3
Bounds and G-Closures

In structural optimization, the effective properties of layouts are controls: An optimal structure adapts itself to the local fields. The layout is no longer periodic but almost periodic function. Here we introduce the corresponding technique which is the G-convergence of a sequence of linear operators.

In control problems, it is essential to know the range of effective properties. Here we establish some bounds for the effective tensors. We also introduce the notion of the G-closure: the set of effective tensors of a composite with arbitrary microstructures.

3.1 Effective Tensors: Variational Approach

Here we compute the effective tensors from the variational principles and we establish inequalities for these tensors.

3.1.1 Calculation of Effective Tensors

The Energy of a Homogenized Body

Consider the sequence σ_ε of periodic layouts. The solution w_ε of the conductivity equations is a minimizer of a corresponding variational functional (2.1.23):

$$\int_\Omega (W(\boldsymbol{\sigma}_\varepsilon, \nabla w_\varepsilon) + f w_\varepsilon), \tag{3.1.1}$$

where

$$W(\boldsymbol{\sigma}_\varepsilon, \nabla w_\varepsilon) = \frac{1}{2}\nabla w_\varepsilon \cdot \boldsymbol{\sigma}_\varepsilon \nabla w_\varepsilon.$$

Also, the solution w_0 (2.2.5) minimizes the energy of the homogenized body:

$$\int_\Omega (W(\boldsymbol{\sigma}_*, \nabla w_0) + f w_0). \tag{3.1.2}$$

The Euler–Lagrange equation for the last functional, $\nabla \cdot \boldsymbol{\sigma}_* \nabla w_0 = f$, coincides with the homogenized equation.

The minimizer w_ε of the variational problem (3.1.1) tends to the minimizer w_0 of the homogenized medium when $\varepsilon \to 0$. Hence, the sequence of Lagrangians $\{W(\boldsymbol{\sigma}_\varepsilon, \nabla w_\varepsilon) - f w_\varepsilon\}$ tends to the Lagrangian $W(\boldsymbol{\sigma}_*, \nabla w_0) - f w_0$. In other words, the average of the energy over a small region in an inhomogeneous body is arbitrarily close to the energy of an equivalent homogeneous material[1].

The sequence of energies weakly converges (in $L_1(\Omega)$) to the energy of the homogenized material

$$\langle W(\boldsymbol{\sigma}_\varepsilon, \nabla w_\varepsilon)\rangle \rightharpoonup W(\boldsymbol{\sigma}_*, \nabla w_0). \tag{3.1.3}$$

The last relationship can be rewritten as either

$$\langle \mathbf{e}_\varepsilon \cdot \boldsymbol{\sigma}_\varepsilon \mathbf{e}_\varepsilon\rangle \rightharpoonup \langle \mathbf{e}_0\rangle \cdot \boldsymbol{\sigma}_* \langle \mathbf{e}_0\rangle$$

or

$$\langle \mathbf{j}_\varepsilon \cdot \boldsymbol{\sigma}_\varepsilon^{-1} \cdot \mathbf{j}_\varepsilon\rangle \rightharpoonup \langle \mathbf{j}_0\rangle \cdot \boldsymbol{\sigma}_*^{-1} \cdot \langle \mathbf{j}_0\rangle.$$

Essentially, these formulas introduce the effective tensor $\boldsymbol{\sigma}_*$. One can check that this definition is equivalent to the earlier definition of the effective tensor as the proportionality coefficients between the averaged current and field (Bensoussan et al., 1978; Jikov et al., 1994).

Remark 3.1.1 *The symmetric form $\mathbf{e}_\varepsilon \cdot \mathbf{j}_\varepsilon$ of the energy deals explicitly only with the currents and fields but not with the properties. The limiting equality (3.1.3) takes the form:*

$$\langle \mathbf{e}_\varepsilon \cdot \mathbf{j}_\varepsilon\rangle \rightharpoonup \langle \mathbf{e}_0\rangle \cdot \langle \mathbf{j}_0\rangle.$$

This representation looks surprising because the operation of integration (averaging) commutes with the scalar product operation. This relation follows from the variational principle; it will be analyzed and explained later using the theory of compensated compactness(see Chapter 7).

---

[1] Generally speaking, these energies can differ by a *null-Lagrangian*, that is, by a term for which the Euler–Lagrange equation is identically zero (see the discussion in Chapters 5, 7, and 12).

Calculation of the Effective Tensor Using Variational Approach

We use the variational principle to compute the effective tensor because a cell of periodicity Ω in an inhomogeneous medium stores the same amount of energy as the effective material:

$$\langle \mathbf{e} \cdot \boldsymbol{\sigma} \mathbf{e} \rangle = \langle \mathbf{e} \rangle \cdot \boldsymbol{\sigma}_* \langle \mathbf{e} \rangle.$$

This equation can be used to determine the effective properties tensor itself. For example, applying a field $\mathbf{e} = \mathbf{i}_1$ of unit magnitude and calculating the energy in the unit cell, we find that this energy is equal to the upper-left element σ_{11}^* of the tensor $\boldsymbol{\sigma}_*$.

This element is the cost of the variational problem (3.1.2):

$$(\sigma_*)_{11} = \min_{\mathbf{e} \in \mathcal{E}} \langle \mathbf{e} \cdot \boldsymbol{\sigma} \mathbf{e} \rangle, \tag{3.1.4}$$

where

$$\mathcal{E} = \{ \mathbf{e} : \nabla \times \mathbf{e} = 0, \quad \langle \mathbf{e} \rangle = \mathbf{i}_1, \quad \mathbf{e} \text{ is 1-periodic} \}. \tag{3.1.5}$$

Repeating this procedure several times with differently oriented external fields $\mathbf{e}$, one can calculate all elements of $\boldsymbol{\sigma}_*$.

3.1.2 Wiener Bounds

The variational method allows us to derive the bounds for coefficients of the effective tensor. Indeed, any admissible trial function $\mathbf{e}_{\text{trial}}(\mathbf{x})$ that satisfies (3.1.5) provides an upper bound for a diagonal coefficient of $\boldsymbol{\sigma}_*$ due to (3.1.4).

