers. The references on the original papers that are used in the course are given at the end of each section.

1.2 Notations

Let introduce some notations that are used in the course. First, let us denote all vectors and tensors as a bold characters, unit tensor as $\boldsymbol{I}$

$$\boldsymbol{I} = \delta_i \delta_j = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{1.1}$$

symbol $(\cdot)$ denotes the convolution of the tensors over one index, namely

$$\boldsymbol{a} \cdot \boldsymbol{b} = a_i b_i, \quad \boldsymbol{A} \cdot \boldsymbol{b} = A_{ij} b_j \boldsymbol{l}_i, \quad \boldsymbol{A} \cdot \boldsymbol{B} = A_{ij} B_{jk} \boldsymbol{l}_i \boldsymbol{l}_k, \quad \boldsymbol{b} \cdot \boldsymbol{D} \cdot \boldsymbol{b} = D_{ij} b_i b_j, \tag{1.2}$$

etc., where a_i, b_i, A_{ij} , and B_{ij} are the elements of the vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and tensors $\boldsymbol{A}$, and $\boldsymbol{B}$ respectively in the Cartesian basis, $\boldsymbol{l}_i$ is the ort of the axis x_i. We use summation agreement that sum is taken over the repeating indices from 1 to N, where N is the dimension of the space, $N = 2$ or $N = 3$. Two dots are used in the elasticity theory notations as follows

$$\boldsymbol{\epsilon} \cdot \cdot \boldsymbol{\sigma} = \epsilon_{ij} \sigma_{ji}, \quad \boldsymbol{\epsilon} \cdot \cdot \boldsymbol{C} \cdot \cdot \boldsymbol{\epsilon} = C_{ijkl} \epsilon_{ji} \epsilon_{lk}. \tag{1.3}$$

We also denote as ∇ the Hamiltonian operator

$$\nabla = \boldsymbol{l}_i \frac{\delta}{\delta x_1}. \tag{1.4}$$

1.3 Composite materials and their effective properties.

We begin with formulation of the homogenization problem for two isotropic conducting materials. To study the effective properties of a mixture it is sufficient to deal with space periodic structures. The case of random composite has some specific features but most of the results are simplier to prove and describe for the periodic structures, generalization on random case is a technical problem. A composite which is not periodic, but say statistically homogeneous, can be replaced by a periodic one with negligible change in its effective properties: one can take a sufficiently large cubic representative sample of the statistically homogeneous composite and extend it periodically. For simplicity we start with a description of a two-dimensional two-phase composite combined from two conducting materials.

We assume that each element of periodicity S is divided into the parts S_1 and S_2 with the prescribed volume fractions m_1 and m_2 respectively, see Figure 1.

$$\begin{gathered} S_1 \cup S_2 = S, \\ (volS_1)/(volS) = m_1, \\ (volS_2)/(volS) = m_2, \\ m_1 + m_2 = 1 \end{gathered} \tag{1.5}$$

We can assume that $volS = 1$ without loss of generality.

Figure 1: two-phase composite material.

Suppose that these two parts are occupied by two isotropic materials with different conductivities $\mathbf{\Sigma}_1 = \sigma_1 \boldsymbol{I}$ and $\mathbf{\Sigma}_2 = \sigma_2 \boldsymbol{I}$ respectively. The state of the media is described by the linear elliptic system of differential equations of electrostatic

$$\nabla \cdot \boldsymbol{j} = 0, \quad \boldsymbol{j} = \mathbf{\Sigma} \cdot \boldsymbol{e}, \quad \boldsymbol{e} = -\nabla \phi, \tag{1.6}$$

where ϕ is the electrical potential, $\boldsymbol{j}$ is a current and $\boldsymbol{e}$ is an electrical field. The conductivity tensor $\mathbf{\Sigma}$ has the form

$$\Sigma(\boldsymbol{x}) = (\sigma_1 \chi_1(\boldsymbol{x}) + \sigma_2 \chi_2(\boldsymbol{x}))\ \boldsymbol{I}, \tag{1.7}$$

where $\chi_i(\boldsymbol{x}),\ i = 1, 2$ are the characteristic functions of the subdomains S_1, S_2

$$\chi_i(\boldsymbol{x}) = \begin{cases} 1, & \text{if } x \in S_i \\ 0, & \text{otherwise.} \end{cases} \tag{1.8}$$

We denote also $\mathbf{\Sigma}_i = \sigma_i\ \boldsymbol{I}, \quad i = 1, 2$

Remark: The conductivity equations (1.6) describe also heat conductance, diffusion of particles or liquid in a porous medium, magnetic permeability etc. as it is summarized in the following table, but we use the notations of electrical conductivity problem.

Problem	$\mathbf{j}$	$\mathbf{e}$	ϕ	$\mathbf{\Sigma}$
Thermal Conduction	Heat current	Temperature gradient	Temperature	Thermal conductivity
Electrical Conduction	Electrical current	Electrical field	Electrical potential	Conductivity
Dielectrics	Displacement field	Electric field	Potential	Permittivity
Diffusion	Particle current	Gradient of concentration	Concentration	Diffusivity
Magnetism	Magnetic induction	Magnetic field intensity	Potential	Permeability
Stoke's flow	Current	Pressure gradient	Pressure	Viscosity
Homogenized flow in porous media	Fluid current	Pressure gradient	Pressure	Permeability

Described periodical structure acts in a smooth external field as a homogeneous anisotropic conductor, that can be described by the effective properties tensor $\mathbf{\Sigma}_0$. There exist two equivalent definitions of the effective properties tensor.

Let put the composite into the homogeneous external fields. The local fields in the cell of periodicity are S-periodic. Let compute the average values of the current and electrical fields over the cell of periodicity S

$$< \boldsymbol{j} >= \int_S \boldsymbol{j}(\boldsymbol{x}) dS, \qquad < \boldsymbol{e} >= \int_S \boldsymbol{e}(\boldsymbol{x}) dS, \tag{1.9}$$

One can prove that these values are connected by linear relationship

$$< \boldsymbol{j} >= \mathbf{\Sigma}_0 \cdot < \boldsymbol{e} >, \tag{1.10}$$

Here and below the symbol $< \cdot >$ denotes the average value of $(\cdot)$, i.e.

$$< (\cdot) >= \int_S (\cdot) dS / \ vol S, \tag{1.11}$$

Definition 1. Symmetric, positive definite (2×2) tensor Σ_0 defined by the above procedure is called the tensor of effective conductivity of the composite.

Due to the linearity of the state law (1.6), the tensor $\mathbf{\Sigma}_0$ is independent of external fields, that make this definition meaningful. Effective properties tensor $\mathbf{\Sigma}_0$ depends on the properties of the components, on their volume fractions, and also strongly depends on geometrical structure of the composite.

This derivation can be done rigorously using the technic of multiscale decomposition, but we omit these details. Interested reader can find the details in the book by Sanchez-Palencia.

Basing on this definition one can calculate the effective properties tensor for any given microgeometry. Indeed, let study the following boundary value problem combining the equations (1.6) with boundary conditions

$$\phi = -e_{01} x_1, \quad if \ \ \boldsymbol{x} = \{x_1, x_2\} \in \Gamma. \tag{1.12}$$

Here e_{01} is some constant and Γ is the boundary of the periodic cell. Let assume that we solve this problem either analytically or numerically and denote as $\boldsymbol{j}_0 = \boldsymbol{j}(\boldsymbol{x})$, $\boldsymbol{e}_0 = \boldsymbol{e}(\boldsymbol{x})$, where $\boldsymbol{j}_(\boldsymbol{x})$ and $\boldsymbol{e}(\boldsymbol{x})$ is the solution of (1.6), (1.12). One can check that $\boldsymbol{e}_0 = \{e_{01}, 0\}$. Indeed

$$\boldsymbol{e}_0 = -\int_S \nabla\phi dS = \int_\Gamma \boldsymbol{n}\; e_{01} d\Gamma = e_{01}\boldsymbol{l}_1. \tag{1.13}$$

Here $\boldsymbol{l}_1$ is the ort of the axis x_1 and $\boldsymbol{n}$ is the external normal to the Γ. Now let us rewrite the effective state law (1.10) in a component form

$$j_{01} = \sigma^0_{11} e_{01} + \sigma^0_{12} e_{02}, \qquad j_{02} = \sigma^0_{21} \boldsymbol{e}_{01} + \sigma^0_{22} e_{02}, \tag{1.14}$$

where σ^0_{ij} are the elements of the effective conductivity tensor $\boldsymbol{\Sigma}_0$, and substitute the value $\boldsymbol{e}_{02} = 0$ in it. We immediately arrive at the relations

$$\sigma^0_{11} = j_{01}/e_{01}, \quad \sigma^0_{21} = j_{02}/e_{01}. \tag{1.15}$$

Similarly, by solving the equations (1.6) in conjunction with the boundary conditions

$$\phi = -e_{02} x_2 \quad if \quad \boldsymbol{x} = \{x_1, x_2\} \in \Gamma \tag{1.16}$$

we arrive at the relations

$$\sigma^0_{22} = j_{02}/e_{02}, \quad \sigma^0_{12} = j_{01}/e_{02} \tag{1.17}$$

where j_{01}, and j_{02} are the averaged over the periodic cell current fields for the problem with boundary conditions (1.16)

In general, for more complicated problems, we need to solve as many boundary value problems as the dimension of the space of phase variables. Namely, this number is equal to N for N-dimensional conductivity problem, equal to 3 for two-dimensional elasticity and equal to 6 for the three-dimensional elasticity.

There exists the other definition of the effective properties tensor based on the energy arguments.

Definition 2. Tensor of the effective properties of a composite is defined as a tensor of properties of the medium that in the homogeneous external filed $\boldsymbol{e}_0$ stores exactly the same amount of energy as a composite medium subject to the same homogeneous field

$$\boldsymbol{e}_0 \cdot \boldsymbol{\Sigma}_0 \cdot \boldsymbol{e}_0 = < \boldsymbol{e}(\boldsymbol{x}) \cdot \boldsymbol{\Sigma}(\boldsymbol{x}) \cdot \boldsymbol{e}(\boldsymbol{x}) > . \tag{1.18}$$

Here $\boldsymbol{e}(\boldsymbol{x})$ is the solution of the problem (1.6) with periodic boundary conditions and with an additional condition $\boldsymbol{e}_0 = < \boldsymbol{e}(\boldsymbol{x}) >$. Using Dirichlet variational principle one can write

$$\boldsymbol{e}_0 \cdot \boldsymbol{\Sigma}_0 \cdot \boldsymbol{e}_0 = \inf_{\substack{\boldsymbol{e}\,:\,\boldsymbol{e} = \nabla\phi \\ <\boldsymbol{e}> = \boldsymbol{e}_0}} < \boldsymbol{e}(\boldsymbol{x}) \cdot \boldsymbol{\Sigma}(\boldsymbol{x}) \cdot \boldsymbol{e}(\boldsymbol{x}) >, \tag{1.19}$$

Similarly, by using Thompson variational principle, one can write

$$\boldsymbol{j}_0 \cdot \boldsymbol{\Sigma}_0^{-1} \cdot \boldsymbol{j}_0 = \inf_{\substack{\boldsymbol{j}\,:\,\nabla\cdot\boldsymbol{j} = 0, \\ <\boldsymbol{j}> = \boldsymbol{j}_0}} < \boldsymbol{j}(\boldsymbol{x}) \cdot \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}) \cdot \boldsymbol{j}(\boldsymbol{x}) >, \tag{1.20}$$

The definitions (1.10) and (1.19)-(1.20) are equivalent. The first one is useful to compute the effective properties for given structures, the second one is a key that provides an opportunity to use variational methods to construct the bounds on the effective properties. To prove the equivalence we mention first that

$$< \boldsymbol{e}(\boldsymbol{x}) \cdot \boldsymbol{\Sigma}(\boldsymbol{x}) \cdot \boldsymbol{e}(\boldsymbol{x}) >=< \boldsymbol{e}(\boldsymbol{x}) \cdot \boldsymbol{j}(\boldsymbol{x}) >= \boldsymbol{e}_0 \cdot \boldsymbol{j}_0 + \sum_{\boldsymbol{k} \neq 0} \hat{\boldsymbol{e}}(\boldsymbol{k}) \cdot \hat{\boldsymbol{j}}(\boldsymbol{k}), \tag{1.21}$$

where we used the Fourier transformation and the Plancherel's equality to justify the second equality. Here $\boldsymbol{k}$ is a wave vector of the Fourier transformation, $\hat{\boldsymbol{e}}(\boldsymbol{k})$ and $\hat{\boldsymbol{j}}(\boldsymbol{k})$ are the Fourier coefficients of the electrical and current fields respectively. Electrical field is a potential one

$$\boldsymbol{e} = -\nabla \phi. \tag{1.22}$$

Current field is divergence free ($\nabla \cdot \boldsymbol{j} = 0$); therefore one can introduce vector potential $\boldsymbol{A}$ such that

$$\boldsymbol{j} = \nabla \times \boldsymbol{A}, \tag{1.23}$$

where ($\times$) is a sign of vector product. Conditions (1.22) and (1.23) can be presented in terms of the Fourier images of these fields as

$$\hat{\boldsymbol{e(k)}} = -\boldsymbol{k}\hat{\phi(\boldsymbol{k})}, \qquad \hat{\boldsymbol{j(k)}} = \boldsymbol{k} \times \hat{\boldsymbol{A}}(\boldsymbol{k}). \tag{1.24}$$

Therefore

$$\hat{\boldsymbol{e(k)}} \cdot \hat{\boldsymbol{j(k)}} = \phi(\boldsymbol{k})\boldsymbol{k} \cdot \boldsymbol{k} \times \hat{\boldsymbol{A}}(\boldsymbol{k}) = 0. \tag{1.25}$$

Let define the effective properties tensor via energy relationship (1.19). Substituting (1.19), (1.25) into (1.21) we arrive at the relation

$$\boldsymbol{e}_0 \cdot \boldsymbol{\Sigma}_0 \cdot \boldsymbol{e}_0 = \boldsymbol{e}_0 \cdot \boldsymbol{j}_0 \tag{1.26}$$

that is valid for any field $\boldsymbol{e}_0$. Therefore $\boldsymbol{j}_0 = \boldsymbol{\Sigma}_0 \cdot \boldsymbol{e}_0$ as it is stated by (1.10); thus we proved the equivalence of two definitions.

