TWO APPROACHES TO SOLVE A NONCONVEX VECTORIAL VARIATIONAL PROBLEM: REVISED TRANSLATION METHOD AND YOUNG MEASURES

by

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ABSTRACT

In this dissertation, several problems are solved using different approaches.

The first problem is the two-dimensional three-material G-closure problem: finding all possible effective tensors from given conductivities of three materials and volume fractions. We solve this problem by establishing lower bounds on effective tensors, and finding the (sequences of) microstructures that attain the lower bounds.

The lower bound is a piece wise analytic function that depends on the conductivity and volume fraction of each component. They are derived using a combination of the translation method, and additional constraints on the field in the materials. The found bound extend their results to the anisotropic case. Furthermore, the lower bound obtained in this dissertation is also the improvement of the Hashin-Shtrikman and translation bounds, in the sense that it is optimal in a range of parameters where previously known bounds are not; and in the region where both the new bound and previously known bounds are not optimal, the bound derived here is tighter.

In the case when the established bound is optimal, structures that attain the bound are presented. All structures are laminates of finite rank. While the bound cannot be obtained by laminate structures, we estimate the bound by comparing it with some particular structure. The numerical experiment shows that the gap between the two is rather small, hence the bound is very close to the optimal bound.

The next two problems are typical problems in optimal design, and are solved using the variational method in the frame of Young measures developed by Pedregal. The key idea of this approach is to find the quasiconvex envelope of sets and functions. Those ideas have been used before for optimal design problems with two materials at disposal. Our goal here is to explore how those ideas can be extended to three or more materials situations. In particular, we focus on two paradigmatic cases, where we consider a linear-in-the-gradient cost functional and a typical quadratic situation. In both cases, we are able to formulate, quite explicitly, a full relaxation of the

problem through which optimal microstructures for the original nonconvex problem can be understood.

In principle, this approach can be also used to find the G-closure problem as long as one can find the quasiconvex hull of the set, composed of the gradient fields and their associated divergence free fields determined by the governing equations in the G-closure problem.

To my husband Carlos and our son Juan-Luis Maria

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CHAPTER 1

INTRODUCTION

In this dissertation, we study several constrained optimization problems given by:

$$(GP) \qquad \text{minimize in } \chi \quad \int_{\Omega} \Psi(\nabla u)\, dx \tag{1.1}$$

subjected to:

$$\chi = \{\chi_i\} \in \{0,1\}^3, \quad \int_{\Omega} \chi(x)\, dx = \mathbf{r}|\Omega|,$$

and

$$\operatorname{div}(\sum_{i=1}^{3} A_i \chi_i \nabla u(x)) = 0, \text{ in } \Omega, \quad u = u_0, \text{ on } \partial\Omega \tag{1.2}$$

Here $\Omega \subset \mathbf{R}^N$ is a regular, bounded domain, $\mathbf{r} \in [0,1]^3$, $\mathbf{r} \cdot \mathbf{1} = 1$, $\mathbf{1} = (1,1,1)$. The matrices A_i are conductivity tensors for the constituents, assumed to be positive definite and such that $A_i - A_j$ is invertible for every pair $i \neq j$.

1.1 G-closure problem

In the first part of the dissertation, we focus on two-dimensional three-material G-closure problem-characterizing the set of all possible effective tensors K_{eff} from given $(A, \mathbf{r})$. This set is completely determined by its boundary due to its properties.

In Chapter 2, we define K_{eff} in the context of periodic homogenization through problem (GP) with some particular integrand Ψ and proper space where u is sitting. We also pose the G-closure problem, and discuss how this boundary of G-closure can be found by constructing lower bounds on the energy stored in the homogeneous media with effective conductivity K_{eff}, and seeking the micro-geometry of three-material composites with equal energy. It is assumed that

$$A_i = a_i I, \; a_1 < a_2 < a_3 = \infty.$$

which significantly simplifies the calculation. The same assumption was made in [22] for the two material case. In the end of chapter, we review all known bounds on the G-closure.