The simplest bound is given by a *constant* trial function

$$\mathbf{e}_{\text{trial}}(\mathbf{x}) = \text{constant}(\mathbf{x}) = \mathbf{i}_1 \quad \forall \mathbf{x} \tag{3.1.6}$$

that obviously belongs to the set $\mathcal{E}$ (see (3.1.5)). If we substitute $\mathbf{e}_{\text{trial}}$ into (3.1.4) and recall that $\boldsymbol{\sigma}(\mathbf{x}) = \sigma(\mathbf{x})I$, we obtain

$$(\sigma_*)_{11} \leq \langle \mathbf{i}_1 \cdot \boldsymbol{\sigma} \mathbf{i}_1 \rangle = \langle \boldsymbol{\sigma}_{11} \rangle.$$

Varying the orientation of the vector of $\mathbf{i}$, we obtain the matrix inequality:

$$\boldsymbol{\sigma}_* \leq \langle \boldsymbol{\sigma} \rangle. \tag{3.1.7}$$

Particularly, the maximal eigenvalue of $\boldsymbol{\sigma}_*$ is bounded from above by the maximal eigenvalue of $\langle \boldsymbol{\sigma} \rangle$.

For a composite assembled from several materials with volume fractions m_i and conductivity tensors $\boldsymbol{\sigma}_i$ we have

$$\langle \boldsymbol{\sigma} \rangle = \sum_{i=1}^{N} m_i \boldsymbol{\sigma}_i = \boldsymbol{\sigma}_a, \tag{3.1.8}$$

where subindex $_a$ denotes the arithmetic mean. The bound (3.1.7) is called the *Reuss bound* (Reuss, 1929) or the *arithmetic mean bound*.

The dual variational principle (Thompson's principle) also determines a bound for the effective tensor $\boldsymbol{\sigma}_*$. The diagonal coefficient β_*^{11} of the inverse tensor $\boldsymbol{\beta} = \boldsymbol{\sigma}^{-1}$ is

$$\beta_*^{11} = \min_{\mathbf{j} \in \mathcal{J}} \langle \mathbf{j} \cdot \boldsymbol{\sigma}^{-1} \mathbf{j} \rangle,$$

where

$$\mathcal{J} = \{ \mathbf{j} : \nabla \cdot \mathbf{j} = 0, \quad \langle \mathbf{j} \rangle = \mathbf{i}_1, \quad \mathbf{j} \text{ is 1-periodic} \}.$$

Thompson's principle leads to upper estimates of the coefficients of the inverse tensor $\boldsymbol{\sigma}_*^{-1}$ (which are the *lower* estimates of the tensor $\boldsymbol{\sigma}_*$). Again, using the constant trial function, one obtains the inequality

$$\beta_*^{11} \leq \langle \mathbf{i}_1 \cdot \boldsymbol{\sigma}^{-1} \mathbf{i}_1 \rangle,$$

which leads to

$$\boldsymbol{\sigma}_*^{-1} \leq \langle \boldsymbol{\sigma}^{-1} \rangle = \sum_{i=1}^{N} m_i \boldsymbol{\sigma}_i^{-1} = \boldsymbol{\sigma}_h^{-1},$$

where

$$\boldsymbol{\sigma}_h = \left(\sum_{i=1}^{N} m_i \boldsymbol{\sigma}_i^{-1} \right)^{-1} \tag{3.1.9}$$

denotes the harmonic mean. This bound is called the *Voigt bound* (Voigt, 1928) or the *harmonic mean bound*.

Together, inequalities (3.1.7) and (3.1.9) provide two-sided bounds of the range of variation of the effective properties tensor:

$$\boldsymbol{\sigma}_h \leq \boldsymbol{\sigma}_* \leq \boldsymbol{\sigma}_a. \tag{3.1.10}$$

The range $[\boldsymbol{\sigma}_h, \boldsymbol{\sigma}_a]$ is called the *Wiener box*. It depends only on the properties of the initial materials and their fractions in the composite. The inequalities (3.1.10) are valid for any composite regardless of its geometry; we call them geometrically independent bounds. These inequalities are also called *Wiener inequalities* (Wiener, 1912).

Remark 3.1.2 *Similar bounds can be established for other equilibria that satisfy a minimum variational principle. Indeed, the constant trial function similar to (3.1.6) trivially satisfies any linear differential restrictions.*

Note that the Wiener bounds are invariant to interchanging the properties tensors with their inverses:

$$\left(\boldsymbol{\sigma}^{-1}\right)_h \leq \boldsymbol{\sigma}_*^{-1} \leq \left(\boldsymbol{\sigma}^{-1}\right)_a.$$

The equivalence follows from obvious identities

$$\left(\boldsymbol{\sigma}^{-1}\right)_h = \left(\boldsymbol{\sigma}_a\right)^{-1}, \quad \left(\boldsymbol{\sigma}^{-1}\right)_a = \left(\boldsymbol{\sigma}_h\right)^{-1}.$$

They demonstrate that the upper bound for the "direct" tensor $\boldsymbol{\sigma}$ becomes the lower estimate for the inverse tensor $\boldsymbol{\sigma}^{-1}$ and vice versa.

Bounds on Composites' Properties

The derived Wiener bounds are the simplest examples of the bounds on effective properties. More complicated procedures take into account the differential properties of the acting fields like the curlfree nature of the fields $\mathbf{e}$. In this book, we will develop several methods of this kind. However, a number of the approaches is not discussed because our main focus is structural optimization. Instead, we refer to the collections and monographs (Hashin, 1970b; Christensen, 1979; Berdichevsky, 1983; Nemat-Nasser and Hori, 1993; Berdichevsky et al., 1999; Markov and Preziosi, 1999; Markov and Inan, 1999) where the reader can find these approaches.

A number of papers deals with bounds on the overall properties of composites from nonlinear materials. We mention (Hashin, 1983; Talbot and Willis, 1985; Ponte Castañeda and Willis, 1988; Bergman, 1991; Hashin, 1992; Talbot and Willis, 1992; Bourgeat et al., 1995; Khruslov, 1995; Oleĭnik, Yosifian, and Temam, 1995; Talbot, Willis, and Nesi, 1995; Talbot and Willis, 1995; Telega, 1995; Zhikov, 1995; Ponte Castañeda, 1996; Ponte Castañeda, 1997; Talbot and Willis, 1997; Milton and Serkov, 1999; Torquato, 1999) where a number of bounding methods is developed.