1.4 Examples of calculations of the effective moduli of some particular structures

For the most of the structures the effective properties can be calculated only numerically because the boundary value problems (that are needed to be solved to find these moduli) can be solved only numerically. But there exist a limited number of special classes of composites that allow the analytical calculation of the properties, these composites are of special interest and we study them in more details.

1.4.1 Laminate composite.

Let us assume that the component materials are laminated in a proportions m_1 and m_2 and let denote the ort in the direction of lamination as $\boldsymbol{n}$, and the ort along the laminate as $\boldsymbol{t}$, see Figure 2.

Figure 2: laminate composite of two phases.

To calculate the effective properties let put this composite into the homogeneous external field $\boldsymbol{e}_0$. The local fields in the materials are peace-wise constant in this case, namely

$$\boldsymbol{e}(\boldsymbol{x}) = \boldsymbol{e}_1\chi_1(\boldsymbol{x}) + \boldsymbol{e}_2\chi_2(\boldsymbol{x}), \quad \boldsymbol{j}(\boldsymbol{x}) = \boldsymbol{j}_1\chi_1(\boldsymbol{x}) + \boldsymbol{j}_2\chi_2(\boldsymbol{x}) \tag{1.27}$$

Now the average fields are calculated as

$$\boldsymbol{e}_0 = m_1\boldsymbol{e}_1 + m_2\boldsymbol{e}_2, \quad \boldsymbol{j}_0 = m_1\boldsymbol{j}_1 + m_2\boldsymbol{j}_2. \tag{1.28}$$

Due to the differential restriction on the electrical and current fields the following jump conditions should be satisfied on the boundary of the layers

$$(\boldsymbol{e}_1 - \boldsymbol{e}_2)\cdot\boldsymbol{t} = 0, \quad (\boldsymbol{j}_1 - \boldsymbol{j}_2)\cdot\boldsymbol{n} = 0. \tag{1.29}$$

Therefore, by taking into account the jump conditions (1.29) for the electrical field we get

$$\boldsymbol{e}_1 = \boldsymbol{e}_0 + e'\boldsymbol{n}, \quad \boldsymbol{e}_2 = \boldsymbol{e}_0 - \frac{m_1}{m_2}e'\boldsymbol{n}, \tag{1.30}$$

where e' is some scalar constant. Note also that

$$\boldsymbol{j}_1 = \boldsymbol{\Sigma}_1\cdot\boldsymbol{e}_1, \quad \boldsymbol{j}_2 = \boldsymbol{\Sigma}_2\cdot\boldsymbol{e}_2. \tag{1.31}$$

Let assume now that the field $\boldsymbol{e}_0$ is given and let calculate $\boldsymbol{j}_0$. The following equalities are obvious consequences of (1.30)-(1.31)

$$\boldsymbol{j}_0 = m_1\boldsymbol{j}_1 + m_2\boldsymbol{j}_2 = m_1\boldsymbol{\Sigma}_1\cdot\boldsymbol{e}_1 + m_2\boldsymbol{\Sigma}_2\cdot\boldsymbol{e}_2 = (m_1\boldsymbol{\Sigma}_1 + m_2\boldsymbol{\Sigma}_2)\boldsymbol{e}_0 + m_1e'(\boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_2)\cdot\boldsymbol{n} \tag{1.32}$$

The constant e' can be found from jump conditions (1.29) for the current field. Namely, from the equations (1.30) -(1.31) we get

$$\boldsymbol{j}_1 - \boldsymbol{j}_2 = (\boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_2)\cdot\boldsymbol{e}_0 + \frac{e'}{m_2}(m_2\boldsymbol{\Sigma}_1 + m_1\boldsymbol{\Sigma}_2)\cdot\boldsymbol{n} \tag{1.33}$$

Projecting (1.33) on the direction $\boldsymbol{n}$ we obtain

$$e' = -m_2[\boldsymbol{n} \cdot (m_2\boldsymbol{\Sigma}_1 + m_1\boldsymbol{\Sigma}_2) \cdot \boldsymbol{n}]^{-1}\boldsymbol{n} \cdot (\boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_2) \cdot \boldsymbol{e}_0 \tag{1.34}$$

Combining (1.32) and (1.34) we get the result

$$\boldsymbol{j}_0 = \boldsymbol{\Sigma}_0 \cdot \boldsymbol{e}_0, \tag{1.35}$$

where

$$\boldsymbol{\Sigma}_0 = (m_1\boldsymbol{\Sigma}_1 + m_2\boldsymbol{\Sigma}_2) - m_1m_2(\boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_2) \cdot \boldsymbol{n}[\boldsymbol{n} \cdot (m_2\boldsymbol{\Sigma}_1 + m_1\boldsymbol{\Sigma}_2) \cdot \boldsymbol{n}]^{-1}\boldsymbol{n} \cdot (\boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_2) \tag{1.36}$$

In a more general setting for the state law

$$\boldsymbol{J} = \boldsymbol{D} \cdot \boldsymbol{E} \tag{1.37}$$

with the jump conditions on the boundary with the normal $\boldsymbol{n}$

$$\boldsymbol{P}(\boldsymbol{n}) \cdot (\boldsymbol{E}_1 - \boldsymbol{E}_2) = 0, \qquad \boldsymbol{P}_\perp(\boldsymbol{n}) \cdot (\boldsymbol{J}_1 - \boldsymbol{J}_2) = 0 \tag{1.38}$$

we obtain

$$\boldsymbol{D}_0 = m_1\boldsymbol{D}_1 + m_2\boldsymbol{D}_2 - \tag{1.39}$$

$$-m_1m_2(\boldsymbol{D}_1 - \boldsymbol{D}_2) \cdot \boldsymbol{P}_\perp(n)[\boldsymbol{P}_\perp(\boldsymbol{n}) \cdot (m_2\boldsymbol{D}_1 + m_1\boldsymbol{D}_2) \cdot \boldsymbol{P}_\perp(\boldsymbol{n})]^{-1}\boldsymbol{P}_\perp(\boldsymbol{n}) \cdot (\boldsymbol{D}_1 - \boldsymbol{D}_2). \tag{1.40}$$

Here $\boldsymbol{P}_\perp(\boldsymbol{n})$ is a projector operator on the subspace of the discontinuous components of the vector $\boldsymbol{E}$ on the boundary with the normal $\boldsymbol{n}$.

The derivation is literally the same. We just need to use more general projection operator and more general definition of the convolution $(\cdot)$.

1.4.2 Hashin structures

The other example of the structures whose effective moduli can be computed analytically was suggested by Hashin and used by Hashin and Shtrikman in order to prove the attainability of the bound on the effective properties of a composite. They study the following process. Let put into the space filled by the conducting material with the properties σ_0 an inclusions consisting of a core of the material σ_1 and surrounded by the sphere of the material σ_2, see Figure 3.

Figure 3: Hashin-Shtrikman construction.

Let put this construction into the homogeneous on infinity electrical field $\boldsymbol{e}_0$. In the polar coordinates we look for the solution of the conductivity problem in a form

$$\phi_1 = a_1 r \cos\alpha, \quad \text{in the core,} \tag{1.41}$$
$$\phi_2 = (a_2 r + b_2/r^2)\cos\alpha, \quad \text{in the coating,} \tag{1.42}$$
$$\phi_0 = a_0 r \cos\alpha, \quad \text{in the medium,} \tag{1.43}$$

where r is a radial coordinate $r = \sqrt{\boldsymbol{x}\cdot\boldsymbol{x}}$, α is an angle between the direction of the applied field $\boldsymbol{v}$ and radius vector $\boldsymbol{x}$. The electrical and current fields in this case expressed as

$$\boldsymbol{e}_1 = -\nabla\phi_1 = -a_1\boldsymbol{v} = -a_1[\cos\alpha\boldsymbol{v}_r - \sin\alpha\boldsymbol{v}_\alpha], \tag{1.44}$$
$$\boldsymbol{j}_1 = \sigma_1\boldsymbol{e}_1 = -\sigma_1 a_1[\cos\alpha\boldsymbol{v}_r - \sin\alpha\boldsymbol{v}_\alpha], \tag{1.45}$$
$$\boldsymbol{e}_2 = -\nabla\phi_2 = -[a_2 - 2b_2/r^3]\cos\alpha\boldsymbol{v}_r + [a_2 + b_2/r^3]\sin\alpha\boldsymbol{v}_\alpha], \tag{1.46}$$
$$\boldsymbol{j}_2 = \sigma_2\boldsymbol{e}_2 = -\sigma_2[a_2 - 2b_2/r^3]\cos\alpha\boldsymbol{v}_r + \sigma_2[a_2 + b_2/r^3]\sin\alpha\boldsymbol{v}_\alpha], \tag{1.47}$$
$$\boldsymbol{e}_0 = -\nabla\phi_0 = -a_0\boldsymbol{v} = -a_0[\cos\alpha\boldsymbol{v}_r - \sin\alpha\boldsymbol{v}_\alpha], \tag{1.48}$$
$$\boldsymbol{j}_0 = \sigma_0\boldsymbol{e}_0 = -\sigma_0 a_0[\cos\alpha\boldsymbol{v}_r - \sin\alpha\boldsymbol{v}_\alpha], \tag{1.49}$$

where $\boldsymbol{v}_r$ and $\boldsymbol{v}_\alpha$ are the unit radial and tangential vectors in terms of which $\boldsymbol{v} = \cos\alpha\boldsymbol{v}_r - \sin\alpha\boldsymbol{v}_\alpha$. These potentials satisfy the conductivity equations in each of the regions. We only need to find the constant to satisfy the jump conditions on the interface of these regions. Continuity of the potential leads to the conditions

$$a_1 = a_2 + b_2/r_1^3, \qquad a_0 = a_2 + b_2/r_2^3 \tag{1.50}$$

Jump conditions on the current field give

$$\sigma_1 a_1 = \sigma_2[a_2 - b_2/r_1^3], \qquad \sigma_0 a_0 = \sigma_2[a_2 - 2b_2/r_2^3]. \tag{1.51}$$

By substituting (1.50) into (1.51) we arrive at the system of equations

$$a_2 = -b_2[\sigma_1 + 2\sigma_2]/[r_1^3(\sigma_1 - \sigma_2)] = -b_2[1 + 3\sigma_2/(\sigma_1 - \sigma_2)]/r_1^3 \tag{1.52}$$
$$a_2 = -b_2[\sigma_0 + 2\sigma_2]/[r_2^3(\sigma_0 - \sigma_2)] = -b_2[1 + 3\sigma_2/(\sigma_0 - \sigma_2)]/r_2^3. \tag{1.53}$$

From these equations we deduce that

$$\frac{1}{\sigma_0 - \sigma_2} = \frac{1}{m_1}\frac{1}{\sigma_1 - \sigma_2} + \frac{m_2}{3m_1\sigma_2}, \tag{1.54}$$

where

$$m_1 = 1 - m_2 = r_1^3/r_2^3, \tag{1.55}$$

m_1 and m_2 are the volume fractions of the materials in the inclusion. If the constant σ_0 satisfies the relation (1.54) the solution of the conductivity problem for the described geometry is given by (1.41)-(1.43). As we see, the field outside the inclusion is exactly the same as it would be without it. It means that we can put the other inclusions in the space without changing the average electrical field. Let fill all the space by such inclusions (we need infinitely many scales of the inclusion's sizes to do it). Resulting medium possesses the effective conductivity constant σ_0. It consists of the materials σ_1 and σ_2 taken in the proportions m_1 and m_2.

We can do the same for the two-dimensional conductivity, the result is given be the relation

$$\frac{1}{\sigma_0 - \sigma_2} = \frac{1}{m_1}\frac{1}{\sigma_1 - \sigma_2} + \frac{m_2}{2m_1\sigma_2}. \tag{1.56}$$

Let denote the conductivity of such a medium as $\sigma_{HS}^2 = \sigma_0$ Changing the order of the materials in a structure (i.e. studying the composite with inclusions consisting of the core of the second material surrounded by the first material) we obtain the other media with conductivity (in two dimensions)

$$\frac{1}{\sigma_{HS}^1 - \sigma_1} = \frac{1}{m_2}\frac{1}{\sigma_2 - \sigma_1} + \frac{m_1}{2m_2\sigma_1} \tag{1.57}$$

As we will see later, conductivity σ_0 of any isotropic composite lies between these values

$$\sigma_0 \in [\sigma_{HS}^1, \sigma_{HS}^2] \tag{1.58}$$

1.5 Conclusions

As we see, the effective properties of the composite depend on the properties of component materials, their volume fractions in the composite, but also depend very strongly on the microstructure. When the microstructure is known the properties of the composite can be computed. We face absolutely different situation when we know a little or nothing about the microstructure of the material but are interested in their effective moduli. Such problems often arise in optimal design of composite materials when we want to create the composite that is the best according to some optimality criteria In this situation the microstructure is unknown, it needs to be determined. But some *a-priory* information that does not depend on the structure would be helpful and desirable. We address this kind of problems in the next lecture.

1.6 References

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2 Bounds on the effective properties of composite materials

As we saw, the effective moduli of the composite strongly depend on their microstructure. To illustrate it let study the example of the two-dimensional conductivity problem. For such a case the tensor of effective properties is a second order tensor that can be completely characterized by two rotationally invariant parameters, namely, by their eigenvalues λ_1 and λ_2, and by the orientation ϕ. The space of invariant characteristic is two-dimensional and can be easily illustrated, see Figure 4.

Figure 4. Plane of invariants of conductivity matrices in two dimensions.