In Chapter 3, we describe the technique of constructing the lower bound, which inherits the translation method, described in [5, 12, 28] etc., and incorporate the idea in [32] of imposing extra constraints derived in [4] on the field ∇u. A similar technique was applied in [14]. Because of the constraint, the translated energy-wells can become nonconvex but are still bounded from below, a new bound is obtained in this case. During the derivation of the bounds, the associated optimality conditions on the field are found naturally. This new bound is a piece-wise analytic function whose algebraic expressions vary depending on the problem parameters: conductivity of each constituent, volume fractions and external loading. In one subset of parameters, it matches the translation bound. In the isotropic case, the bound derived in this dissertation coincides with those found by Cherkaev [14]. In the remaining cases, the new bound either improves the known bounds or extends the isotropic optimal bounds [14, 32] to the anisotropic case. Precisely, the new bounds are optimal in a big part of the region, where the known translation bounds are not optimal. And based on the optimal energy bounds, the G-closure boundary is calculated. In the rest of this region, the new bound is tighter than those previously known, and we have a better outer bound on the G-closure.

In Chapter 4, we construct optimal structures to attain the bounds, guided by the optimality conditions obtained in Chapter 3. More exactly, we found structures realizing the bound in almost all ranges of problem parameters, except a subset where we suggest the best possible structure. This method was suggested in [2]. All structures are orthogonal laminates of some finite rank, and the fields in two neighboring layers are rank-1 connected. Also the fields in each layer are assumed to comply with the optimality conditions. We construct optimal structures by finding ways to join the materials by rank-1 connections. In the subset where the bound cannot be attained by laminate structures, numerical experiments are performed. The result shows that the gap between the bound and the energy of specially constructed structure is rather small.

Remark 1.1 *Generally, optimal structures are not necessarily laminates: for example, Hashin and Shtrikman first suggested "coated spheres" geometry [20], Milton [27] proved optimality of parallel coated spheres, and later developed a method of transformation of optimal shapes [28], Lurie and Cherkaev showed the optimality of multilayer coated circles [26], Vigdergauz [42], Grabovsky and Kohn [19], and recently Liu [24] suggested special convex oval-shaped inclusions, Gibiansky and Sigmund suggested "bulk blocks" [18], Albin and Cherkaev proved the optimality of "haired spheres" [1], and a recent paper by Benveniste and Milton investigated "coated ellipsoids" [8]. All these structures admit separation of variables when effective properties are computed. It is not clear yet if the laminate structure approximates any other optimal structure, see for example [3, 11, 34]. We show, however, that proper laminates are optimal for the considered problem.*

The first part of dissertation ends with a summary of the result about the new bound, and structures that either attain it or best approximate it.

1.2 Optimal design problem

The second part of the dissertation focuses on finding the (quasi) convex envelope of the admissible set and the quasiconvexification of the integrand of some optimization problems. Those issues are intimately related to relaxation of nonconvex vectorial problems.

Unlike in the first part, u is a scalar field, but we do not limit ourselves to the two-dimensional case, we work in arbitrary dimensions. The assumption $a_3 = \infty$ is not needed either. Besides, we consider the integrand as both linear and quadratic with respect to the gradient of the state, i.e.,

1. the linear case: $\Psi(x, \xi) = G(x) \cdot \nabla u$, for some fixed field $G \in L^2(\Omega, R^N)$;

2. a quadratic case: $\Psi(x, \xi) = (1/2)|\nabla u|^2$.

Notice that the cost functional in the first part can be treated as linear because of the governing equation. This type of problem is very typical in optimal design. It is well known that in general, such problems do not admit optimal solutions, because the oscillating behavior of a minimizing sequence of characteristic functions persists to a degree that relaxation is needed. These relaxed versions might provide some insight in understanding optimal microstructures, and eventually lay down the foundation for setting up suitable numerical simulations [16].

The main tool in the analysis is an appropriate reformulation of the optimal design problem as a nonconvex, vector variational problem for which, due to the underlying structure carried by the conductivity law, a relaxation can be either fully computed, or appropriately estimated. This procedure leads one to work with div-curl Young measures as introduced in [36]. This program has been carried out for two materials in [9]. The objective of current work is to understand the differences in the more complex situation of multimaterials, and how the various ingredients and computations change for three or more materials.

In Chapter 5, we briefly recall some features of div-curl Young measures that is related to our analysis. Afterwards, we review the key ingredients of the variational method for optimal design problems in the frame of Young measures associated with pairs of gradient-divergence free vector field.