3.2 G-Closure Problem

3.2.1 G-convergence

Definition

Generalization of the homogenization procedure for linear operators leads to the introduction of the G-convergence. The theory of G-convergence studies the behavior of sequences of linear operators L^s and of corresponding solutions w^s of the boundary value problems:

$$L^s w^s = f, \quad \text{in } \Omega, \quad w^s|_{\partial\Omega} = \rho. \tag{3.2.1}$$

The family of the conductivity operators in inhomogeneous media

$$L^s = \nabla \cdot \boldsymbol{\sigma}(\chi^s)\, \nabla,$$

where χ^s is periodic in the cube Ω^s with side $\frac{1}{2^s}$, gives an example of such an operator sequence. The almost periodic layout gives another example.

Consider a sequence $\{L^s\}$ of the operators (3.2.1) and the sequence of their solutions $\{w^s = (L^s)^{-1} f\}$. Suppose that the sequence of the solutions converges weakly (in H^1) to a function w_0:

$$w^s \rightharpoonup w_0 \quad \text{weakly in } H^1(\Omega).$$

Definition 3.2.1 The weak convergence of solutions $w^s = (L^s)^{-1}f$ implies a certain convergence of the operator's sequence, which is called *G-convergence*:

$$L^s \overset{G}{\to} L_* \quad \text{if } (L^s)^{-1}f \rightharpoonup L_*^{-1}f \quad \forall f \in H^{-1}(\Omega).$$

The limiting operator L_* exists for a family of linear elliptic coercive operators L^s if their solutions weakly converge, and this limit is an elliptic operator of the same order as the operators in the sequence, (Marino and Spagnolo, 1969; Bensoussan et al., 1978; Jikov et al., 1994).

More exactly, the sequence $L^s = \nabla \cdot \boldsymbol{\sigma}^s \nabla$ of the conductivity operators G-converges to an operator $L_* = \nabla \cdot \boldsymbol{\sigma}_* \nabla$,

$$L^s = \nabla \cdot \boldsymbol{\sigma}^s \nabla \ \overset{G}{\longrightarrow} \ \nabla \cdot \boldsymbol{\sigma}_* \nabla = L_*, \tag{3.2.2}$$

if the eigenvalues of tensors $\boldsymbol{\sigma}^s$ are constrained,

$$\|\boldsymbol{\sigma}^s\| \le c_1, \quad \|\boldsymbol{\sigma}^{s\,-1}\| \le c_2, \quad c_1 > 0, c_2 > 0.$$

These conditions mean that the mixed materials are not ideal conductors of insulators. They guarantee that the G-limit of a sequence of the conductivity operators is also a conductivity operator.

The G-convergence of operators is a more general type of convergence than homogenization, but it includes homogenization. Particularly, we can view the limiting operator L_* as the conductivity operator corresponding to an inhomogeneous medium with infinitely fine-scale oscillating properties. The weak limit w_0 of solutions w^s is the averaged potential and the G-limiting operator is the homogenized conductivity operator that depends on the effective conductivity $\boldsymbol{\sigma}_*$.

Instead of a convergence of the conductivity operators we may consider a convergence of the layouts $\{\boldsymbol{\sigma}^s\}$ that define these operators. The notion of G-convergence can be applied to the sequence $\{\boldsymbol{\sigma}^s\}$.

Definition 3.2.2 We say that the sequence of the layouts $\{\boldsymbol{\sigma}^s\}$ *G-converges* to the effective layout $\boldsymbol{\sigma}_*$ if the corresponding sequence $L(\boldsymbol{\sigma}^k)$ G-converges to the conductivity operator $L(\boldsymbol{\sigma}_*)$, $L(\boldsymbol{\sigma}^s) \overset{G}{\longrightarrow} L(\boldsymbol{\sigma}_*)$; see (3.2.2).

Also, we call the layout $\boldsymbol{\sigma}_*$ the G-limit of the sequence $\{\boldsymbol{\sigma}^s\}$:

$$\boldsymbol{\sigma}^s \ \overset{G}{\longrightarrow} \ \boldsymbol{\sigma}_*.$$

The homogenization procedure corresponds to the case where a G-limiting tensor is independent of $\mathbf{x}$. The G-limiting tensor $\boldsymbol{\sigma}_*$ describes the conductivity of the homogenized media.

Various generalizations for the concept of G-convergence is discussed in (Tartar, 1990; Bensoussan, Boccardo, and Murat, 1992; Dal Maso, 1993; Pedregal, 1997; Chiheb and Panasenko, 1998); see also references therein, and in (Raĭtum, 1999).

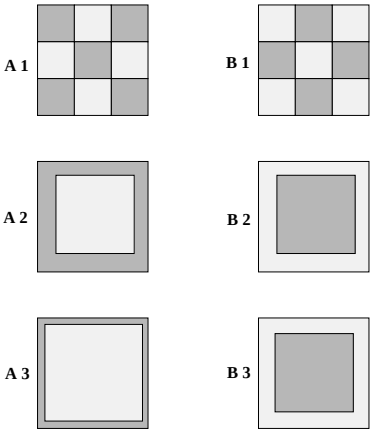

FIGURE 3.1. Various limits in the description of the materials layouts.

G-Convergence and Other Types of Convergence

The following examples (Figure 3.1) illustrate relationships between G-convergence and other types of convergence of sequences of materials' layouts.

Example 3.2.1 First, we comment on the relation between the G-convergence and strong convergence.

Suppose that an optimal layout $\mathcal{R}_\varepsilon$ of conducting materials is given by a checkerboard structure with squares of size ε made of "white" and "black" materials with conductivities σ_1 and σ_2 ($\sigma_1 < \sigma_2$), respectively (Figure 3.1, **A**1). The structure fills in a domain much larger than a square of the checkerboard and is submerged into a uniform external electrical field. The structure can be replaced with a homogeneous material with isotropic effective conductivity σ_*.