Let us put on this plane the effective properties of the structures that we calculated at the last lecture. Let rewrite the formula for the effective conductivity of laminate material in the basis that is connected with the normal $\boldsymbol{n}$ to the laminates. We get

$$\lambda_1 = \sigma_h = (m_1/\sigma_1 + m_2/\sigma_2)^{-1}, \quad \lambda_2 = \sigma_a = m_1\sigma_1 + m_2\sigma_2 \tag{2.1}$$

Points A and B on the Figure 3 correspond to the laminate composites with the normal to layers $\boldsymbol{n}$ oriented along and perpendicular to the direction of the x_1 axis, respectively. Note, that the diagonal of the first sector (see Figure 4) is the axis of symmetry for the picture, because we always may rotate composite possessing the eigenvalues (λ_1, λ_2) and get the material with the pair of eigenvalues (λ_2, λ_1). Points C and D correspond to the Hashin-Shtrikman assemblages of coated circles. They differ by the order of the materials: for the more conducting one (with the higher conductivity) the inclusion consists of the core of the less conducting material surrounded by the circle of more conducting material and vise-versa for the other point. All these media were composed from the same amounts of the same component materials, but the effective properties of these media are absolutely different. The only reason is the difference in the microstructure. Arbitrary composite corresponds to some point G in the plane (λ_1, λ_2). The question arises how far can we change the properties by changing the microstructure of a composite, how large is the region in the space of invariants of the effective properties tensors that corresponds to some composite materials. Let me give two definitions that are essential:

Definitions:

1. $\boldsymbol{G_m}$ **-closure**: Let assume that we have in our disposal the set $\{U\}$ of the component materials. The set of the effective properties tensors of the composites combined from the *given amounts* of the component materials is called the G_m-closure of the set U

and is denoted as G_mU-set.

$$G_mU = \cup_{\chi_i(x):<\chi_i(x)>=m_i} \boldsymbol{D}_0(\chi_i(x)) \tag{2.2}$$

The union of all such G_mU sets over the volume fractions m_i is called G-closure of the set U and is denoted as GU

$$G_U = \cup_{m_i} G_mU, \tag{2.3}$$

see Figure 4 for the conductivity example.

In the other words, ***G*-closure** or ***GU*-set** is the set of the effective properties of all the composites that can be prepared from *arbitrary amounts* of the component materials.

Knowledge of these sets is important for many reasons. They provide a benchmark for testing experimental results and approximation theories, and can provide an indicator as to whether the average response of a given composite is extreme in the sense of being close to the edge of these sets. There exists a simple way (2.3) to find G-closure if we know the G_m-closure set. Therefore we concentrate our attention on the problem of finding G_m-closure.

There is no direct and straightforward way (at least it is not known) to find G_mU set. The way how people do it is the following:

1. First one need to construct the bounds on the effective properties of composites that do not depend on microstructure. They depend on the properties of component materials, their volume fractions, but do not depend on the details of the microstructure. They are valid for a composite material of any structure with fixed volume fractions of the components. In the space of invariants of the effective properties tensors they define the set P_mU such that

$$G_mU \subset P_mU. \tag{2.4}$$

2. Then one can look for the set of the effective properties tensors of a particular structures combined from given component materials (laminate composite, laminate composite of laminate composite, Hashin-Shtrikman - type structures etc.) to define the set L_mU such that

$$L_mU \subset G_mU. \tag{2.5}$$

It gives the bound of the G_mU-set from inside. If both bounds coincide it allows us to define G_mU itself;

$$\text{If} \quad L_mU = P_mU, \quad \text{then} \quad L_mU = G_mU = P_mU. \tag{2.6}$$

The goal of our course is to describe the method for constructing geometrically independent bounds on the effective properties of a composite, i.e. the method to find the P_mU-set. We also describe the microgeometries that are candidates to be optimal, i.e. that are extremal in the sense that they correspond to the bounds of the G-sets. It is now recognized that optimal bounds are important in the context of structural optimization: the microstructures that achieve the bounds are often the best candidates for use in the design of a structure.

There exist just few examples where the whole G or G_m sets are known. They include the bounds on the conductivity tensor of two- and three-dimensional two-phase composite, bounds on effective complex conductivity for two-phase two-dimensional composite, coupled problem of two second order diffusion equations for two-dimensional two-component composite. There are much more problems for which some bounds on the properties are known, there exist the composites that correspond to some parts of bounds, but there are no such structures for some other parts of the boundary. Among such examples are three-dimensional two-phase complex-conducting composites, elastic composite, bounds on the effective properties for three-phase composites, etc. Now we are going to discuss the method of constructing geometrically independent bounds on the effective properties of composite materials.

2.1 Bounds on the effective properties tensor

For a long time people tried to suggest different approximations for the effective moduli of the mixtures. Voigt suggested the arithmetic mean

$$\boldsymbol{D}_0 = < \boldsymbol{D}(x) > = \sum_i m_i \boldsymbol{D}_i \tag{2.7}$$

as a good approximation for the effective properties. The other approximation was suggested by Reuss who proposed the harmonic mean expression for the effective moduli of a composite

$$\boldsymbol{D}_0 = < \boldsymbol{D}^{-1}(x) >^{-1} = [\sum_i m_i \boldsymbol{D}_i^{-1}]^{-1} \tag{2.8}$$

Wiener proved that (2.7) and (2.8) are actually the upper and low bounds on the effective moduli of the mixture. These bounds are now known as Reuss-Voigt bounds or, in the context of elasticity, as Hill's bounds

$$< \boldsymbol{D}^{-1}(x) >^{-1} \quad \leq \quad \boldsymbol{D}_0 \quad \leq \quad < \boldsymbol{D}(x) > \tag{2.9}$$

Remark: We say that $\boldsymbol{A} \geq \boldsymbol{B}$ *if the difference of these two tensors* $\boldsymbol{C} = \boldsymbol{A} - \boldsymbol{B}$ *is positive semidefinite tensor , i.e. all the eigenvalues of this tensor* $\boldsymbol{C}$ *are greater or equal to zero.*

Note that for the conductivity case these bounds are exact in a sense that there exists a composite (namely, laminate composite) that has one eigenvalue (across the laminate) equal to the harmonic mean of the component conductivities whereas the other ones are equal to the arithmetic mean of phases conductivities. So, in the Figure 4 these bounds form the square that contains $G_m U$ set and this square is the minimal one because two corner points of it correspond to the laminate composites.

Now I'd like to show how to prove these bounds, because it is the key point of the following discussion.

2.2 Proof of the Reuss-Voigt-Wiener bounds.

To prove the bounds one can start with the variational definition of the effective properties. Namely, we have

$$\boldsymbol{e}_0 \cdot \boldsymbol{D}_0 \cdot \boldsymbol{e}_0 = \inf_{\boldsymbol{e}=\nabla\phi, <\boldsymbol{e}>=\boldsymbol{e}_0} < \boldsymbol{e} \cdot \boldsymbol{D} \cdot \boldsymbol{e} > . \tag{2.10}$$

By substituting the constant field $\boldsymbol{e}(x) = \boldsymbol{e}_0$ into the right hand side of the equation (2.10) we get

$$\boldsymbol{e}_0 \cdot \boldsymbol{D}_0 \cdot \boldsymbol{e}_0 \quad \leq \quad <\boldsymbol{e}_0 \cdot \boldsymbol{D} \cdot \boldsymbol{e}_0> \quad = \quad \boldsymbol{e}_0 \cdot <\boldsymbol{D}> \cdot \boldsymbol{e}_0. \tag{2.11}$$

These arguments are valid for any value of the average field $\boldsymbol{e}_0$. Therefore we can deduce the inequality for the matrices

$$\boldsymbol{D}_0 \quad \leq \quad <\boldsymbol{D}> \tag{2.12}$$

from the inequality (2.11) for the quadratic forms. Similarly,

$$\boldsymbol{j}_0 \cdot \boldsymbol{D}_0^{-1} \cdot \boldsymbol{j}_0 = \inf_{\boldsymbol{j}:\nabla\cdot\boldsymbol{j}=0,<\boldsymbol{j}>=\boldsymbol{j}_0} <\boldsymbol{j} \cdot \boldsymbol{D}^{-1} \cdot \boldsymbol{j}> \quad \leq \quad <\boldsymbol{j}_0 \cdot \boldsymbol{D}^{-1} \cdot \boldsymbol{j}_0> \quad = \quad \boldsymbol{j}_0 \cdot <\boldsymbol{D}^{-1}> \cdot \boldsymbol{j}_0, \tag{2.13}$$

and therefore

$$\boldsymbol{D}_0^{-1} \quad \leq \quad <\boldsymbol{D}^{-1}>. \tag{2.14}$$

Reuss bound follows immediately from this statement.

As we see the procedure is based on the assumption that either electrical or current field is constant throughout the composite. It may be true for some structures and some fields, as we will see. In that situations the bounds are exact in a sense that there exists a composite that has the effective properties tensor that corresponds to the equality in the expressions (2.9) .

2. Variational proof.

The other proof (that is not so elementary but more useful for us because it can be improved in order to receive more restrictive bounds) is the following. As earlier we start with the variational definition of the effective properties tensor but now we construct the bound by omitting the differential restrictions $\boldsymbol{e} = -\nabla\phi$ on the fields. Namely,

$$\boldsymbol{e}_0 \cdot \boldsymbol{D}_0 \cdot \boldsymbol{e}_0 = \inf_{\boldsymbol{e}:\boldsymbol{e}=\nabla\phi,<\boldsymbol{e}>=\boldsymbol{e}_0} <\boldsymbol{e} \cdot \boldsymbol{D} \cdot \boldsymbol{e}> \quad \geq \quad \inf_{\boldsymbol{e}:<\boldsymbol{e}>=\boldsymbol{e}_0} <\boldsymbol{e} \cdot \boldsymbol{D} \cdot \boldsymbol{e}>. \tag{2.15}$$

Note, that when we drop off the differential restriction we decrease the value of the functional. The last problem is the standard problem of calculus of variations and can be easily solved. The main idea is that we drop of the local (i.e. point-wise) restrictions that we can not investigate, but save the integral restrictions that are easy to handle. Let take into account the remaining restriction by vector Lagrange multiplier $\boldsymbol{\gamma}$

$$\inf_{\boldsymbol{e}:<\boldsymbol{e}>=\boldsymbol{e}_0} <\boldsymbol{e} \cdot \boldsymbol{D} \cdot \boldsymbol{e}> = \sup_{\gamma} \inf_{e} <\boldsymbol{e} \cdot \boldsymbol{D} \cdot \boldsymbol{e} + 2\boldsymbol{\gamma} \cdot (\boldsymbol{e} - \boldsymbol{e}_0)> \tag{2.16}$$

Stationary conditions lead to the equations

$$2\boldsymbol{D} \cdot \boldsymbol{e} + 2\boldsymbol{\gamma} = 0, \tag{2.17}$$

or

$$\boldsymbol{e} = -\boldsymbol{D}^{-1} \cdot \boldsymbol{\gamma}. \tag{2.18}$$

Note that the equation (2.17) requires the current field $\boldsymbol{j} = \boldsymbol{D} \cdot \boldsymbol{e}$ to be constant throughout the composite. Here the constant vector parameter $\boldsymbol{\gamma}$ can be found from the restriction $<\boldsymbol{e}>= \boldsymbol{e}_0$, namely

$$\boldsymbol{\gamma} = - <\boldsymbol{D}^{-1}>^{-1} \cdot \boldsymbol{e}_0 \tag{2.19}$$

By substituting (2.18), (2.19) into (2.15) we get

$$
\begin{aligned}
<\boldsymbol{e}\cdot\boldsymbol{D}\cdot\boldsymbol{e}> \quad &= \quad <\boldsymbol{e}_0\cdot <\boldsymbol{D}^{-1}>^{-1}\cdot\boldsymbol{D}^{-1}\cdot\boldsymbol{D}\cdot\boldsymbol{D}^{-1}\cdot <\boldsymbol{D}^{-1}>^{-1}\cdot\boldsymbol{e}_0> \\
&= \quad \boldsymbol{e}_0\cdot <\boldsymbol{D}^{-1}>^{-1}\cdot\boldsymbol{e}_0 \qquad (2.20)
\end{aligned}
$$

that proves the Reuss bound. Note that the condition

$$\boldsymbol{D}(\boldsymbol{x}) \geq 0, \tag{2.21}$$

is required in order for the stationary solution of the problem to be a minimum of the functional. This condition for the two-phase composite can be rewritten as

$$\boldsymbol{D}_1 \geq 0, \qquad \boldsymbol{D}_2 \geq 0. \tag{2.22}$$

It will be essential in a future for the procedure of improving of Reuss-Voigt bounds.

Similarly, one can get Voigt bounds starting from the variational principle in terms of the current fields.

As we see, any information about the microstructure of the composite disappears from the problem when we drop off the differential restrictions on the fields like $\boldsymbol{e} = -\nabla\phi$. So, the key idea to improve the bound is to take these differential restrictions into account by some way. We concentrate our attention on so called translation method that use the integral corollaries of the differential restriction to improve the Reuss-Voigt bounds, but before I'd like to mention very briefly the other methods that can be used to obtain the bounds on the effective properties.

1. Hashin-Shtrikman method was suggested by the authors in 1962 when they assumed the isotropy of the composite and found the bounds on the effective conductivity and on the bulk and shear moduli of elastic composites. This method was reformulated for the anisotropic materials later by Avellaneda, Kohn, Lipton, and Milton and the bounds that can be obtained by this method are proved to be equivalent to the translation bounds for some special choice of the parameters. Whereas Reuss-Voigt bounds require one of the fields to be constant throughout the composite, this method requires the constant field only in one of the phases and allows fluctuations of the fields in the others components.

2. Analytical method (see Bergman, Milton) is based on the analytic properties of the effective conductivity as a function $\sigma_0 = \sigma_0(\sigma_1, \sigma_2)$ of the two component conductivities. In fact, because this is a homogeneous function it suffices to set one of the component conductivities equal to 1 and to study the effective conductivity as a function of the remaining component conductivity $\sigma_0 = \sigma_1\sigma_0(1, \sigma_2/\sigma_1)$. The resulting function of one complex variable is essentially a so called Stieltjes function and many of the bounds on the complex effective conductivity correspond to bounds on this Stieltjes function. This method has an advantage of being able to handle complex moduli case, but it is difficult to generalize it to more general problems because it requires studying of analytic functions of several variables. This theory is not too developed to be used for the construction of the bounds.