In Chapter 6, we deal with the linear cost functional whose relaxation amounts to determining the set of all generalized admissible pairs, or more precisely, the weak limits of all admissible pairs from the original problem. Because of the weak continuity of linear cost functionals with respect to weak convergence, this suffices for the linear case. A full relaxation is obtained and stated in Theorem 6.2.

In Chapter 7, the quadratic cost functional is studied. The analysis and computation are much harder than the linear cost functional case. In general, one only gets a lower bound of the relaxation, or subrelaxation (see [17] for two materials case). We first compute the subrelaxation using the variational method described in Chapter 5, after verifying it is fruitless to continue in this direction, we turn to the JBOC condition introduced in [36]. Following its idea of studying a few appropriately built problems, we succeed in finding a relaxation as stated in Theorem 7.2.

In Chapter 8, we describe the microstructure based on the relaxation result achieved in Chapter 7. The microstructures are local laminates of arbitrary finite order (Theorem 8.1). The diversity of microstructures is due to the fact that optimal solutions of the relaxed problem are sitting in a two-dimensional space where we have three independent rank-1 connections.

1.3 Connection between two parts

The problem of bounding the energy of multimaterial linear composites is equivalent to the problem of finding the quasiconvexification of the multiwell energy [21], (discussed in)[28]. In other words, one could obtain the G-closure through the quasiconvexification of corresponding multiwell energy. In principle, if we could find the quasiconvexification of the integrand defined in the first part, then we would have achieved the whole G-closure. G-closure could also be achieved by finding the quasiconvex hull of all $M^{2\times 4}$ matrices in the form of $(\nabla U, F)$ using the method described in the second part, where

$$\nabla U = (\nabla u_1, \nabla u_2)^T, \quad F = (F_1, F_2)^T, \quad \operatorname{div} F_j = 0,$$

and

$$F = \sum_i \chi_i A_i \nabla U, \qquad i = 1, 2, 3.$$

However, due to the technical difficulty of identifying Young measures associated with sequences $\{(\nabla U_j,\ F^j)\}$, we have not succeeded in doing so. This will be part of the future plans.

CHAPTER 2

PROBLEM AND NOTATION

In this chapter, we briefly review the problems of homogenization and G-closure. The references for this chapter can be found in [5, 12, 28], for example.

2.1 Three material conductivity composite

Consider three materials that form a two-dimensional periodic composite. The materials with isotropic conductivity tensor $k_i I$ occupy disjoint sets $\Omega_i \subset \mathbf{R}^2$, $i = 1, 2, 3$, that form a unit periodicity cell Ω:

$$\Omega = \bigcup_{i=1,2,3} \Omega_i, \quad \Omega = \{(x_1, x_2) :\ 0 \le x_1 < 1,\ 0 \le x_2 < 1\},$$

where I is the two-by-two identity matrix. It is assumed that

$$k_1 < k_2 < k_3, \quad \textit{and} \quad k_3 = \infty$$

The areas $m_i = \|\Omega_i\|$ of Ω_i are fixed and satisfy:

$$m_1 + m_2 + m_3 = 1,\ m_i \ge 0,\ \forall i = 1, 2, 3.$$

The governing equations applied to the composite are described as:

$$\operatorname{div}(K \nabla u) = 0, \quad \int_\Omega \nabla u(x) = E_0, \quad x \in \mathbf{R}^2, \tag{2.1}$$

where E_0 is the average field prescribed by the distant external loadings, and $K : \Omega \to \{K_1, K_2, K_3\}$ is the conductivity tensor defined by:

$$K(x) = \sum_i \chi_i(x) K_i, \quad K_i = k_i I, \tag{2.2}$$

where

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

Notice that $K(x)$ is actually determined through the partition Ω_i or $\{\chi_i\}$.

The assumption that $k_3 = \infty$ forces the field $u(x), x \in \Omega_3$ to be zero, and so is the energy density in Ω_3. The energy stored in the material with layout $K(x)$ is defined as:

$$W(K, E_0) = \inf_{u \in H^1_\#(\Omega) + E_0 \cdot x} \int_\Omega \nabla u(x) \cdot K(x) \nabla u(x)\, dx,$$

where $H^1_\#(\Omega)$ is the space of local H^1 functions that are Ω periodic with zero mean.