Interchange the materials in the fields and call the new structure $\mathcal{R}'_\varepsilon$ (Figure 3.1, **B**1). Consider the conductivity of the structure $\mathcal{R}'_\varepsilon$ in the same domain and external field. The difference $w' - w$ of the solutions to the corresponding conductivity problems will be as small as the scale of the board is. In the limit, these solutions coincide:

$$w - w' \to 0 \quad \text{as} \quad \varepsilon \to 0.$$

The G-convergence does not distinguish between these two layouts that lead to equal solutions to the conductivity problem,

$$\sigma_*(\mathcal{R}_\varepsilon) = \sigma_*(\mathcal{R}'_\varepsilon).$$

However, the pointwise tensor properties of these two layouts are extremely different. The norm of the difference is maximal,

$$|\sigma(\mathcal{R}_\varepsilon) - \sigma(\mathcal{R}'_\varepsilon)| = \sigma_2 - \sigma_1 \quad \forall \mathbf{x} \in \Omega,$$

because the material is switched in each point of the domain.

Therefore, G-convergence does not imply the strong convergence. However, the strong convergence does imply the G-convergence (the consideration is left to the reader).

Example 3.2.2 Consider the relation between weak convergence (averaging) of the materials' layouts and G-convergence. We demonstrate first that the weak limit does not define the G-limit.

Consider a conducting plane of a good conductor σ_2 with periodic square inclusions of a bad conductor (insulator) σ_1 (structure $\mathcal{R}_A$) and suppose that the volume fraction of inclusions is equal to one-half (Figure 3.1, **A**2). Again, consider a sequence of structures in which the size of the periodicity element tends to zero.

The average value of conductivity $\langle\sigma\rangle$ (that is, the weak limit of the conductivity layout) of the structure is $\langle\sigma(\mathcal{R}_A)\rangle = \frac{\sigma_1+\sigma_2}{2}$. The structure has an isotropic effective conductivity $\boldsymbol{\sigma}_*(\mathcal{R}_A) = \sigma_*(\mathcal{R}_A)I$ due to its symmetry. Physically, it is clear that the effective conductivity of the plane σ_* will remain close to σ_2 ($\sigma_*(\mathcal{R}_A) \approx \sigma_2$), because the conductance is mainly provided by the material σ_2 in the connected phase.

Interchange materials in the composite and call the resulting structure $\mathcal{R}_B$ (Figure 3.1, **B**2). The average conductivity of the structures $\mathcal{R}_A$ and $\mathcal{R}_B$ stays the same, because the same amounts of the materials is used, but the effective conductivity of the structure $\mathcal{R}_B$ is lower; $\sigma_*(\mathcal{R}_B) < \sigma_*(\mathcal{R}_A)$ because its conductance is now mainly determined by the first material ($\sigma_*(\mathcal{R}_B) \approx \sigma_1$) that forms the connected phase.

These two structures have the same mean value of conductivity but different G-limits:

$$\langle\sigma(\mathcal{R}_A)\rangle = \langle\sigma(\mathcal{R}_B)\rangle, \quad \text{but} \quad \sigma_*(\mathcal{R}_B) < \sigma_*(\mathcal{R}_A).$$

Example 3.2.3 On the other hand, the G-limit does not determine the weak limit either. Let us demonstrate the structures (Figure 3.1, **A**3, **B**3) that have the same G-limit of conductivity but different mean conductivities.

Consider again the configuration $\mathcal{R}_A$ (Figure 3.1, **A**2) with square inclusions occupied by the bad conductor σ_1. Let us increase the fraction m of the inclusions in the element of periodicity from $\frac{1}{2}$ to 1 and let us call the structures obtained $\mathcal{R}_A(m)$. The structure $\mathcal{R}_B$ (Figure 3.1) corresponds to the volume fraction $\frac{1}{2}$ and is denoted $\mathcal{R}_B\left(\frac{1}{2}\right)$.

We already mentioned that

$$\sigma_*\left(\mathcal{R}_A\left(\frac{1}{2}\right)\right) > \sigma_*\left(\mathcal{R}_B\left(\frac{1}{2}\right)\right).$$

Following the increase of m, $\mathcal{R}_A(m)$ continuously decreases down to the value $\sigma_*(\mathcal{R}_A(1)) = \sigma_1$, which is obviously less than $\sigma_*(\mathcal{R}_B)\left(\frac{1}{2}\right)$. Therefore

$\mathcal{R}_A(m)$ meets the effective conductivity $\sigma_*\left(\mathcal{R}_B\left(\frac{1}{2}\right)\right)$ of the configuration $\mathcal{R}_B$ (Figure 3.1, **B**2) somewhere during this process (Figure 3.1, **A**3):

$$\exists\ m_0 \in \left[\frac{1}{2},\ 1\right]: \quad \sigma_*(\mathcal{R}_A(m_0)) = \sigma_*\left(\mathcal{R}_B\left(\frac{1}{2}\right)\right).$$

The two composites (Figure 3.1, **A**3, **B**3) have the same effective conductivity but different mean values of the conductivities, whereas different relative amounts of materials are needed to obtain the same effective conductivity in the configurations $\mathcal{R}_A$ and $\mathcal{R}_B$, $m_0 \neq \frac{1}{2}$.

Thus, the weak limit cannot be determined by the G-limit, either.

Moreover, the G-limit of an asymmetric structure such as a laminate depends on the direction of the applied field, but the weak limit does not. Thus, the G-limit cannot be determined by the weak limit. However, the range of G-limits may depend on it.

3.2.2 G-Closure: Definition and Properties

Here we introduce the central idea of the G-closure of a set of material properties. The G-closure is the set of effective properties of all possible composites assembled from given materials. The problem of its description was addressed at the turn of the twentieth century, when the bounds of all possible effective tensors were established in (Wiener, 1912). Hashin and Shtrikman came out with the exact description of isotropic points of G-closure in (Hashin and Shtrikman, 1962a). Their work has demonstrated that the bounds for the G-closure corresponds to simple explicit formulas. Another simple example was built in (Tartar, 1975; Raĭtum, 1978): we discuss it in the next Section.

The concept of the G-closure and the term itself was introduced in (Lurie and Cherkaev, 1981a; Lurie and Cherkaev, 1981c) as the problem of completeness of the G-limits. This consideration was motivated by the problem of existence of an optimal layout (Lurie and Cherkaev, 1981a; Armand, Lurie, and Cherkaev, 1984). Here we use the results of the review article (Lurie and Cherkaev, 1986a), where the properties of G-closures are systematically studied.