3. Translation method was suggested in different but close forms by Murat & Tartar and Lurie & Cherkaev around ten years ago. The main idea of the translation method

is to bound the functional (2.10) (and therefore the effective tensor $\boldsymbol{D}_0$) by taking into account the differential restrictions

$$\boldsymbol{e} = -\nabla\phi \tag{2.23}$$

through their integral corollaries

$$\langle \mathbf{e} \cdot \boldsymbol{T}\mathbf{e} \rangle \quad \geq \quad \langle \mathbf{e} \rangle \cdot \boldsymbol{T} \langle \mathbf{e} \rangle, \tag{2.24}$$

which are hold for every field $\mathbf{e}$ satisfying (2.23) for some special choices of the matrix $\boldsymbol{T}$. Here $\boldsymbol{T}$ is the so called translation matrix which may possess several free parameters. The choice of this matrix is dictated by the differential properties (2.23) of the field $\boldsymbol{e}$. Functions that possess properties similar to (2.24) under averaging are called quasiconvex functions. For a general discussion of quasiconvexity and methods for finding quadratic quasiconvex function see, for example, Tartar, Ball, and Dacorogna.

We discuss this method in details in the next lecture.

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3 The translation method to bound the effective moduli of composites.

The translation method is based on the variational definition of the effective properties and on bounds on some energy type functionals. It consists of several well-formulated steps, namely

1. choosing appropriate functionals to study;
2. studying the differential properties of the phase variables in order to define quadratic quasiconvex functions.
3. finding the lower bounds for these functionals by using existence of the quasiconvex quadratic forms; finding the bounds on effective properties tensor by using the bounds for the functionals;
4. checking the attainability of the bounds by examining particular microstructures.

We discuss first three steps in this and in the next lecture, last lecture of the course is devoted to the description of optimal structures.

3.1 Choosing appropriate functionals.

Let start with figure similar to the Figure 4 that was discussed during the previous lecture.

Figure 5: Construction of the functionals that give the bound for the G_mU set for the conductivity problem.

It shows approximate form of the G_mU set for the conductivity problem. Let study what kind of functionals we need to estimate in order to obtain the desired bound for the

G_mU set. Let minimize (over all microstructures, i.e. over all characteristic functions χ_i) the energy stored by the composite in the homogeneous external field $\boldsymbol{e}_{01}$

$$W_{01} = \inf_{\chi_i : <\chi_i(\boldsymbol{x})> = m_i} \boldsymbol{e}_{01} \cdot \boldsymbol{D}_0(\chi_i) \cdot \boldsymbol{e}_{01}. \tag{3.1}$$

We find out first, that it is optimal to rotate composite so that the minimal conductivity direction be oriented along the vector $\boldsymbol{e}_{01}$. In fact, the structure tries to minimize the lowest eigenvalue because

$$W_{01} = \inf_{\chi_i : <\chi_i(\boldsymbol{x})> = m_i} \lambda_{min}(\chi_i) \boldsymbol{e}_{01} \cdot \boldsymbol{e}_{01} \tag{3.2}$$

It means that the optimal composite corresponds to the corner point of the set G_mU, see Figure 5, say to the point A if the direction $\boldsymbol{e}_{01}$ coincides with the axis λ_1. As we see, this functional reflects only properties of the medium in the direction of the applied field $\boldsymbol{e}_{01}$ and can not "feel" the properties in the orthogonal direction. Let now minimize the energy stored by the composite placed into the external field $\boldsymbol{e}_{02}$ that is orthogonal to $\boldsymbol{e}_{01}$

$$W_{02} = \inf_{\chi_i : <\chi_i(\boldsymbol{x})> = m_i} \boldsymbol{e}_{02} \cdot \boldsymbol{D}_0(\chi_i) \cdot \boldsymbol{e}_{02} \tag{3.3}$$

The optimal composite (that gives a solution to the problem (3.3)) corresponds to the points B on the Figure 5 and possesses the minimal conductivity direction λ_2 oriented along the vector $\boldsymbol{e}_{02}$. As we see, by bounding the functionals W_{01} and W_{02} we can only bound the minimal eigenvalue of the conductivity matrix that corresponds to the Reuss bounds. We can bound the eigenvalues of the conductivity matrix only independently. It happens because the functional of the type (3.2)-(3.3) reflects the properties of the medium only in one particular direction. In order to take into account the properties of the composite in the other direction we may combine the above two functionals and study the quadratic form

$$\begin{aligned} W_e = W_{01} + W_{02} &= \inf_{\chi_i : <\chi_i(\boldsymbol{x})> = m_i} [\boldsymbol{e}_{01} \cdot \boldsymbol{D}_0(\chi_i) \cdot \boldsymbol{e}_{01} + \boldsymbol{e}_{02} \cdot \boldsymbol{D}_0(\chi_i) \cdot \boldsymbol{e}_{02}] \\ &= \inf_{\chi_i : <\chi_i(\boldsymbol{x})> = m_i} [\lambda_1(\chi_i) \boldsymbol{e}_{01} \cdot \boldsymbol{e}_{01} + \lambda_2(\chi_i) \boldsymbol{e}_{02} \cdot \boldsymbol{e}_{02}] \end{aligned} \tag{3.4}$$

This functional is a weighted sum of the eigenvalues. In order to minimize such functional the composite has to minimize the sum of its eigenvalues. Bound for this functional shows how far can we move the point that corresponds to the effective properties of the composite in the direction of arrow on the Figure 5. They define the position of the straight line that is tangential to the set $P_mU : \ G_mU \in P_mU$. Changing the "weights" of each eigenvalue (by changing an amplitude of the vectors $\boldsymbol{e}_{01}$ and $\boldsymbol{e}_{02}$) we change this direction within the third sector as it is shown in the Figure 5. As we see, one can construct the lower bound of the set G_mU for the two-dimensional conducting composite by bounding the functional (3.4). In the three dimensional space we need to study also the functional that is the sum of three terms. Each of these terms is an energy stored by the composite in the homogeneous external field. These three fields should be orthogonal to each other in order for the functional to reflect the properties of the medium in three orthogonal directions. In order to find the upper bound we need to construct an energy type functional that "move" the composite in the direction toward the upper bound, namely

$$W_j = W_{01} + W_{02} = \inf_{\chi_i: <\chi_i(\boldsymbol{x})>=m_i} [\boldsymbol{j}_{01} \cdot \boldsymbol{D}_0^{-1}(\chi_i) \cdot \boldsymbol{j}_{01} + \boldsymbol{j}_{02} \cdot \boldsymbol{D}_0^{-1}(\chi_i) \cdot \boldsymbol{j}_{02}]$$
$$= \inf_{\chi_i: <\chi_i(\boldsymbol{x})>=m_i} [\lambda_1^{-1}(\chi_i) \boldsymbol{j}_{01} \cdot \boldsymbol{j}_{01} + \lambda_2^{-1}(\chi_i) \boldsymbol{j}_{02} \cdot \boldsymbol{j}_{02}] \tag{3.5}$$

By using similar arguments one can define the functionals to be minimized for any specific problem under study. The key idea is the following: to find the bound one need to find the energy type functional that achieves its minimum on the boundary that one is looking for.

3.2 Formulation of the variational problem and specific features of this problem.

Now we want to transform the functional under study into some standard form and to study the properties of the resulting variational problem. Let us do it on the example of the functional W_e. By using the variational definition of the effective properties tensor we can rewrite (3.4) as

$$W_e = \inf_{\chi_i:\ \chi_i=m_i} \ \inf_{\substack{\boldsymbol{e}_1 :\, \boldsymbol{e}_1 = \nabla\phi_1, \\ <\boldsymbol{e}_1>=\boldsymbol{e}_{01}}} \ \inf_{\substack{\boldsymbol{e}_2 :\, \boldsymbol{e}_2 = \nabla\phi_2, \\ <\boldsymbol{e}_2>=\boldsymbol{e}_{02}}} < \boldsymbol{e}_1 \cdot \boldsymbol{D}(\chi_i) \cdot \boldsymbol{e}_1 + \boldsymbol{e}_2 \cdot \boldsymbol{D}(\chi_i) \cdot \boldsymbol{e}_2 > . \tag{3.6}$$

It is a quadratic form that can be rewritten as

$$W_e = W = \inf_{\chi_i:\ \chi_i(\boldsymbol{x})=m_i} \ \inf_{\boldsymbol{E}: <\boldsymbol{E}>=\boldsymbol{E}_0, \boldsymbol{E} \in EK} < \boldsymbol{E} \cdot \boldsymbol{\mathcal{D}}(\chi_i) \cdot \boldsymbol{E} >, \tag{3.7}$$

where $\boldsymbol{E}$ is a vector of phase variables, $\boldsymbol{E} = (\boldsymbol{e}_1, \boldsymbol{e}_2)$ in this example, EK is the set of admissible vector fields $\boldsymbol{E}$

$$EK = \{\boldsymbol{E} :\ \boldsymbol{E}(\boldsymbol{x}) \ \text{ is S} - \text{periodic and satisfy some differential restrictions}\}, \tag{3.8}$$

and $\boldsymbol{\mathcal{D}}$ is the block-diagonal matrix of properties

$$\boldsymbol{\mathcal{D}} = \begin{pmatrix} \boldsymbol{D} & 0 \\ 0 & \boldsymbol{D} \end{pmatrix} \tag{3.9}$$

in this example. The definition of the set EK includes the differential restrictions that depend on the particular problem. For the problem under study, the differential restrictions require for the first and the last two elements of the vector $\boldsymbol{E}$ to be gradients of some potentials, i.e.

$$EK_e = \{\boldsymbol{E} :\ \boldsymbol{E}(\boldsymbol{x}), \quad \boldsymbol{E} = (E_1, E_2, E_3, E_4) = (\boldsymbol{e}_1, \boldsymbol{e}_2), \quad \boldsymbol{e}_1 = -\nabla\phi_1, \quad \boldsymbol{e}_2 = -\nabla\phi_2\}. \tag{3.10}$$

Remark: The other functional W_j also can be presented in the same form where

$$\boldsymbol{E} = \boldsymbol{j}_1, \boldsymbol{j}_2, \qquad \boldsymbol{\mathcal{D}} = \begin{pmatrix} \boldsymbol{D}^{-1} & 0 \\ 0 & \boldsymbol{D}^{-1} \end{pmatrix}, \tag{3.11}$$

and

$$EK_j = \{\boldsymbol{E}: \ \boldsymbol{E} = (\boldsymbol{j}_1, \boldsymbol{j}_2), \quad \nabla \cdot \boldsymbol{j}_1 = 0, \quad \nabla \cdot \boldsymbol{j}_2 = 0\}. \tag{3.12}$$

We arrive at the variational problem with quadratic integrand. Note, that this problem is not a classical problem of calculus of variations because it contains differential restrictions that are local for the phase variable $\boldsymbol{E}$. The other specific feature is that the integrand of this problem is not a convex function. To see it we note that the set of the values of the tensor $\boldsymbol{\mathcal{D}}$ has only two values:

$$\boldsymbol{\mathcal{D}}(\boldsymbol{x}) = \boldsymbol{\mathcal{D}}_1\chi_1(\boldsymbol{x}) + \boldsymbol{\mathcal{D}}_1\chi_2(\boldsymbol{x}) \tag{3.13}$$

We can also check that the function $F(\boldsymbol{E}, \boldsymbol{\mathcal{D}}) = \boldsymbol{E} \cdot \boldsymbol{\mathcal{D}} \cdot \boldsymbol{E}$ is not convex as a function of several variables $\boldsymbol{E}$ and $\boldsymbol{\mathcal{D}}$. Let try to solve this problem in order to understand the difficulties that arise here. First, let us interchange the order of the infimums and take into account the restrictions on the functions χ_i by Lagrange multipliers γ_i.

$$\begin{aligned} W = \inf_{\chi_i:\ <\chi_i(\boldsymbol{x})>=m_i} \ \inf_{\substack{\boldsymbol{E}:<\boldsymbol{E}>=\boldsymbol{E}_0,\\ \boldsymbol{E}\in EK}} < \boldsymbol{E} \cdot \boldsymbol{\mathcal{D}}(\chi_i) \cdot E >= \\ \inf_{\substack{\boldsymbol{E}:<\boldsymbol{E}>=\boldsymbol{E}_0,\\ \boldsymbol{E}\in EK}} \max_{\gamma_i}\{ \ < \inf_{\chi_i} \ [\boldsymbol{E} \cdot \boldsymbol{\mathcal{D}}(\chi_i) \cdot \boldsymbol{E} + \gamma_i(\chi_i(\boldsymbol{x}) - m_i)] >= \\ \inf_{\substack{\boldsymbol{E}:<\boldsymbol{E}>=\boldsymbol{E}_0,\\ \boldsymbol{E}\in EK}} \max_{\gamma_i}\{< \min_i [\boldsymbol{E} \cdot \boldsymbol{\mathcal{D}}_i \cdot \boldsymbol{E} + \gamma_i] > -\gamma_i m_i\} \end{aligned} \tag{3.14}$$

The internal maximum over the Lagrange multiplies γ_i is not essential, because γ_i are just the parameters, one can handle this problem by using the standard arguments. The most difficult part is the solution of the minimization problem

$$\inf_{\substack{\boldsymbol{E}:<\boldsymbol{E}>=\boldsymbol{E}_0,\\ \boldsymbol{E}\in EK}} < W' >, \quad W' = \min_i [\boldsymbol{E} \cdot \boldsymbol{\mathcal{D}}_i \cdot \boldsymbol{E} + \gamma_i] \tag{3.15}$$

Figure 6 illustrates the integrand of this variational problem for the two-phase composite by a schematic picture. Each of the functions $W_i = \boldsymbol{E} \cdot \boldsymbol{\mathcal{D}}_i \cdot \boldsymbol{E} + \gamma_i$ is represented by a parabola that crosses the vertical axis at the point γ_i.

The result of the minimum over i is the nonconvex function W' that is highlighted in the Figure 6.

Figure 6: Energy minimization problem for two-phase composite material (a) and the schematic picture of the solution to this problem (b).