The effective conductivity K_{eff} of the composite with layout $\{\chi_i\}$ is defined as the conductivity tensor of homogeneous material storing the same energy, subjected to the same external loading. Hence, we have:

$$E_0 \cdot K_{eff} E_0 = \inf_{u \in H^1_\#(\Omega) + E_0 \cdot x} \int_\Omega \nabla u(x) \cdot K(x) \nabla u(x)\, dx \quad \forall E_0 \in R^2.$$

In order to completely determine effective properties of the composite, we subject the mixture to two orthogonal loadings

$$\lim_{|x| \to \infty} e_a(x) = e_{0a} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \text{and} \lim_{|x| \to \infty} e_b(x) = e_{0b} = \begin{pmatrix} 0 \\ r \end{pmatrix},$$

and calculate the sum of energies, which can be rewritten in terms of the vector potential $U = (u_1, u_2)$, in response to the external loading

$$E_0 = (e_{0a} | e_{0b}) = \mathrm{diag}(1, r).$$

The gradient matrix of potentials is defined as:

$$DU = \begin{pmatrix} DU_1 \\ DU_2 \end{pmatrix}, \quad DU_i = \begin{pmatrix} \frac{\partial u_i}{\partial x_1} & \frac{\partial u_i}{\partial x_2} \end{pmatrix}, \quad i = 1, 2.$$

The sum of energies is:

$$\mathcal{W}(K, E_0) = \inf_{U \in H^1_\#(\Omega, R^2) + E_0 x} \int_\Omega (DU(x) \cdot K(x) DU(x))\, dx, \tag{2.3}$$

where the inner product defined over two-by-two matrices is:

$$A \cdot B = \mathrm{Tr}(A^T B),$$

and the energy in the corresponding homogeneous material with conductivity tensor K_{eff}, subjected to the external loadings E_0 is:

$$E_0 K_{eff} \cdot E_0 = W(K, e_{0a}) + W(K, e_{0b}) = k_{*1} + k_{*2} r^2, \quad \forall r \in R, \tag{2.4}$$

where k_{*1} and k_{*2} are the eigenvalues of K_{eff}. Without loss of generality, it is assumed that $0 \leq r \leq 1$. Following the definition of the effective tensor K_{eff}, one gets:

$$E_0 K_{eff} \cdot E_0 = \inf_{U \in H^1_{\#}(\Omega, R^2)+E_0 x} \int_\Omega (DU(x) \cdot K(x) DU(x))\, dx = \mathcal{W}(K, E_0). \qquad (2.5)$$

2.2 G-closure boundary and optimal energy bounds

The G-closure $G(m_i, k_i)$ is defined as the closure of the set of all possible K_{eff} obtained for parameters m_i and k_i. We say $K_* \in G(m_i, k_i)$, if there exists a sequence of structures with layout $\{\chi_i^\epsilon\}$ whose effective tensor K^ϵ_{eff} is such that $K^\epsilon_{eff} \to K_*$. The G-closure is a bounded subset of two-by-two symmetric matrices. It is also known to be rotationally invariant, so it is enough to consider the projection of the set in the two-dimensional eigenvalues plane. Two types of bounds are used to find G-closure: inner and outer bounds. An outer bound is a set $\mathcal{B}(m_i, k_i)$ that contains $G(m_i, k_i)$. An inner bound $\mathcal{S}(m_i, k_i)$, on the other hand, is a smaller set that lies inside $G(m_i, k_i)$. If we can construct sets $\mathcal{S}$ and $\mathcal{B}$ such that $\mathcal{S} = \mathcal{B}$, then we have fully characterized the G-closure.

We define outer bound $\mathcal{B}$ by a set of inequalities in the eigenvalues plane, that any tensor $K_* \in G(m_i, k_i)$ must satisfy. For example, the known Wiener bounds and translation bounds are given by:

1. Wiener bound

$$\lambda_{min}(K_*) \geq \left(\sum_{i=1}^N \frac{m_i}{k_i} \right)^{-1}, \quad \lambda_{max}(K_*) \leq \sum_{i=1}^N m_i k_i,$$

   where λ_{min} and λ_{max} are the minimum and maximum eigenvalues of K_* respectively.