Definitions

Consider a family of materials with known properties D_i, where $i = 1, \ldots, N$ is a parameter of the family[2], and let us call this set $\mathcal{U} = \{D_i\}$.

Consider a composite assembled from these materials. Suppose that the materials are presented in the composite with volume fractions m_i. This

[2]The notation D for the materials' properties emphasizes that the linear material may correspond to an equilibrium different from conductivity. For example, elastic materials may be considered with proper exchange in the notation.

composite material is equivalent in the sense of G-convergence to a uniform medium with tensor of effective properties D_*. We recall that the tensor $\mathcal{D}_*$ is independent of external fields. It is determined only by properties of the mixed materials and by the geometrical structure of the composite.

G_m-Closure. We call the G_m-closure of the set $\mathcal{U}$ the set of all possible values of the effective tensors $\mathcal{D}_*$ that correspond to arbitrary microstructures with the fixed volume fractions of materials. We denote the G_m-closure of $\mathcal{U}$ by $G_m\mathcal{U}$. It depends only on the set $\mathcal{U}$ of the properties of those materials and on their volume fractions m_i in a composite:

$$G_m\mathcal{U} = G_m(D_i, m_i).$$

Any tensor $D_* \in G_m\mathcal{U}$ is characterized by angles of orientation of the coordinate system and by rotationally invariant parameters such as the eigenvalues. The G_m-closure set depends only on these invariants, and it is represented as a domain in a corresponding finite-dimensional space. Each microstructure corresponds to a point in this domain.

G-Closure. We define the G-closure of the set of properties of the materials, that is, the set of possible values of the tensor $\mathcal{D}_*$ corresponding to an arbitrary microstructure and arbitrary volume fractions of the materials. The G-closure depends only on the properties of the materials in the set $\mathcal{U}$:

$$G\mathcal{U} = \bigcup_{m_i \in \mathbf{m}} G_m\mathcal{U}, \quad G\mathcal{U} = G\mathcal{U}(D_i).$$

The G-closures are of special interest for the study of polycrystals, where they naturally represent a variety of all composites made from differently oriented fragments of an anisotropic material.

Where Is the Description of G_m-Closure Used?

The following problems are examples where G_m-closures are needed:

- G_m-closures provide a priori bounds for calculation of the effective properties of any prescribed structure. It is useful to know G_m-closures dealing with structures that are either unknown or random.
- It is necessary to know the G_m-closure if a structure of a composite is to be chosen to improve its properties.
- In structural optimization, G_m-closures describe the set of admissible controls, because it is not known a priori what composite is the most effective at a specific point of a construction.

Remark 3.2.1 *For some optimization problems it is enough to find only some components of the G_m-closures. For example, we could be interested in structures of composites that store the minimal energy in an arbitrary external field.*

We also notice that a description of the closures is often presented in an explicit form; they are described by rather simple inequalities that connect invariants of any possible effective tensor. On the other hand, the problem of calculating the effective properties of a given structure typically can only be solved numerically.

G-Closeness of Sets of Materials

Most applications deal with sets of available materials $\mathcal{U}$ that are not G-closed, i.e., they do not coincide with their G-closure. We cite a few examples:

1. Discrete set that consists of several materials (the composites have intermediate effective properties).
2. Arbitrary set of isotropic media (laminates of isotropic materials are generally not isotropic).[3]
3. Set of anisotropic crystals that differ only in the orientation of their principal axes (a polycrystal composite could be isotropic).

Finally, let us give an example of the G-closed set of conducting materials. It is the set of anisotropic materials $\boldsymbol{\sigma}$ with the eigenvalues $\lambda_i,\ i = 1, \dots d$ that are restricted by two constants a and b:

$$0 < a \le \lambda_i \le b < \infty.$$

Proof of the G-closeness is left to the reader.

Notice that this example is not very natural. It is much easier to find not-G-closed sets of materials than to find a G-closed set.

Properties of G-Closures and G_m-Closures

Finiteness, Connectedness

Consider the G-closure of a set of conductivity tensors $\boldsymbol{\sigma}_*$. Each tensor is characterized by its eigenvalues $\lambda_i,\ i = 1, \dots, d$, and by angles of orientation of the tensor in space. We are interested in a description of the set of eigenvalues only, because the orientation of an effective tensor can be arbitrarily chosen by an orientation of the periodic structure as a whole. It is easy to find that the G_m-closure is a closed, simply connected, and bounded set in the space of invariants of tensor properties.[4]

Indeed, it is bounded by the Wiener inequalities

$$\sigma_h I \le \boldsymbol{\sigma}_* \le \sigma_a I,$$

[3] An exclusive counterexample of isotropic G-closure is discussed in Chapter 15.

[4] The properties discussed are valid for the G-closures of the set of linear materials with arbitrary, not only conducting, properties. Additional consideration is needed to describe the proper invariants of the materials' characteristics.

which imply that every eigenvalue belongs to the interval

$$\lambda_i \in [\sigma_h, \sigma_a]\,.$$

Therefore the G-closure is bounded.

A G-closure is connected. Indeed, any two points $\boldsymbol{\sigma}_A$, $\boldsymbol{\sigma}_B$ of a G-closure can be linked by a family of continuous curves that also belong to the G-closure. These curves correspond, for example, to the effective properties of laminates assembled from the materials $\boldsymbol{\sigma}_A$ and $\boldsymbol{\sigma}_B$ or to another family of microstructures with variable volume fractions. Obviously, the properties of a structure continuously depend on the volume fractions. Different curves correspond to different orientations of the normal to the layers in the laminates. Motion along the curve corresponds to varying the fractions of materials $\boldsymbol{\sigma}_A$ and $\boldsymbol{\sigma}_B$ in the composite, and the ends of the curve correspond to the vanishing of one of the materials in the composite.

A G_m-closure set is connected, too. If $\boldsymbol{\sigma}_A$ and $\boldsymbol{\sigma}_B$ represent composites with equal concentration of some initial materials, then a composite of $\boldsymbol{\sigma}_A$ and $\boldsymbol{\sigma}_B$ obviously has the same concentrations of these materials, which means that any such composite belongs to G_m-closure.