Let study the variational problem (3.15). First, drop off the differential restriction EK and find the function

$$CW(\boldsymbol{E}_0) = \inf_{\boldsymbol{E}:<\boldsymbol{E}>=\boldsymbol{E}_0} < W'(\boldsymbol{E}) > \tag{3.16}$$

We have already solved the similar problem while were proving the the Reuss-Voigt-Wiener bounds. The solution of the problem oscillates from the parabola representing the energy of the first material to the other parabola that corresponds to the second one in order to preserve the average value of the phase variable $\boldsymbol{E}$ and minimize the functional $CW(\boldsymbol{E}_0)$. The cell of periodicity is divided into two parts S_1 and S_2 in the proportions m_1 and m_2 (see Figure 6b), and $\boldsymbol{E} = \boldsymbol{E}_1$ when $\boldsymbol{x} \in S_1$, $\boldsymbol{E} = \boldsymbol{E}_2$ when $\boldsymbol{x} \in S_2$. The average values of the fields and the energy are given by

$$\boldsymbol{E}_0 = m_1\boldsymbol{E}_1 + m_2\boldsymbol{E}_2, \quad CW(\boldsymbol{E}_0) = m_1 W_1(\boldsymbol{E}_1) + m_2 W_2(\boldsymbol{E}_2), \tag{3.17}$$

The value $CW(\boldsymbol{E}_0)$ is clearly less than the value $W'(\boldsymbol{E}_0)$. It is clear from the picture that the value $CW(\boldsymbol{E}_0)$ is given by the convex envelope of the function W', straight line in the Figure 6 is tangential to the both parabolas W_1 and W_2. The volume fractions are defined by the values $\boldsymbol{E}_1$ and $\boldsymbol{E}_2$. For the one dimensional example where E is a scalar we have

$$m_1 = \frac{E_0 - E_1}{E_2 - E_1}, \quad m_2 = \frac{E_2 - E_0}{E_2 - E_1}, \tag{3.18}$$

The Lagrange multipliers γ_i are chosen to modify the function W' in order to satisfy the restrictions $< \chi_i >= m_1$.

The situation changes when we take into account the differential restrictions on the field $\boldsymbol{E} \in EK$. In this case the field $\boldsymbol{E}$ is no more arbitrary, there exist jump conditions on the boundary of the sets S_1 and S_2. For example, if the field $\boldsymbol{E}$ is a gradient of some potential then $(\boldsymbol{E}_1 - \boldsymbol{E}_2) \cdot \boldsymbol{t} = 0$, where $\boldsymbol{t}$ is the tangential vector to the boundary of the regions S_1 and S_2. If $\boldsymbol{E}$ is a current field, then $(\boldsymbol{E}_1 - \boldsymbol{E}_2) \cdot \boldsymbol{n} = 0$, where $\boldsymbol{n}$ is the normal vector to the boundary of S_1 and S_2, etc. In such a situation the values $\boldsymbol{E}_1$ and $\boldsymbol{E}_2$ are no more arbitrary. They satisfy the jump conditions and therefore depend on the form of the boundary, i.e. on functions χ_i. Therefore, the function $QW(\boldsymbol{E}_0)$

$$QW(\boldsymbol{E}_0) = \inf_{\boldsymbol{E}:<\boldsymbol{E}>=\boldsymbol{E}_0, \quad \boldsymbol{E} \in EK} < W' > \tag{3.19}$$

lies above the function $CW(\boldsymbol{E}_0)$, but below the function W'. This function is called a quasiconvex envelope of the function $W'(\boldsymbol{E}_0)$; it is a largest quasiconvex function that is less or equal to $W'(\boldsymbol{E}_0)$. We need to find the bounds on the function $QW(\boldsymbol{E}_0)$ in order to find the bound on the effective properties. The main problem is that there exists no general procedure like convexification to find such kind of function, i.e. to solve the variational problems like (3.19). We construct the bounds on the functional (3.19) by taking into account not the differential restrictions $\boldsymbol{e} \in EK$ themselves, but their integral corollaries.

3.3 Quasiconvex functions.

Let me introduce briefly some definitions and notations of so called quasiconvexity theory that is closely related to our problem under study.

1.Definition of quasiconvexity.

We start with the definition of convexity: The function $F(\boldsymbol{v})$ is called convex if

$$F(\boldsymbol{v}_0) \leq < F(\boldsymbol{v}_0 + \xi) > \quad \text{for all } \xi : \quad \xi \in L_p, < \xi >= 0, \tag{3.20}$$

Here $\boldsymbol{v}_0$ is a constant vector that in our examples represents the average value of the phase variable $\boldsymbol{v}$ over the periodic cell and $\xi = \boldsymbol{v} - \boldsymbol{v}_0$ is a fluctuatiing part of it. Let us add to this inequality the requirement that the "trial fields" ξ satisfies the differential restrictions EK. We come to the definition of so called A-quasiconvexity, which is due to Morrey (1953): The function $F(\boldsymbol{v})$ is called A-quasiconvex in the point $\boldsymbol{v}_0$, if

$$F(\boldsymbol{v}_0) \quad \leq \quad < F(v_0 + \xi) >, \quad \text{for all} \quad \xi \in \Xi, \tag{3.21}$$

where

$$\Xi = \{\xi : \quad < \xi >= 0, \tag{3.22}$$

$$A(\xi) = \sum a_{ijk} \frac{\partial \xi_j}{\partial x} = 0, \tag{3.23}$$

$$\xi_j \in L_p, \ j = 1, ..m, \quad \xi_j \ \text{ are } \ \text{S} \ \text{ periodic}\}, \tag{3.24}$$

and S is an arbitrary unit hypercube in R_n.

We observe that the difference between convexity and quasiconvexity is in the requirement (3.23). One can see that any convex function is also quasiconvex, because the set of the trial functions ξ is larger in the case of convexity than in case of quasiconvexity. The inverse statement is not true. Differential restrictions $\boldsymbol{E} \in EK$ enlarge the set of the functions that satisfy the convexity inequality (3.20). We can use these functions as follows. Let assume that we found some quasiconvex functions. Then we can add the conditions (3.21) as integral restriction on the phase variables that follows from the differential one. Now if we drop off the differential restriction (3.23) from the problem (3.19) but add their integral corollaries (3.21) we end up with the new problem that possesses some good properties. First, it can be solved, because it contains only integral restrictions. Then, it takes into account some of the properties of the fields in the form (3.21). We may hope, that the obtained function is a good low bound for the function $QW(\boldsymbol{E}_0)$.

3.4 Examples of quasiconvex but not convex function.

Consider the function

$$F(\boldsymbol{v}) = \det \boldsymbol{v}, \tag{3.25}$$

where $\boldsymbol{v}$ is given by

$$\boldsymbol{v} = [\boldsymbol{e}_1, \boldsymbol{e}_2] = \begin{pmatrix} \frac{\delta\phi_1}{\delta x_1} & \frac{\delta\phi_2}{\delta x_1} \\ \frac{\delta\phi_1}{\delta x_2} & \frac{\delta\phi_2}{\delta x_2} \end{pmatrix}. \tag{3.26}$$

Obviously, $F(\boldsymbol{v})$ is not convex. Let us prove, however, that it is quasiconvex. The simplest and the most visible way to prove quasiconvexity of the quadratic functions is to use the Fourier transformation. Indeed, one can check that the function $F(\boldsymbol{v})$ can be presented as a quadratic form of the vector $\boldsymbol{E}$ that we have introduced earlier

$$< F(\boldsymbol{v}) >=< \boldsymbol{E} \cdot \boldsymbol{T} \cdot \boldsymbol{E} >, \tag{3.27}$$

where

$$\boldsymbol{E} = (e_1, e_2) = \begin{pmatrix} \frac{-\delta\phi_1}{\delta x_1} \\ \frac{-\delta\phi_1}{\delta x_2} \\ \frac{-\delta\phi_2}{\delta x_1} \\ \frac{-\delta\phi_2}{\delta x_2} \end{pmatrix}, \quad T = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{3.28}$$

By using the Plancherel's equality we rewrite (3.27) as

$$< F(\boldsymbol{v}) >= \sum_{\boldsymbol{k}} \hat{\boldsymbol{E}} \cdot \boldsymbol{T} \cdot \hat{\boldsymbol{E}} = \boldsymbol{E}_0 \cdot \boldsymbol{T} \cdot \boldsymbol{E}_0 + \sum_{\boldsymbol{k} \neq 0} \hat{\boldsymbol{E}}(\boldsymbol{k}) \cdot \boldsymbol{T} \cdot \hat{\boldsymbol{E}}(\boldsymbol{k}), \tag{3.29}$$

where $\boldsymbol{k}$ is a Fourier wave vector, $\boldsymbol{E}_0 =< \boldsymbol{E} >$ is the average field and $\hat{\boldsymbol{E}}(\boldsymbol{k})$ are the Fourier coefficients of the field $\boldsymbol{E}(\boldsymbol{x})$ that have the following representation, see (3.28)

$$\hat{\boldsymbol{E}} = - \begin{pmatrix} k_1 \hat{\phi}_1 \\ k_2 \hat{\phi}_1 \\ k_1 \hat{\phi}_2 \\ k_2 \hat{\phi}_2 \end{pmatrix}. \tag{3.30}$$

Here k_1 and k_2 are the coordinates of the wave vector $\boldsymbol{k}$ and $\hat{\phi}_1$ and $\hat{\phi}_2$ are the Fourier images of the potentials. By substituting (3.30) into (3.29) we immediately arrive at

(3.20) with the equality sign in it. Such functions $F(\boldsymbol{v})$ that satisfy the quasiconvexity condition with an equality sign are called quasiaffine functions.

For any set of the differential restrictions EK one can find the quasiconvex quadratic forms using this approach of Fourier analyses. We mention that such functions can depend on several parameters. For example, the function

$$F(\boldsymbol{E}) = t\boldsymbol{E} \cdot \boldsymbol{T} \cdot \boldsymbol{E}, \tag{3.31}$$

where $\boldsymbol{E}$ and $\boldsymbol{T}$ are given by (3.28) is quasiconvex for any t. Using similar analysis in a Fourier space one can check that the same function (3.31) is quasiconvex for any value of the parameter t if

$$\boldsymbol{E} = (\boldsymbol{j}_1, \boldsymbol{j}_2), \qquad \nabla \cdot \boldsymbol{j}_1 = 0, \quad \nabla \cdot \boldsymbol{j}_2 = 0. \tag{3.32}$$

3.5 Bound on the functional and on the effective properties by using the quasiconvex functions.

Having in mind the existence of quasiconvex quadratic functions for any set of differential restrictions EK we continue studying the minimization problem (3.7). We can drop off the differential restrictions, take into account the existence of the quasiconvex functions such that

$$< \boldsymbol{E} \cdot \boldsymbol{T} \cdot \boldsymbol{E} > \geq \boldsymbol{E}_0 \cdot \boldsymbol{T} \cdot \boldsymbol{E}_0 \tag{3.33}$$

by Lagrange multipliers and solve the problem similar to how we did it before for the case without differential restrictions. I'd like to show the other way to do it. Namely, let me add and subtract the quasiaffine combination from the original functional and use the condition (3.33). We get

$$\begin{aligned} &\boldsymbol{E}_0 \cdot \boldsymbol{\mathcal{D}}_0 \cdot \boldsymbol{E}_0 = \\ &\inf_{\substack{\boldsymbol{E} :< \boldsymbol{E} >= \boldsymbol{E}_0, \\ \boldsymbol{E} \in EK}} < \boldsymbol{E} \cdot (\boldsymbol{\mathcal{D}} - t\boldsymbol{T}) \cdot \boldsymbol{E} + t\boldsymbol{E} \cdot \boldsymbol{T} \cdot \boldsymbol{E} > \\ \geq &\inf_{\substack{\boldsymbol{E} :< \boldsymbol{E} >= \boldsymbol{E}_0, \\ \boldsymbol{E} \in EK}} < \boldsymbol{E}(\boldsymbol{\mathcal{D}} - t\boldsymbol{T}) \cdot \boldsymbol{E} > + t\boldsymbol{E}_0 \cdot \boldsymbol{T} \cdot \boldsymbol{E}_0 \end{aligned} \tag{3.34}$$

Now let bound the first term from below by Reuss bound

$$\begin{aligned} \boldsymbol{E}_0 \cdot \boldsymbol{\mathcal{D}}_0 \cdot \boldsymbol{E}_0 \quad \geq \quad &\inf_{\boldsymbol{E}:<\boldsymbol{E}>=\boldsymbol{E}_0} < \boldsymbol{E} \cdot (\boldsymbol{\mathcal{D}} - t\boldsymbol{T}) \cdot \boldsymbol{E} > + t\boldsymbol{E}_0 \cdot \boldsymbol{T} \cdot \boldsymbol{E}_0 = \\ &\boldsymbol{E}_0 \cdot < (\boldsymbol{\mathcal{D}} - t\boldsymbol{T})^{-1} >^{-1} \cdot \boldsymbol{E}_0 + t\boldsymbol{E}_0 \cdot \boldsymbol{T} \cdot \boldsymbol{E}_0. \end{aligned} \tag{3.35}$$

(Remember that in order to obtain Reuss bound we need to drop of the differential restriction and solve remaining variational problem). Note, that we need to insure (by choosing an appropriate value of the parameter t) that $(\boldsymbol{\mathcal{D}} - t\boldsymbol{T}) \geq 0$, i.e. that this matrix is positive semidefinite throughout the composite. This bound is valid for any average field $\boldsymbol{E}_0$. Therefore we arrive at the inequality for the matrices

$$\boldsymbol{\mathcal{D}}_0 \quad \geq \quad < (\boldsymbol{\mathcal{D}} - t\boldsymbol{T})^{-1} >^{-1} + t\boldsymbol{T} \tag{3.36}$$

that bounds the effective properties tensor $\boldsymbol{\mathcal{D}}_0$. This bound contains one free parameter t that should be chosen in order to make this bound the most restrictive, but keeping in mind that $(\boldsymbol{\mathcal{D}} - t\boldsymbol{T})$ is positive in any of the phases:

$$\boldsymbol{\mathcal{D}}_0 \ \geq \ <(\boldsymbol{\mathcal{D}} - t\boldsymbol{T})^{-1}>^{-1} + t\,\boldsymbol{T} \quad \text{for any} \quad \mathrm{t} : \boldsymbol{\mathcal{D}}_1 - t\boldsymbol{T} \ \geq 0, \ \ \boldsymbol{\mathcal{D}}_1 - t\boldsymbol{T} \ \geq 0, \quad (3.37)$$