2. The translation bound

$$\frac{\mathrm{Tr} K_* - 2k_1}{\det K_* - k_1^2} \leq 2 \sum_{i=1}^N \frac{m_i}{k_i + k_1}, \quad \frac{\mathrm{Tr} K_* - 2k_N}{\det K_* - k_N^2} \geq 2 \sum_{i=1}^N \frac{m_i}{k_i + k_N}.$$

The outer bounds depend only on the parameters k_i and m_i. Because G-closure contains all possible effective tensor K_{eff} of certain m_i and k_i, and K_{eff} is associated with $\mathcal{W}(K, E_0)$ through (2.4), we construct outer bounds by finding a lower bound on $\mathcal{W}(K, E_0)$. Its complementary upper bound can be established by solving a dual problem in the same way, replacing the conductivity k_i by the resistivity $\rho_i = 1/k_i$. Our attention is then brought to the lower bound defined by:

$$B(E_0, k_i, m_i) = \inf_{\chi} \mathcal{W}(K, E_0), \tag{2.6}$$

where χ satisfies

$$\chi = \{\chi_i\} \in \{0, 1\}^3, \quad \int_{\Omega} \chi_i \, dx = m_i, \quad i = 1, 2, 3.$$

It depends on the ratio r of magnitudes of the two external loadings, and will be written as $B = B(r)$ from now on, with other parameters fixed.

The inner bound of the G-closure or $\mathcal{S}$ is formed by the effective tensor of the structures. Therefore if the lower bounds equal to the energy of some structure, or can be approached by the energy of a sequence of structures with fixed (m_i, k_i) and layout χ^{ϵ}, then we conclude we have reached the G-closure boundary. And the G-closure can be completely characterized by its boundary, because it is closed, bounded, and simply connected. This sequence of structures are called optimal structures, and the bound $B(r)$ is said to be optimal. The optimal bounds $B(r)$ and eigenvalues k_{*1} and k_{*2} of K_* located on the G-closure boundary are related through

$$B(r) = k_{*1} + k_{*2} r^2 \tag{2.7}$$

by (2.4)-(2.6). And the eigenvalues can be computed as:

$$k_{*1}(r) = B - \frac{r}{2} \frac{d\,B}{d\,r}, \quad k_{*2}(r) = \frac{1}{2\,r} \frac{d\,B}{d\,r}. \tag{2.8}$$

The pairs $(k_{*1}(r), k_{*2}(r))$ form a parametric equation for the boundary of the G-closure set. If the parameter r can be explicitly excluded from system (2.8), one obtains an explicit relation between $k_{*1}(r)$ and $k_{*2}(r)$.

2.3 Known bounds on G-closure

2.3.1 Outer bounds

The problem of exact bounds has a long history. It started with the bounds by Voigt and Reuss, called also Wiener bounds or the arithmetic and harmonic mean bounds. The bounds are valid for all microstructures and become in a sense exact for laminates: one of the eigenvalues of K_* of a laminate is equal to the harmonic mean of the mixed materials' conductivities, and the other one, to the arithmetic mean of them. The pioneering paper by Hashin and Shtrikman [20] found the bounds and the matching structures for optimal isotropic two-component composites, and suggested bounds for multicomponent ones. The exact bounds and optimal structures of *anisotropic* two-material composites were found in earlier papers [22, 23, 25, 39] using a version of the translation method (see its description in the books [5, 12, 15, 28]. The method is equivalent to building the polyconvex envelope of a multiwell Lagrangian, as it was shown by Kohn and Strang [22, 23]; the wells are the energy of the materials plus their cost (here, "cost" is the dual variable to the volume fraction of material in the composite). The theory of bounds for the two-material composite is now well developed and applied to elastic, viscoelastic, and other linear materials.

Bounds for multicomponent composites turn out to be much more difficult. Milton [27] showed that the Hashin-Shtrikman bound is not exact everywhere (it tends to an incorrect limit when $m_1 \to 0$), but is exact when m_1 is larger than a threshold,

$$m_1 \geq 2\theta(1 - m_2), \tag{2.9}$$

where

$$\theta = \frac{k_1(k_3 - k_2)}{(k_2 + k_1)(k_3 - k_1)} \leq \frac{1}{2}.$$

Milton and Kohn [29] suggested an extension of the translation method to anisotropic multimaterial composites, computed the anisotropic bounds for multicomponent composites and the optimal structures. Nesi [32] suggested a new tighter bound for *isotropic* multicomponent structures, and Cherkaev [14] further improved it and found optimal structures.