Both the G-closure and the G_m-closure contain a family of curves that link any two points in it and that correspond to different microstructures with different properties. Generally (but not always), the G-closures are sets with nonempty interior in the space of eigenvalues of $\boldsymbol{\sigma}_*$.

Other Properties

We notice some properties of the G-closure of a set $\mathcal{U}$ that are similar to properties of convex envelopes:

1. The envelope rule: Each set $\mathcal{U}$ belongs to its G-closure $G\mathcal{U}$:

$$\mathcal{U} \in G\mathcal{U}.$$

2. The closure rule: The G-closure of a G-closed set coincides with the set:

$$G(G\mathcal{U}) = G\mathcal{U}.$$

3. The junction rule: The union of the G-closures of two sets is smaller than or equal to the G-closure of the union of these sets:

$$G(\mathcal{U}_1 \cup \mathcal{U}_2) \supset G(\mathcal{U}_1) \cup G(\mathcal{U}_2).$$

4. The swallow rule: If a set M belongs to the G-closure of the set $\mathcal{U}$ (but not necessarily to $\mathcal{U}$ itself), then the G-closure of the set $\mathcal{U} \cup M$ is equal to the G-closure of $\mathcal{U}$:

$$M \in G\mathcal{U} \quad \Rightarrow \quad G(\mathcal{U} \cup M) = G\mathcal{U}.$$

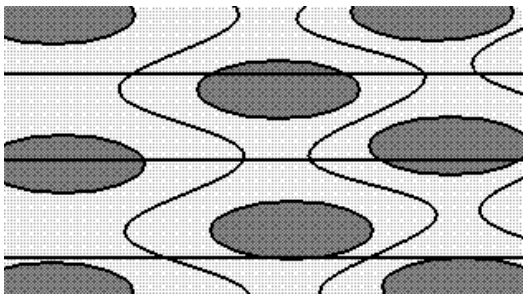

FIGURE 3.2. Illustration of the conservation property of G-closure. The phases have a common conductivity λ_0 in the horizontal direction. The applied homogeneous horizontal field causes a constant field everywhere. The applied homogeneous vertical field causes a variable field inside the structure.

These properties are physically obvious; for example, the last one means that if a material from the set M is in the G-closure of $\mathcal{U}$, then it could be replaced by a composite of materials from $\mathcal{U}$, and therefore adding this material to the set $\mathcal{U}$ does not change the G-closure. The formal proofs of these properties are left to the reader.

The Conservation Property of the G-Closure

Consider the case where the mixed anisotropic materials are represented by the tensors $\boldsymbol{\sigma}_i$ that all have a common eigenvalue and common eigenvector. Let us denote the common eigenvalue by λ_0 and the common eigenvector by $\mathbf{a}$. The conductivity tensors $\boldsymbol{\sigma}_i$ of mixing materials are of the form

$$\boldsymbol{\sigma}^i = \lambda_0 \, (\mathbf{a} \otimes \mathbf{a}) + \sum_{j=2}^{d} \lambda_j^i (\mathbf{a}_j^i \otimes \mathbf{a}_j^i), \tag{3.2.3}$$

where j is the number of an eigenvalue, i is the number of a material, and $\otimes$ denotes the *dyadic product* as follows: $C = \{c_{ij} = \mathbf{a} \otimes \mathbf{b}$ if $c_{ij} = a_i b_j\}$.

Let us demonstrate that any matrix of material properties $\boldsymbol{\sigma}_*$ from the G-closure has the same eigenvalue and eigenvector:

$$\boldsymbol{\sigma}_* = \lambda_0 \, (\mathbf{a} \otimes \mathbf{a}) + \sum_{j=2}^{d} \lambda_{*j} (\mathbf{a}_{*j} \otimes \mathbf{a}_{*j}) \; \forall \boldsymbol{\sigma}_* \in G\text{-closure}.$$

Indeed, consider a composite with arbitrary shapes of the fragments (see Figure 3.2) and calculate the fields in the composite in the response to the external field $\mathbf{e}_0 = \gamma \mathbf{a}$ applied in the direction $\mathbf{a}$. The pair of the uniform field

$$\mathbf{e}_0(\mathbf{x}) = \gamma \mathbf{a} = \text{constant}(\mathbf{x})$$

and the uniform current

$$\mathbf{j}(\mathbf{x}) = \lambda_0 \mathbf{e}_0(\mathbf{x}) = \lambda_0 \gamma \mathbf{a} = \text{constant}(\mathbf{x})$$

represents a solution to the problem: These constant fields trivially satisfy differential constraints, they satisfy the constitutive equations, and the boundary conditions do not imply any discontinuities in the fields because the only property λ_0 involved in the conductance has the same value in all fragments of the structure. Therefore, the continuity of the normal component of the current $[\mathbf{j}] = 0$ implies the continuity of this component of the field: $[\mathbf{j}] = \lambda_0[\mathbf{e}] = 0$. The current $\mathbf{j}$ that corresponds to the applied field $\mathbf{e}$ is constant everywhere and is aligned with $\mathbf{e}$. Informally speaking, the fragments of the microstructure become "clear" or "invisible" in that field. However, the microstructure manifests itself if any other field $\mathbf{e}_1(\infty)$ is applied. This time, the current $\mathbf{j}_1(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x})\mathbf{e}_1(\mathbf{x})$ is inhomogeneous and so is the field $\mathbf{e}_1(\mathbf{x})$ (see Figure 3.2).

Remark 3.2.2 *The conservation property can also be established for elastic materials. We discuss an example in Chapter 15. Moreover, it is valid even for nonlinear composites if their property λ_0 in a direction depends on the field: $\lambda_0 = \lambda_0(\mathbf{e})$ but is constant in all fragments. The reason is the same: The applied constant field $\mathbf{e}$ corresponds to the aligned current $\mathbf{j}$ that is constant everywhere.*

The investigation of the conservation property of G-closures can be formulated as the search for properties of composites that are "stable under homogenization" (Grabovsky and Milton, 1998). Namely, one can ask what sets of material properties $\mathcal{U}$ lead to the set $G\mathcal{U}$ with empty interior. Such G-closures are characterized by equalities called *exact relations* rather than by inequalities. The G-closure of the materials with a common eigenvalue and eigenvector is an example of a set with empty interior, whereas one of the eigenvalues of the G-limit is fixed.