In fact, we found the required bound. The only problem remains that matrices $\boldsymbol{\mathcal{D}}_i$ and $\boldsymbol{T}$ can be of a large dimension. But we need to manipulate with them in order to find the answer in an appropriate form. The matrix $\boldsymbol{T}$ may depend on several free parameters and we need to find their suitable values that optimize the bounds (3.37). Note, that the bound (3.37) is valid for a composite of an arbitrary number of phases. For the two-phase materials there exists a fraction linear transformation (so called Y-transformation) that greatly simplifies the expressions. Namely, let denote

$$\mathbf{Y}(\boldsymbol{\mathcal{D}}_0) = m_2\boldsymbol{\mathcal{D}}_1 + m_1\boldsymbol{\mathcal{D}}_2 - m_1 m_2(\boldsymbol{\mathcal{D}}_1 - \boldsymbol{\mathcal{D}}_2)\cdot(\boldsymbol{\mathcal{D}}_0 - m_1\boldsymbol{\mathcal{D}}_1 - m_2\boldsymbol{D}_2)^{-1}\cdot(\boldsymbol{\mathcal{D}}_1 - \boldsymbol{\mathcal{D}}_2). \quad (3.38)$$

In terms of the tensor $\boldsymbol{Y}$ the effective properties tensor $\boldsymbol{D}_0$ is expressed as

$$\boldsymbol{\mathcal{D}}_0 = m_1\boldsymbol{\mathcal{D}}_1 + m_2\boldsymbol{\mathcal{D}}_2 - m_1 m_2(\boldsymbol{\mathcal{D}}_1 - \boldsymbol{\mathcal{D}}_2)\cdot(m_2\boldsymbol{\mathcal{D}}_1 + m_1\boldsymbol{D}_2 + \boldsymbol{Y})^{-1}\cdot(\boldsymbol{\mathcal{D}}_1 - \boldsymbol{\mathcal{D}}_2). \quad (3.39)$$

If the matrix $(\boldsymbol{\mathcal{D}}_1 - \boldsymbol{\mathcal{D}}_2)$ does not degenerate, then the bounds (3.37) can be represented in a surprisingly simple form

$$\mathbf{Y}(\boldsymbol{\mathcal{D}}_0) + \mathbf{T} \ \geq \ 0, \quad (3.40)$$

as follows from (3.37) and the definition of the tensor $\boldsymbol{Y}$. Here we omit the parameter t, it can be inserted in the definition of the matrix $\boldsymbol{T}$. The scalar inequality

$$\det\ [\mathbf{Y}(\boldsymbol{\mathcal{D}}_0) + \mathbf{T}] \ \geq \ 0. \quad (3.41)$$

that follows from (3.40) gives us a simple form of the bound of the G_mU set. It is valid for any matrix $\boldsymbol{T}$ of the quasiconvex quadratic form such that

$$\boldsymbol{D}_1 - \boldsymbol{T} \ \geq \ 0, \quad \boldsymbol{D}_2 - \boldsymbol{T} \ \geq \ 0, \quad (3.42)$$

One should choose the matrix $\boldsymbol{T}$ in order to make the bounds (3.41) as restrictive as possible. One can argue that it is optimal to choose matrix $\boldsymbol{T}$ in order to minimize the sum of the ranks of the matrices

$$\mathrm{rank}[\boldsymbol{D}_1 - \boldsymbol{T}] + \mathrm{rank}[\boldsymbol{D}_2 - \boldsymbol{T}] \quad (3.43)$$

(a lot of examples and arguments suggest this rule although the rigorous proof for the general case is not found yet). Note some useful property of the bound in the form (3.41): it does not depend on the volume fractions of the materials in the composite. All information about the volume fraction is "hidden" in the definition of the Y-tensor. Let also mention some helpful properties of the Y-transformation, namely

$$\boldsymbol{Y}(\boldsymbol{\mathcal{D}}_i) = -\boldsymbol{\mathcal{D}}_1, \quad \boldsymbol{Y}(\boldsymbol{\mathcal{D}}_0^{-1}) = \boldsymbol{Y}^{-1}(\boldsymbol{\mathcal{D}}_0) \quad (3.44)$$

3.6 The example of the translation bounds: conductivity problem.

To give you a flavor of the method let me illustrate it by the simplest example of the G_m-closure bounds for the composite of two isotropic conducting materials in two dimensions. For this example we need to study the functionals (3.4) and (3.5). For the first one we have

$$\boldsymbol{\mathcal{D}}_0 = \begin{pmatrix} \boldsymbol{\Sigma}_0 & 0 \\ 0 & \boldsymbol{\Sigma}_0 \end{pmatrix} = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_1 & 0 \\ 0 & 0 & 0 & \lambda_2 \end{pmatrix}, \tag{3.45}$$

$$\boldsymbol{Y}(\boldsymbol{\mathcal{D}}_0) = \begin{pmatrix} \boldsymbol{Y}(\boldsymbol{\Sigma}_0) & 0 \\ 0 & \boldsymbol{Y}(\boldsymbol{\Sigma}_0) \end{pmatrix} = \begin{pmatrix} y(\lambda_1) & 0 & 0 & 0 \\ 0 & y(\lambda_2) & 0 & 0 \\ 0 & 0 & y(\lambda_1) & 0 \\ 0 & 0 & 0 & y(\lambda_2) \end{pmatrix}. \tag{3.46}$$

Here

$$y(\lambda_i) = m_2\sigma_1 + m_1\sigma_2 - \frac{m_1 m_2(\sigma_1 - \sigma_2)^2}{\lambda_i - m_1\sigma_1 - m_2\sigma_2} \tag{3.47}$$

is a scalar form of Y-transformation (3.38);

$$\boldsymbol{\mathcal{D}}_i = \begin{pmatrix} \sigma_i & 0 & 0 & 0 \\ 0 & \sigma_1 & 0 & 0 \\ 0 & 0 & \sigma_i & 0 \\ 0 & 0 & 0 & \sigma_i \end{pmatrix}, \quad \boldsymbol{T} = \begin{pmatrix} 0 & 0 & 0 & t \\ 0 & 0 & -t & 0 \\ 0 & -t & 0 & 0 \\ t & 0 & 0 & 0 \end{pmatrix}. \tag{3.48}$$

The bound (3.41) can be written as

$$\det\ [\boldsymbol{Y}(\boldsymbol{\Sigma}_0) + \boldsymbol{T}(t)] = y(\lambda_1)y(\lambda_2) - t^2 \geq 0, \tag{3.49}$$

where t subjects to the restrictions

$$\sigma_1^2 - t^2 \geq 0, \quad \sigma_2^2 - t^2 \geq 0. \tag{3.50}$$

The resulting bound gives

$$y(\lambda_1)y(\lambda_2) - \sigma_{min}^2 \geq 0, \quad \sigma_{min} = \min[\sigma_1, \sigma_2]. \tag{3.51}$$

This bound defines hyperbola in the $(y(\lambda_1), y(\lambda_2))$ plane that passes through the point $y(\lambda_1) = y(\lambda_2) = \sigma_{min}$. Studying the functional (3.5) of two current fields in a similar way we get the bound

$$y(\frac{1}{\lambda_1})y(\frac{1}{\lambda_2}) - \sigma_{max}^{-2} \geq 0, \quad \sigma_{max} = \max[\sigma_1, \sigma_2]. \tag{3.52}$$

By using the remarkable property of the Y-transformation

$$\boldsymbol{Y}(\boldsymbol{D}_0^{-1}) = \boldsymbol{Y}^{-1}(\boldsymbol{D}_0) \tag{3.53}$$

we end up with the upper bound

$$y(\lambda_1)y(\lambda_2) - \sigma_{max}^2 \leq 0. \tag{3.54}$$

It is the other hyperbola that passes through the point $y(\lambda_1) = y(\lambda_2) = \sigma_{max}$.

Now we need to map these bounds into the plane of invariants of the tensor $\mathbf{\Sigma}_0$ instead of the plane $\boldsymbol{Y}(\mathbf{\Sigma}_0)$. In order to do it we mention that

$$\lambda_i = m_1\sigma_1 + m_2\sigma_2 - \frac{m_1 m_2(\sigma_1 - \sigma_2)^2}{m_2\sigma_1 + m_1\sigma_2 + y(\lambda_i)}, \quad i = 1, 2, \tag{3.55}$$

is a fraction linear transformation, it maps hyperbola in the Y-plane into the hyperbola in the Σ-plane. Any hyperbola can be defined by three points that it comes through. Hyperbola (3.51) passes through the points

$$A = (0, \infty), \quad B = (\infty, 0), \quad C = (\sigma_1, \sigma_1). \tag{3.56}$$

Therefore corresponding hyperbola in Σ plane passes through the points

$$A = (\sigma_h, \sigma_a), \quad B = (\sigma_a, \sigma_h), \quad C = (\sigma_{HS}^1, \sigma_{HS}^1), \tag{3.57}$$

where

$$\sigma_h = [m_1/\sigma_1 + m_2/\sigma_2]^{-1}, \quad \sigma_h = m_1\sigma_1 + m_2\sigma_2, \tag{3.58}$$

and the expression σ_{HS}^1 is defined by the formula (1.53). Similarly, the upper boundary hyperbola (3.54) passes (in the Σ plane) through the points

$$A = (\sigma_h, \sigma_a), \quad B = (\sigma_a, \sigma_h), \quad C = (\sigma_{HS}^2, \sigma_{HS}^2), \tag{3.59}$$

see (1.52). Obviously, the points A and B correspond to the laminate structures and points σ_{HS}^2 and σ_{HS}^2 correspond to the Hashin-Shtrikman constructions. At last, let me give you the expressions that define boundary hyperbolas

$$\frac{1}{\lambda_1 - \sigma_1} + \frac{1}{\lambda_2 - \sigma_1} = \frac{1}{m_2}\frac{1}{\lambda_2 - \sigma_1} + \frac{m_1}{m_2}\frac{1}{2\sigma_1} \tag{3.60}$$

(lower bound) and

$$\frac{1}{\lambda_1 - \sigma_2} + \frac{1}{\lambda_1 - \sigma_2} = \frac{1}{m_1}\frac{1}{\lambda_1 - \sigma_2} + \frac{m_2}{m_1}\frac{1}{2\sigma_2} \tag{3.61}$$

(upper bound).

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4 Implementation of the translation method to the plane elasticity problem

In this lecture we prove the bounds on the effective properties of an isotropic composite made from two isotropic elastic materials with known properties. The materials are supposed to be mixed in an arbitrary way but with fixed volume fractions. First we adopt the translation method for the planar elasticity. Then we give an elementary proof of the known Hashin–Shtrikman and Walpole bounds and show how to apply the same method to prove the coupled bounds for the shear and bulk moduli of an isotropic elastic composite. The results are also valid for the effective moduli of a transversally isotropic three-dimensional composite with arbitrary cylindrical inclusions.

First we describe the equations of the plane elasticity, introduce the notations, and give the statement of the problem.

4.1 Basic equations and notations.

We deal with the plane problem of the elasticity. Let $\boldsymbol{x} = (x_1, x_2)$ be the Cartesian coordinates, $\boldsymbol{u} = (u_1, u_2)$ be the displacement vector, $\boldsymbol{\epsilon}$ be the strain tensor, $\boldsymbol{\sigma}$ be the stress tensor. The state of an isotropic body is characterized by the following system:

$$\begin{gathered} \boldsymbol{\epsilon} = \tfrac{1}{2}(\boldsymbol{\nabla u} + (\nabla \boldsymbol{u})^T), \\ \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}^T, \\ \boldsymbol{\sigma} = \boldsymbol{C}(K, \mu) \cdot \cdot \boldsymbol{\epsilon}, \end{gathered} \tag{4.1}$$

where $\boldsymbol{\nabla}$ is the two-dimensional Hamilton operator, $\boldsymbol{C}(K(\boldsymbol{x}), \mu(\boldsymbol{x}))$ is the tensor of rigidity of an isotropic material - the fourth order symmetric positively defined tensor, and $(\cdot\cdot)$ are the convolutions with regard to two indices.

It is convenient to introduce the following orthonormal basis in the space of the symmetric second order tensors :

$$\begin{gathered} \boldsymbol{a}_1 = (\boldsymbol{ii} + \boldsymbol{jj})/\sqrt{2}, \qquad \boldsymbol{a}_2 = (\boldsymbol{ii} - \boldsymbol{jj})/\sqrt{2}, \\ \boldsymbol{a}_3 = (\boldsymbol{ij} + \boldsymbol{ji})/\sqrt{2}, \qquad \boldsymbol{a}_i \cdot \cdot \boldsymbol{a}_j = \delta_{ij}, \end{gathered} \tag{4.2}$$

where $\boldsymbol{i}$ and $\boldsymbol{j}$ are the unit vectors of the Cartesian axis x_1 and x_2, δ_{ij} is the Kronecker symbol. In this basis the isotropic tensor $C(K, \mu)$ of rigidity is represented by the diagonal matrix

$$\boldsymbol{C}(K, \mu) = \begin{pmatrix} 2K & 0 & 0 \\ 0 & 2\mu & 0 \\ 0 & 0 & 2\mu \end{pmatrix}. \tag{4.3}$$

The elastic energy density can be represented either as a quadratic form of strains

$$W_{\boldsymbol{\epsilon}} = \boldsymbol{\epsilon} \cdot \cdot \boldsymbol{C} \cdot \cdot \boldsymbol{\epsilon} \tag{4.4}$$

or as a quadratic form of stresses

$$W_{\boldsymbol{\sigma}} = \boldsymbol{\sigma} \cdot \cdot \boldsymbol{S} \cdot \cdot \boldsymbol{\sigma}, \tag{4.5}$$

where

$$\boldsymbol{S} = \boldsymbol{C}^{-1} = \begin{pmatrix} \frac{1}{2K} & 0 & 0 \\ 0 & \frac{1}{2\mu} & 0 \\ 0 & 0 & \frac{1}{2\mu} \end{pmatrix} \tag{4.6}$$

is the compliance tensor.