2.3.2 Inner bound (optimal structures)

2.3.2.1 Two-material optimal structures

The topology of two-material optimal structures is simple and intuitively clear: for isotropic or moderately anisotropic loading, the material with smaller conductivity k_1 "wraps" the one with bigger conductivity k_2 ($k_2 > k_1$), so that k_2 forms a nucleus and k_1 forms a core. The G-closure in this case is completely known due to the work in [20, 25, 39].

2.3.2.2 Multimaterial optimal structures

The multimaterial structures are more diverse and nonunique, and require new ideas for constructing. Milton [27], Lurie and Cherkaev [26], and later Barbarosie [7] described two types of isotropic structures that realize the multicomponent bound for sufficiently large volume fractions (see (2.9)). Gibiansky and Sigmund ([18]) expand the domain of applicability of Hashin-Shtrikman bounds to

$$2\theta(\sqrt{m_2} - m_2) \leq m_1 \leq 2\theta(1 - m_2).$$

They demonstrated new isotropic nonlaminate microstructures (bulk structures) that realize this bound. Albin et al. [2] extended the results of Gibiansky and Sigmund [18], finding laminates that realize translation bounds for both isotropic and anisotropic case in a range of parameters

$$m_1 \geq g_{acn}, \quad \text{and } \frac{|k_{*2} - k_{*1}|}{k_{*1} + k_{*2}} \leq \hat{g}_{acn},$$

where k_{*1} and k_{*2} are the eigenvalues of K_*. These inequalities represent the range of volume fractions and degree of anisotropy of a composite where the translation bound is optimal. For isotropic composites ($k_{*1} = k_{*2}$), the range of applicability of the found laminates coincides with the one of bulk structures suggested by Gibiansky and Sigmund.

Remark 2.1 *This region corresponds to case D1 in Chapter 3 and 4, where our new results of bounds and optimal structures are identical to those found by Albin et al. [2]. We describe this region explicit in those chapters.*

Structures that realize the isotropic bound for the whole range of volume fractions were found in [14].

CHAPTER 3

ENERGY BOUNDS AND BOUNDS ON G-CLOSURE

In this chapter, we describe the analysis involved to derive the lower bounds on the energy of composites and provide details on how those bounds are found, which turns out to be by solving some nonlinear programming problem. Such lower bounds vary depending on the problem parameter (m_i, k_i) as well as external loading $E_0 = diag(1, r)$, or precisely r . They are piece-wise analytic functions. The bounds on the G-closure follows, after the energy bounds are obtained.

3.1 Basis

Prior to the analysis of the bound, we introduce an orthonormal basis

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

of two-by-two matrices. In terms of this basis, any matrix $E \in M^{2\times 2}$ can be written as

$$E = \frac{1}{\sqrt{2}}s_1(E)\mathbf{a_1} + \frac{1}{\sqrt{2}}d_1(E)\mathbf{a_2} + \frac{1}{\sqrt{2}}d_2(E)\mathbf{a_3} + \frac{1}{\sqrt{2}}s_2(E)\mathbf{a_4} \tag{3.1}$$

where

$$\begin{aligned}
s_1(E) &= \frac{1}{\sqrt{2}}(E_{11} + E_{22}), \quad d_1(E) = \frac{1}{\sqrt{2}}(E_{11} - E_{22})\\
s_2(E) &= \frac{1}{\sqrt{2}}(E_{12} - E_{21}), \quad d_2(E) = \frac{1}{\sqrt{2}}(E_{12} + E_{21}).
\end{aligned} \tag{3.2}$$