Several examples of G-closures with empty interior are discussed in Chapters 10 and 14. Generally, the conserved property may correspond not to a chosen direction of an external field but to a combination of the applied fields. For example, we demonstrate in Chapter 10 that the determinant of a two-dimensional polycrystal is constant independent of the structure. To obtain this conservation property we consider the mutual dependence of the currents corresponding to two applied fields.

We also refer to (Milgrom and Shtrikman, 1989; Bruno, 1991; Cherkaev and Gibiansky, 1992; Benveniste, 1994; Benveniste, 1995), where various exact relations on G-closures have been found. Recent papers (Grabovsky and Milton, 1998; Grabovsky and Sage, 1998; Grabovsky, 1998) treat this problem generally and suggest algebraic algorithms for a systematic search of exact relations.

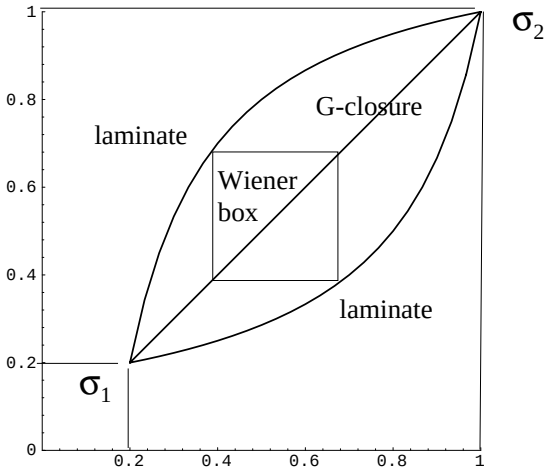

FIGURE 3.3. G-closure set of two isotropic conductors in two dimensions.

3.2.3 Example: The G-Closure of Isotropic Materials

We construct the G-closure of a set of isotropic conductors in two dimensions by using only the simplest properties of G-closures. This set was constructed in (Tartar, 1975; Raĭtum, 1978).

Consider a composite of two isotropic materials with conductivities σ_1 and σ_2 $(0 < \sigma_1 \le \sigma_2 < \infty)$ mixed in an arbitrary proportion. The conductivity of the composite is described by the effective properties tensor σ_*. The material properties of the effective conductivity are presented by the pair $\lambda_1,\ \lambda_2$ of its eigenvalues, $\lambda_1 \le\ \lambda_2$. Let us describe the domain in the $\lambda_1,\ \lambda_2$–plane that corresponds to the G-closure.

The greater eigenvalue λ_2 of an effective tensor of a composite is less than the arithmetic mean of the materials' conductivities (see (3.1.8)), and the smaller eigenvalue of an effective tensor is greater than the harmonic mean of them:

$$\lambda_2 \le m_1\sigma_1 + m_2\sigma_2, \quad \lambda_1 \ge \frac{1}{\frac{m_1}{\sigma_1} + \frac{m_2}{\sigma_2}}.$$

If we exclude the volume fractions $m_1 \ge 0,\ m_2 = 1 - m_1 \ge 0$ from the last two inequalities, we obtain the bound

$$\sigma_1 \le \lambda_1 \le \frac{\sigma_1\sigma_2}{\sigma_2 + \sigma_1 - \lambda_2} \le\ \lambda_2 \le \sigma_2. \tag{3.2.4}$$

The last inequalities provide a complete characterization of the G-closure (see Figure 3.3). Indeed, we can demonstrate the specific composite corresponding to each point of its boundary: It is a laminate with a properly chosen volume fraction. The set of laminates corresponds to the equality (see Figure 3.3)

$$\lambda_1 = \frac{\sigma_1\sigma_2}{\sigma_2 + \sigma_1 - \lambda_2}$$

because the eigenvalue corresponding to the normal component is averaged as a harmonic mean, and the eigenvalue corresponding to the tangent component as an arithmetic mean.

The geometric interpretation of this result is as follows. The G_m-closure set lies inside the Wiener box, which parametrically depends on m. Hence the G-closure lies inside the union of all rectangles corresponding to all volume fractions $m \in [0,\ 1]$ (see Figure 3.3). The boundary of this set is drawn by the motion of two symmetric nondiagonal vertices of those rectangles with coordinates σ_a, σ_h and σ_h, σ_a, respectively. Only the coordinates of these nondiagonal corners of G_m-closure are of importance. Fortunately, these points correspond to the effective properties of the known (laminate) structure. Therefore, laminates form at least a part of the boundary of the G-closure.

In the two-dimensional case, the G-closure is a domain in the plane of eigenvalues of $\boldsymbol{\sigma}_*$. The laminates describe the entire boundary of the G-closure because the set of their properties corresponds to a closed curve in that plane.

Simple-Connectedness

To conclude, we demonstrate that a G-closure is simply connected (it does not contain "holes" inside). The simplest way to demonstrate this is to build a class of microstructures that cover all points inside the domain (3.2.4). We use a two-step procedure to imitate a conductivity tensor with eigenvalues $\sigma', \sigma'' \in G$-closure. First, we build isotropic composites $\boldsymbol{\sigma}_{\text{is}}$ with all intermediate properties $\sigma' \in [\sigma_1, \sigma_2]$ (they correspond, for example, to a class of symmetric microstructures like checkerboards with the volume fraction of one of the materials varying from zero to one). Second, we build a laminate $\boldsymbol{\sigma}_{\text{lam}}$; we choose the volume fraction of materials in that laminate so that one of its eigenvalues becomes equal to σ' (the other eigenvalue $\boldsymbol{\sigma}_{l2}$ is equal to $\sigma_{l2} = \frac{\sigma_1\sigma_2}{\sigma_1+\sigma_2-\sigma'}$). Now mix the materials $\boldsymbol{\sigma}_{\text{is}}$ and $\boldsymbol{\sigma}_{\text{lam}}$. Note that one of the eigenvalues of $\boldsymbol{\sigma}_{\text{lam}}$ is equal to the eigenvalues of $\boldsymbol{\sigma}_{is}$. By the conservation property, one eigenvalue of the composite is equal to σ' (see (3.2.3)), and the other varies in the interval $[\sigma', \sigma_{l2}]$ when the volume fraction of the isotropic phase changes from one to zero. Particularly, we can choose this fraction to make this eigenvalue equal to the given parameter σ''. Therefore, the set of composites of this kind imitates all points of the G-closure (see Figure 3.3).