The energy density W stored in the composite is known to be equal

$$W_{\boldsymbol{\epsilon}} =< \boldsymbol{\epsilon} \ > \cdot \cdot \boldsymbol{C}_0 \cdot \cdot < \boldsymbol{\epsilon} > \tag{4.7}$$

or

$$W_{\boldsymbol{\sigma}} =< \boldsymbol{\sigma} \ > \cdot \cdot \boldsymbol{S}_0 \cdot \cdot < \boldsymbol{\sigma} \ >, \tag{4.8}$$

where the effective compliance tensor $\boldsymbol{S}_0$ is determined as $\boldsymbol{S}_0 = \boldsymbol{C}_0^{-1}$.

The problem of bounds for the elastic moduli has a long history. Hashin and Shtrikman suggested the variational method which allows them to take into account differential restrictions on stress and strain fields; they found new bounds of the elastic moduli of an isotropic mixture made from isotropic materials.

Originally, the Hashin–Shtrikman bounds were formulated for isotropic three dimensional mixtures; however, later they were formulated for the transversal isotropic composites with cylindrical inclusions as well. The above problem is just the case we study here.

The original materials were supposed to be "well ordered". This means that both bulk and shear moduli of the first material are bigger than those of the second one

$$\mu_1 \geq \mu_2, \quad K_1 \geq K_2. \tag{4.9}$$

The obtained bounds have the form

$$K^l_{HS} \leq K_0 \leq K^u_{HS}, \quad \mu^l_{HS} \leq \mu_0 \leq \mu^u_{HS}, \tag{4.10}$$

where

$$K^l_{HS} = K_2 + \frac{m_1}{\frac{1}{K_1 - K_2} + \frac{m_2}{K_2 + \mu_2}}, \tag{4.11}$$

$$K^u_{HS} = K_1 + \frac{m_2}{\frac{1}{K_2 - K_1} + \frac{m_1}{K_1 + \mu_1}}, \tag{4.12}$$

$$\mu^l_{HS} = \mu_2 + \frac{m_1}{\frac{1}{\mu_1 - \mu_2} + \frac{m_2 \ (K_2 + 2\mu_2)}{2\mu_2 \ (K_2 + \mu_2)}}, \tag{4.13}$$

$$\mu^u_{HS} = \mu_1 + \frac{m_2}{\frac{1}{\mu_2 - \mu_1} + \frac{m_1 \ (K_1 + 2\mu_1)}{2\mu_1 \ (K_1 + \mu_1)}}. \tag{4.14}$$

These expressions bound the bulk and shear moduli of a composite independently, see Figure 7.

Figure 7: bounds on bulk and shear moduli of an isotropic two-phase elastic composite.

By using the introduced “Y-transformation” the above values K^l_{HS}, K^u_{HS} and μ^l_{HS}, μ^u_{HS} can be defined as the unique solutions of the equations

$$\begin{aligned} y(K^l_{HS}) &= \mu_2, & y(K^u_{HS}) &= \mu_1, \\ y(\mu^l_{HS}) &= \tfrac{K_2\mu_2}{K_2+2\mu_2}, & y(\mu^u_{HS}) &= \tfrac{K_1\mu_1}{K_1+2\mu_1}. \end{aligned} \tag{4.15}$$

Walpole [9, 10] considered the opposite case of “badly ordered” original materials when

$$\mu_1 \geq \mu_2, \quad K_1 \leq K_2. \tag{4.16}$$

He obtained the bounds for the effective moduli of an isotropic mixture by using similar variational method. The two-dimensional Walpole's bounds we are dealing with also have a simple representation in terms of the “Y-transformation”:

$$K^l_W \leq K_0 \leq K^u_W, \qquad \mu^l_W \leq \mu_0 \leq \mu^u_W, \tag{4.17}$$

where the parameters K^l_W, K^u_W and μ^l_W, μ^u_W satisfy the equations:

$$\begin{aligned} y(K^l_W) &= \mu_2, & y(K^u_W) &= \mu_1, \\ y(\mu^l_W) &= \tfrac{K_1\mu_2}{K_1+2\mu_2}, & y(\mu^u_W) &= \tfrac{K_2\mu_1}{K_2+2\mu_1}. \end{aligned} \tag{4.18}$$

Remark 2.3: Note that the cases (4.9) and (4.16) cover all possible relations between the elastic moduli of two original materials because one can order the materials so that

$$\mu_1 \geq \mu_2. \tag{4.19}$$

Recently we applied the translation method to this problem, reproved all the known bounds, and found new, more restrictive bounds on the elastic moduli of a composite. Let us restrict our attention to the case of well-ordered component materials. The opposite case can be treated similarly. In Figure 7 the Hashin-Shtrikman bounds are presented as a rectangular whereas the new bounds cut the corners of this rectangular.

As we have learned in the previous lectures, the method is based on the lower bound of the functional I

$$I = \sum_{i=1}^{N} W_i. \tag{4.20}$$

This functional is equal to the sum of the values of elastic energy W_i stored in the element of periodicity of a composite which is exposed to N linearly independent external stress or strain fields with fixed mean values. The energy functional is used because its value is equal to the energy stored by an equivalent homogeneous medium in the uniform field. The equivalent medium is characterized by the tensor of the effective properties, and the uniform external field coincides with the mean value of the field in the composite.

Clearly, the lower bound of the functional (4.20) provides also the bounds of the effective tensor we are interest in. Below we get the bounds of the functional (4.20) independent of the microstructure of a mixture and extract the geometrically independent bounds for the effective moduli from them.

4.2 Functionals

Now we specify the functional of the type (4.20) which attains minimal values at the boundary of the set of pairs (K_0, μ_0). We discuss here functionals providing bounds for various components of the boundary.

To obtain the lower bound for the bulk modulus one can expose composite to an external hydrostatic strain $\epsilon_h = \epsilon_1 \boldsymbol{a}_1$ because the energy of an isotropic composite under the action of this field is proportional to the effective bulk modulus K_0.

$$\begin{gathered} I^{\boldsymbol{\epsilon}} =< \ \boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \cdot \boldsymbol{C}(\boldsymbol{x}) \cdot \cdot \boldsymbol{\epsilon}(\boldsymbol{x}) \ >= (2K_0)\epsilon_1^2, \\ \boldsymbol{\epsilon}(\boldsymbol{x}) \in (4.1), \quad < \boldsymbol{\epsilon}(\boldsymbol{x}) >= \epsilon_1 \ \boldsymbol{a}_1. \end{gathered} \tag{4.21}$$

It is clear that the lower bound of the functional (4.21) gives the lower bound of the effective bulk modulus K_0, because the amplitude $\boldsymbol{\epsilon}_1$ of the hydrostatic strain field is assumed to be fixed.

To get the upper bound of this modulus, we need to expose the composite to the hydrostatic stress $\boldsymbol{\sigma}_h = \sigma_1 \ \boldsymbol{a}_1$; this makes the stored energy proportional to $1/K_0$. The lower bound of the corresponding functional gives us the upper bound of K_0. So, this time we minimize the functional

$$\begin{gathered} I^{\boldsymbol{\sigma}} =< \ \boldsymbol{\sigma}(\boldsymbol{x}) \cdot \cdot S(\boldsymbol{x}) \cdot \cdot \boldsymbol{\sigma}(\boldsymbol{x}) \ >= (2K_0)^{-1}\sigma_1^2, \\ \sigma(\boldsymbol{x}) \in (4.1), \quad < \boldsymbol{\sigma}(\boldsymbol{x}) >= \sigma_1 \ \boldsymbol{a}_1, \end{gathered} \tag{4.22}$$

where σ_1 is a given constant.

We will see that the exact bounds of these functionals provide the Hashin - Shtrikman bounds for the bulk modulus.

Similarly, to obtain the lower bound for the shear modulus of a mixture one can examine the energy stored in a composite exposed to the shear-type trial strain. This way we obtain an bound on any of the two shear moduli of the mixture which is anisotropic in general. However, the other shear modulus can have arbitrary value and the energy functionals of the types (4.21), (4.22) are not sensitive to its value. To provide the isotropy of the mixture we should also care about the reaction of the composite on the orthogonal shear field. So, to bound the shear modulus of an isotropic composite we should minimize the functional equal to the sum of two values of energy stored by the medium under the action of two trial orthogonal shear fields $\boldsymbol{\epsilon} = \epsilon_2 \ \boldsymbol{a}_2$ and $\boldsymbol{\epsilon}' = \epsilon_3 \ \boldsymbol{a}_3$.

$$
\begin{gathered}
I^{\boldsymbol{\epsilon}\epsilon} =< \ \boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \cdot \boldsymbol{C}(\boldsymbol{x}) \cdot \cdot \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{\epsilon}'(\boldsymbol{x}) \cdot \cdot \boldsymbol{C}(\boldsymbol{x}) \cdot \cdot \boldsymbol{\epsilon}(\boldsymbol{x}) \ > \\
= 2\mu_0(\epsilon_2^2 + \epsilon_3^2), \\
if \quad \boldsymbol{\epsilon}(\boldsymbol{x}), \ \boldsymbol{\epsilon}'(\boldsymbol{x}) \in \ (4.1), \\
< \boldsymbol{\epsilon}(\boldsymbol{x}) >= \epsilon_2 \boldsymbol{a}_2, \quad < \boldsymbol{\epsilon}'(\boldsymbol{x}) >= \epsilon_3 \boldsymbol{a}_3,
\end{gathered}
\tag{4.23}
$$

where ϵ_2 and ϵ_3 are fixed constants. To find the upper bound of the shear modulus we use the functional equal to the sum of two energies stored in a composite exposed to two orthogonal shear stresses $\boldsymbol{\sigma} = \ \sigma_2 \ \boldsymbol{a}_2$ and $\boldsymbol{\sigma}' = \ \sigma_3 \ \boldsymbol{a}_3$

$$
\begin{gathered}
I^{\boldsymbol{\sigma\sigma}} =< \ \boldsymbol{\sigma}(\boldsymbol{x}) \cdot \cdot \boldsymbol{S}(\boldsymbol{x}) \cdot \cdot \boldsymbol{\sigma}(\boldsymbol{x}) + \boldsymbol{\sigma}'(\boldsymbol{x}) \cdot \cdot \boldsymbol{S}(\boldsymbol{x}) \cdot \cdot \boldsymbol{\sigma}'(\boldsymbol{x}) \ > \\
= \tfrac{1}{2\mu_0}(\sigma_2^2 + \sigma_3^2), \\
if \ \ \boldsymbol{\sigma}, \ \boldsymbol{\sigma}' \in (4.1), \quad < \boldsymbol{\sigma} >= \boldsymbol{\sigma}_2 \ \boldsymbol{a}_2, \quad < \boldsymbol{\sigma}' >= \boldsymbol{\sigma}_3 \ \boldsymbol{a}_3.
\end{gathered}
\tag{4.24}
$$

Here σ_2 and σ_3 are given constants. We show below that the lower bounds of these functionals lead to the Hashin - Shtrikman and Walpole bounds for the shear modulus.

In order to get coupled shear-bulk bounds one can expose a composite to three different fields: a hydrostatic field and two orthogonal shear fields. We have a choice between stress and strain trial fields (two shear fields are supposed to be of the same nature to provide isotropy of the mixture). Therefore the following functionals should be considered:

$$I^{\boldsymbol{\epsilon\epsilon\epsilon}} = I^{\boldsymbol{\epsilon}} + I^{\boldsymbol{\epsilon\epsilon}}, \tag{4.25}$$

$$I^{\boldsymbol{\sigma\sigma\sigma}} = I^{\boldsymbol{\sigma}} + I^{\boldsymbol{\sigma\sigma}}, \tag{4.26}$$

$$I^{\boldsymbol{\sigma\epsilon\epsilon}} = I^{\boldsymbol{\sigma}} + I^{\boldsymbol{\epsilon\epsilon}}, \tag{4.27}$$

$$I^{\boldsymbol{\epsilon\sigma\sigma}} = I^{\boldsymbol{\epsilon}} + I^{\boldsymbol{\sigma\sigma}}. \tag{4.28}$$

The lower bounds on the last two of these functionals give us a required component of the boundary for the well-ordered case.

Indeed, the lower bounds of the functionals $I^{\boldsymbol{\epsilon\epsilon\epsilon}}$ and $I^{\boldsymbol{\sigma\sigma\sigma}}$ provide the lower and upper bounds of the convex combination of the effective bulk and shear moduli because these functionals linearly depend on these moduli (the functional $I^{\epsilon\epsilon\epsilon}$) or on their inverse values (the functional $I^{\sigma\sigma\sigma}$).

In the well ordered case (4.9), however, the points of maximal and minimal values of both moduli (the Hashin - Shtrikman points A and C on Fig.7) are attainable by special microstructures (see [5], for example); and it is clear that the bounds of these functionals cannot improve the classical inequalities (4.10), (4.15).

On the other hand, minimization of the functionals $I^{\sigma\epsilon\epsilon}$ or $I^{\epsilon\sigma\sigma}$ demands to minimize one of the moduli and maximize the other one. We show below that for well ordered materials it leads to coupled bounds of the moduli which are more restrictive then the Hashin - Shtrikman ones.

In the badly ordered case (4.16) we face the opposite situation: the bounds of the functionals $I^{\epsilon\epsilon\epsilon}$ and $I^{\sigma\sigma\sigma}$ improve the Walpole bounds, and the bounds of the functionals $I^{\sigma\epsilon\epsilon}$ and $I^{\epsilon\sigma\sigma}$ leads to known ones.

The situation is illustrated by the Figure 7 where arrows show the directions in the plane (K, μ) that correspond to minimization of the discussed functionals.

4.3 CONSTRUCTION OF QUASIAFFINE FUNCTIONS

To use the translation method for the problem under study we need to find the set of bilinear quasiaffine functions of stresses and strains. In this section we determine some of such functions depending on strain fields, stress fields, and the bilinear function depending on two stress fields.

As before, we use the Fourier transformation to prove the quasiconvexity of the quadratic function. The differential restriction on stress and strain field

$$\nabla \cdot \boldsymbol{\sigma} = 0, \qquad \boldsymbol{\epsilon} = \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T) \tag{4.29}$$

can be rewritten in the Fourier space as

$$\boldsymbol{k} \cdot \hat{\boldsymbol{\sigma}}(\boldsymbol{k}) = 0, \quad \hat{\boldsymbol{\epsilon}}(\boldsymbol{k}) = \frac{1}{2}(\boldsymbol{k}\hat{\boldsymbol{u}}(\boldsymbol{k}) + \hat{\boldsymbol{u}}(\boldsymbol{k})\boldsymbol{k}). \tag{4.30}$$

Let us choose the Cartesian basis where the first basis vector coincides with the Fourier wave vector $\boldsymbol{k}$. In this basis the Fourier coefficients of the fields $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are presented as

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{k}) = \begin{pmatrix} 0 & 0 \\ 0 & \sigma_{22}(\boldsymbol{k}) \end{pmatrix}, \quad \hat{\boldsymbol{\epsilon}}(\boldsymbol{k}) = \begin{pmatrix} k_1\hat{u}_1(\boldsymbol{k}) & (k_2\hat{u}_1(\boldsymbol{k}) + k_1\hat{u}_2(\boldsymbol{k}))/2 \\ (k_2\hat{u}_1(\boldsymbol{k}) + k_1\hat{u}_2(\boldsymbol{k}))/2 & 0 \end{pmatrix}. \tag{4.31}$$

Here k_1, k_2, $\hat{u}_1(\boldsymbol{k})$, $\hat{u}_2(\boldsymbol{k})$, and $\sigma_{22}(\boldsymbol{k})$ are the coordinates of the corresponding vectors and tensor in the chosen basis. Now it is easy to see that

$$< det\boldsymbol{\sigma} > -det < \boldsymbol{\sigma} > = < det\boldsymbol{\sigma} > -det\boldsymbol{\sigma}_0 = \sum_{\boldsymbol{k}\neq 0} det\hat{\boldsymbol{\sigma}}(\boldsymbol{k}) = 0, \tag{4.32}$$

$$< det\boldsymbol{\epsilon} > -det < \boldsymbol{\epsilon} > = \sum_{\boldsymbol{k}\neq 0} det\hat{\boldsymbol{\epsilon}}(\boldsymbol{k}) = det\begin{pmatrix} k_1u_1 & (k_2u_1 + k_1u_2)/2 \\ (k_2u_1 + k_1u_2)/2 & 0 \end{pmatrix} \le 0, \tag{4.33}$$

$$
\begin{aligned}
&< \boldsymbol{\sigma} \cdot \boldsymbol{R} \cdot \boldsymbol{\sigma}' \cdot \boldsymbol{R}^T > - < \boldsymbol{\sigma} > \cdot \boldsymbol{R} \cdot < \boldsymbol{\sigma}' > \cdot \boldsymbol{R}^T \\
= \sum_{\boldsymbol{k} \neq 0} &\begin{pmatrix} 0 & 0 \\ 0 & \sigma_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \sigma'_{22} \end{pmatrix} \begin{pmatrix} 0 & 11 \\ 1 & 0 \end{pmatrix} = 0.
\end{aligned} \tag{4.34}
$$

It completes the prove of the quasiconvexity of the following functions (where we use the tensor basis $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ to present translation matrices):

$$
t \quad \det \boldsymbol{\sigma} = \boldsymbol{\sigma} \cdot \boldsymbol{T}^\sigma \cdot \boldsymbol{\sigma}, \quad \boldsymbol{T}^\sigma(t) = \begin{pmatrix} t & 0 & 0 \\ 0 & -t & 0 \\ 0 & 0 & -t \end{pmatrix}, \quad \text{for} \quad \text{all} \quad t, \tag{4.35}
$$

$$
t \det \boldsymbol{\epsilon} = \boldsymbol{\epsilon} \cdot \boldsymbol{T}^\epsilon \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{T}^\epsilon(t) = \begin{pmatrix} t & 0 & 0 \\ 0 & -t & 0 \\ 0 & 0 & -t \end{pmatrix}, \quad \text{for} \quad \text{all} \quad t \leq 0, \tag{4.36}
$$

$$
\boldsymbol{\sigma} \cdot \boldsymbol{R} \cdot \boldsymbol{\sigma}' \cdot \boldsymbol{R}^T = \boldsymbol{\sigma} \cdot \boldsymbol{T}^\sigma \cdot \boldsymbol{\sigma}, \quad \boldsymbol{T}^{\sigma\sigma} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & t \\ 0 & -t & 0 \end{pmatrix}, \quad \text{for} \quad \text{all} \quad t. \tag{4.37}
$$

Using these functions we show the proof of the Hashin-Shtrikman bounds on the bulk modulus of a composite and Hashin-Shtrikman and Walpole upper bounds on the shear modulus. Quasiconvexity of the other functions that are necessary to use in the prove of the other bounds can be constructed in a similar way.

4.4 Prove of the Hashin-Shtrikman and Walpole bounds

In this section we get some of the Hashin - Shtrikman and Walpole bounds by using a regular procedure of the translation method. We prove it here for the demonstration of a regular procedure on simple examples.

4.5 Bounds for the bulk modulus

4.5.1 The lower bound.

To bound the functional $I^{\boldsymbol{\epsilon}}$ we need the symmetric translation strain-strain matrix $\boldsymbol{T}^{\boldsymbol{\epsilon}}$ (see (4.36)).

To get the result we use the bounds of the third lecture

$$
\boldsymbol{Y}(\boldsymbol{\mathcal{D}}_0) + \boldsymbol{T} \ \geq \ 0, \tag{4.38}
$$

where we should substitute the following matrices

$$
\begin{gathered}
\boldsymbol{\mathcal{D}}_i = \boldsymbol{C}_i, \quad i = 1, 2, \\
\boldsymbol{T} = \boldsymbol{T}^{\boldsymbol{\epsilon}}(t).
\end{gathered} \tag{4.39}
$$

The conditions of the positivity of the matrices $\boldsymbol{C}_1 - \boldsymbol{T}^{\boldsymbol{\epsilon}}(t)$ and $\boldsymbol{C}_2 - \boldsymbol{T}^{\boldsymbol{\epsilon}}(t)$ have the form

$$\begin{pmatrix} 2K_i - t & 0 & 0 \\ 0 & 2\mu_i + t & 0 \\ 0 & 0 & 2\mu_i + t \end{pmatrix} \geq 0, \quad i = 1,\ 2 \tag{4.40}$$

and lead to the scalar inequalities

$$t \leq 0, \quad t \geq -min\{\mu_1, \mu_2\} = -\mu_{min}. \tag{4.41}$$

The bound for the isotropic matrix $\boldsymbol{D}_0^{\boldsymbol{\epsilon}} = \boldsymbol{C}_0'$ associated with the functional $I^{\boldsymbol{\epsilon}}$ has the form

$$\begin{pmatrix} y(2K_0) + t & 0 & 0 \\ 0 & y(2\mu_0) - t & 0 \\ 0 & 0 & y(2\mu_0) - t \end{pmatrix} \geq 0 \tag{4.42}$$

and leads to the inequality for the bulk modulus K_0

$$y(2K_0) \geq -t, \quad t \in (4.41). \tag{4.43}$$

The most restrictive bound corresponds to the critical value

$$t = t^* = -\mu_{min} \tag{4.44}$$

of the parameter t. This bound coincides with the Hashin - Shtrikman and Walpole lower bound for the bulk modulus (see (4.10)–(4.15), (4.17)– (4.18)).

4.5.2 The upper bound.

The upper bound for the bulk modulus can be obtained analogously using the functional $I^{\boldsymbol{\sigma}}$ instead of $I^{\boldsymbol{\epsilon}}$ and the quasiaffine function associated with the translation matrix $\boldsymbol{T}^{\boldsymbol{\sigma}}(t)$. For this functional, the matrices $\boldsymbol{\mathcal{D}}_i,\ i = 0, 1, 2$ are equal

$$\boldsymbol{\mathcal{D}}_i = \boldsymbol{S}_i\ , \quad i = 0, 1, 2. \tag{4.45}$$

Now the restrictions on matrix $\boldsymbol{T}$ have the form

$$\begin{pmatrix} \frac{1}{2K_i} - t_1 & 0 & 0 \\ 0 & \frac{1}{2\mu_i} + t_1 & 0 \\ 0 & 0 & \frac{1}{2\mu_i} + t_1 \end{pmatrix} \geq 0 \tag{4.46}$$

or scalar form

$$-\frac{1}{2\mu_1} = -min\{\frac{1}{2\mu_1},\ \frac{1}{2\mu_2}\} \leq t \leq min\{\frac{1}{2K_1},\ \frac{1}{2K_2}\}. \tag{4.47}$$

The bound for an isotropic effective tensor $\boldsymbol{S}_0$ becomes

$$\begin{pmatrix} y(\frac{1}{2K_0}) + t_1 & 0 & 0 \\ 0 & y(\frac{1}{2\mu_0}) - t_1 & 0 \\ 0 & 0 & y(\frac{1}{2\mu_0}) - t_1 \end{pmatrix} \geq 0. \tag{4.48}$$

The corresponding scalar inequality for a bulk modulus K_0

$$y(\frac{1}{2K_0}) + t_1 \geq 0 \tag{4.49}$$

becomes the most restrictive when the parameter t_1 is chosen as $t_1 = t_1^* = -\frac{1}{2\mu_1}$. By using the properties of the Y-transformation it can be represented in the form

$$y(K_0) \leq \mu_{max}. \tag{4.50}$$

This bound coincides with the Hashin-Shtrikman and Walpole upper bounds for the bulk modulus (see (4.10)–(4.15), (4.17)– (4.18)).

4.6 Upper bounds for the shear modulus

To obtain the upper bound for the shear modulus of the mixture we use the same procedure for estimating the functional $I^{\boldsymbol{\sigma}\boldsymbol{\sigma}}$. In this case

$$\boldsymbol{E} = \{\sigma_1,\ \sigma_2,\ \sigma_3,\ \sigma_1',\ \sigma_2',\ \sigma_3'\} \tag{4.51}$$

is a six-dimensional vector consisting of the components of two stress tensors $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$; the (6×6) matrices

$$\boldsymbol{\mathcal{D}}_i = \begin{pmatrix} \boldsymbol{S}_i & 0 \\ 0 & \boldsymbol{S}_i \end{pmatrix}, \quad i = 0,\ 1,\ 2 \tag{4.52}$$

are block-diagonal. We construct the matrix $\boldsymbol{T}^{\boldsymbol{\sigma}\sigma}$ of a quasiafine quadratic function of the vector $\boldsymbol{E}$ using the bilinear quasiaffine forms (4.35) - (4.37)

$$\boldsymbol{T}^{\boldsymbol{\sigma}\boldsymbol{\sigma}}(t_1,\ t_2) = \begin{pmatrix} -t_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & t_1 & 0 & 0 & 0 & t_2 \\ 0 & 0 & t_1 & 0 & -t_2 & 0 \\ 0 & 0 & 0 & -t_1 & 0 & 0 \\ 0 & 0 & -t_2 & 0 & t_1 & 0 \\ 0 & t_2 & 0 & 0 & 0 & t_1 \end{pmatrix}. \tag{4.53}$$

The restrictions on $\boldsymbol{T}$ now have the matrix form

$$\boldsymbol{D}_i^{\boldsymbol{\sigma}\boldsymbol{\sigma}} - \boldsymbol{T}^{\boldsymbol{\sigma}\boldsymbol{\sigma}}(t_1,\ t_2) =$$

$$\begin{pmatrix} \frac{1}{2K_i} + t_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2\mu_i} - t_1 & 0 & 0 & 0 & -t_2 \\ 0 & 0 & \frac{1}{2\mu_i} - t_1 & 0 & t_2 & 0 \\ 0 & 0 & 0 & \frac{1}{2K_i} + t_1 & 0 & 0 \\ 0 & 0 & t_2 & 0 & \frac{1}{2\mu_i} - t_1 & 0 \\ 0 & -t_2 & 0 & 0 & 0 & \frac{1}{2\mu_i} - t_1 \end{pmatrix} \geq 0, \tag{4.54}$$

$$i = 1,\ 2,$$

or the scalar form

$$t_1 \geq -\frac{1}{2K_{max}}, \tag{4.55}$$

$$\left(\frac{1}{2\mu_{max}} - t_1\right)^2 - t_2^2 \geq 0, \tag{4.56}$$

where

$$\begin{aligned} K_{max} &= \max\{K_1,\ K_2\}, \\ \mu_{max} &= \max\{\mu_1,\ \mu_2\} = \mu_{max}. \end{aligned} \tag{4.57}$$

The critical values $t_1^*,\ t_2^*$ of the parameters $t_1,\ t_2$ are equal

$$t_1^* = -\frac{1}{2K_{max}}, \qquad t_2^* = \frac{1}{2\mu_{max}} + \frac{1}{2K_{max}}. \tag{4.58}$$

The bound becomes

$$\boldsymbol{Y}(\boldsymbol{D}_0^{\boldsymbol{\sigma\sigma}}) + \boldsymbol{T}^{\boldsymbol{\sigma\sigma}}(t_1^*,\ t_2^*) =$$

$$\begin{pmatrix} y(\frac{1}{2K_0}) - t_1^* & 0 & 0 & 0 & 0 & 0 \\ 0 & y(\frac{1}{2\mu_0}) + t_1^* & 0 & 0 & 0 & t_2^* \\ 0 & 0 & y(\frac{1}{2\mu_0}) + t_1^* & 0 & -t_2^* & 0 \\ 0 & 0 & 0 & y(\frac{1}{2K_0}) - t_1^* & 0 & 0 \\ 0 & 0 & -t_2^* & 0 & y(\frac{1}{2\mu_0}) + t_1^* & 0 \\ 0 & t_2^* & 0 & 0 & 0 & y(\frac{1}{2\mu_0}) + t_1^* \end{pmatrix} \geq 0. \tag{4.59}$$

It leads to the scalar inequality

$$y(\frac{1}{2\mu_0}) + t_1^* - t_2^* = y(\frac{1}{2\mu_0}) - \frac{2}{K_{max}} - \frac{1}{\mu_{max}} \geq 0 \tag{4.60}$$

or

$$y(\mu_0) \leq \frac{K_{max}\mu_{max}}{K_{max} + 2\mu_{max}}. \tag{4.61}$$

It coincides with the Hashin – Shtrikman bound (see (4.10)–(4.15)) in the well ordered case (4.9) and with the Walpole bound (see (4.17)–(4.18)) in the badly ordered case (4.16).

The other bounds can be obtained in a similar way, they are presented by the Figure 7.

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