Three-Dimensional Case

In the three-dimensional case, the laminates correspond to curves on the boundary surface of the G-closure. We leave the complete description of three-dimensional G-closure for Chapter 10, because it requires a special technique.

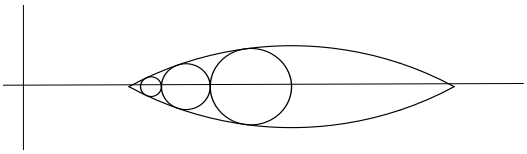

FIGURE 3.4. The domain of attainability of the current $j_{x_1},\ j_{x_2}$. The circles correspond to the fixed volume fractions of materials, the lens corresponds to the G-closure.

3.2.4 Weak G-Closure (Range of Attainability)

Two-Dimensional Case

Another way to characterize the G-closure is to observe the range of the currents $\mathbf{j} = [j_{x_1},\ j_{x_2}]$ that corresponds to the unit field $\mathbf{e} = [1,\ 0]$ and all possible composites. We use the relation $\mathbf{j} = \boldsymbol{\sigma}_*\mathbf{e}$. The current is equal to $\mathbf{j} = [\boldsymbol{\sigma}_{11},\ \boldsymbol{\sigma}_{12}]$. We express the elements of the tensor through its eigenvalues λ_1 and λ_2, and the orientation of an eigenvector Φ:

$$j_{x_1} = \frac{\lambda_1 + \lambda_2}{2} + \frac{\lambda_1 - \lambda_2}{2}\cos 2\Phi, \quad j_{x_2} = \frac{\lambda_1 - \lambda_2}{2}\sin 2\Phi.$$

The set of all possible composites with the fixed volume fractions of materials corresponds to the vector $\mathbf{j}$ that belongs to the disk:

$$F(\lambda_1), \lambda_2, m) = \left(\mathbf{j}_1 - \frac{\lambda_1 + \lambda_2}{2}\right)^2 + \mathbf{j}_2^2 - \left(\frac{\lambda_1 - \lambda_2}{2}\right)^2 \le 0;$$

where the eigenvalues λ_1 and λ_2 take the extreme values $\lambda_1 = (m\sigma_1^{-1} + (1 - m)\sigma_2^{-1})^{-1}$ and $\lambda_2 = m\sigma_1 + (1 - m)\sigma_2$ equal, respectively, to the arithmetic and harmonic means of the mixed materials. The differently oriented laminates correspond to the circumference, and the other structures correspond to the inner points of the disk (see Figure 3.4).

When the volume fraction m varies, the family of circles forms a domain of attainability. This domain is just the envelope of the family of circles. We find it by solving the equation $\frac{\partial}{\partial m}F(\lambda_1, \lambda_2, m) = 0$ and excluding $m \in [0, 1]$.

The equation of the domain of attainability is:

$$|j_{x_2}| \le \sqrt{j_{x_1}(\sigma_1 + \sigma_2 - j_{x_1})} - \sqrt{\sigma_1\sigma_2}.$$

This domain of attainability is shown in Figure 3.4. It is shaped like a lens; the vertices correspond to the pure materials σ_1 and σ_2.

The Three-Dimensional Case

The three-dimensional case is considered similarly. In dealing with the range of currents, we notice that the maximal range of $\mathbf{j}$ corresponds to the situation where the plane of the maximal and minimal eigenvalues

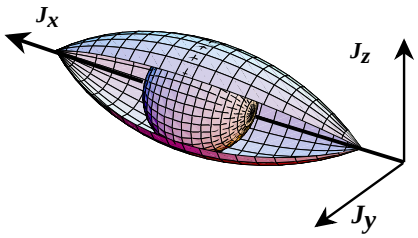

FIGURE 3.5. The domain of attainability of the current in the three-dimensional case. The inner sphere corresponds to the fixed volume fractions; the exterior surface corresponds to the weak G-closure.

of $\boldsymbol{\sigma}_*$ includes both vectors $\mathbf{e}$ and $\mathbf{j}$. In that plane the problem is two-dimensional. Therefore, all the previous results are valid. The value of the intermediate eigenvalue is irrelevant. The domain of attainability in the three-dimensional case is a surface of revolution (Figure 3.5)

$$\sqrt{j_{x_2}^2 + j_{x_3}^2} = \sqrt{j_{x_1}(\sigma_1 + \sigma_2 - j_{x_1})} - \sqrt{\sigma_1 \sigma_2},$$

where x_1 is the direction of the given field.

Notice that the boundary points of the domain correspond to laminate structures. Hence, the class of laminates is sufficient for the solution to a class of structural optimization problems that correspond to optimization of the behavior of electrical fields. A similar concept was used in (Raĭtum, 1989) to prove the existence of the optimal solution in the class of controls that consists of initial materials and their laminates. The set of layouts corresponding to attainability of currents is called the *weak G-closure*.

The advanced generalization of the concept of the weak G-closure to the nonlinear materials and additional references can be found in (Milton and Serkov, 1999).

3.3 Conclusion and Problems

We established simple bounds on the effective properties tensor and introduced the G-closures: sets of all possible effective tensors that correspond to arbitrary microstructures of a composite assembled of material with fixed properties. Their topological properties were studied, and an example was presented.

Now we are prepared to discuss structural optimization problems for conducting media.

Problems

1. How many external fields are needed to compute all coefficients of two- and three-dimensional conductivity tensors by calculating the energy? Suggest an algebraic procedure to calculate the eigenvalues and eigenvectors of an effective tensor.

2. Show that the G-closure is bounded if the mixed materials have finite conductivities.

3. Prove the topological properties of G-closures.

4. Describe the G-closure for the set of two anisotropic materials with conductivities

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda_1 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$