In this basis, the energy of an isotropic material with conductivity tensor kI has the form

$$W(k, E) = kTr(E\,E^T) = k(s_1^2 + s_2^2 + d_1^2 + d_2^2). \tag{3.3}$$

Furthermore the representation for determinant is:

$$\det(E) = \frac{1}{2}(s_1^2 + s_2^2 - d_1^2 - d_2^2). \tag{3.4}$$

The relation among S_{0j}, D_{0j} of average field E_0 and corresponding $s_j, d_j,\ j = 1, 2$, components of the response $E = DU$ in the composite to the external loading is represented by:

$$\begin{aligned} &\int_\Omega s_1(x)\,dx = S_{01} = \frac{(1+r)}{\sqrt{2}}, \quad \int_\Omega s_2(x)\,dx = S_{02} = 0, \\ &\int_\Omega d_1(x)\,dx = D_{01} = \frac{(1-r)}{\sqrt{2}}, \quad \int_\Omega d_2(x)\,dx = D_{02} = 0 \end{aligned} \tag{3.5}$$

The representation of the energy and fields in terms of this basis will simplify computations related to the derivation of a bound, that is to be discussed in the rest of the chapter.

3.2 Technique and relaxation

The technique for the bound derivation, *localized polyconvexification*, is described in [32, 14]. Here, we repeat the argument of Cherkaev [14]. As in the translation method [12, 28], we construct a lower bound using quasi-affiness of the determinant function

$$\int_\Omega \det(E)dx = \det(E_0). \tag{3.6}$$

Start with adding and substracting $2t\det E$ for some $t \in \mathbb{R}$,

$$\mathcal{W}(K, E_0) = \inf_{\substack{E=\nabla U \\ U \in H^1_\#(\Omega)+E_0 x}} \int_\Omega (KE \cdot E) + 2t\det(E))\,dx - 2t\det(E_0). \tag{3.7}$$

Next we relax the point-wise differential constraint on $E = \nabla U$ by replacing the set $H^1_\#(\Omega)^2 + E_0 x$ with the set of $E \in L^2(\Omega, R^{2\times 2})$ such that

$$\int_\Omega E\,dx = E_0.$$

Furthermore, the constraint

$$\det(E) \geq 0, \quad \text{or } s_1^2 + s_2^2 - d_1^2 - d_2^2 \geq 0 \ \text{ a.e. } x \in \Omega, \quad \text{if } \det(E_0) \geq 0 \tag{3.8}$$

is imposed on E. This constraint is proved in [4] to be satisfied by any $U \in H^1_\# + E_0 x$ that is a solution to (2.1). Such constraints are used also in [14, 32]. Now we wind up with a relaxed problem that gives a lower bound of $\mathcal{W}(K, E_0)$

$$\mathcal{W}(K, E_0) \geq \inf_{\mathcal{E}} \int_\Omega ((KE \cdot E) + t\det(E))\, dx - t \det(E_0), \tag{3.9}$$

$$\mathcal{E} = \{E \in L^2(\Omega, \mathbb{R}^{2\times 2}) : \int_\Omega E\, dx = E_0,\ (3.8) \ \text{holds}\} \tag{3.10}$$

which can be rewritten as:

$$\mathcal{W}(K, E_0) \geq Y(E_0(r), t) - 2rt, \tag{3.11}$$

where

$$Y(E_0(r), t) = \inf_{\mathcal{E}} \int_\Omega (k(s_1^2 + s_2^2 + d_1^2 + d_2^2) - t(s_1^2 + s_2^2 - d_1^2 - d_2^2))\, dx, \tag{3.12}$$

using (3.3), (3.4) and (3.5). (3.11) gives a family of lower bounds on $\mathcal{W}(K, E_0)$ parameterized by t. We seek the best possible bound $B(r)$ of this family

$$B(r) = \max_t (Y(E_0(r), t) - t\det E). \tag{3.13}$$

After $B(r)$ is achieved, using (2.8), one can find the bounds for K_*, or the bounds for the G-closure. The constraint (3.8) could be slack or strict in different regions Ω_i, depending on the problem's parameters. If inequality (3.8) is slack everywhere, the procedure coincides with polyconvexification and gives the conventional translation bound.

Remark 3.1 *The bound for isotropic composites obtained in [14] uses a stronger inequality, which, however, coincides with* (3.8) *for the case* $k_3 = \infty$ *considered here.*

3.3 Nonlinear programming problem

The energy bound is found by solving the max-min problem (see (3.13)) where the minimization problem prescribes the condition on the optimal fields. If the minimizer E is a gradient or can be approximated in a proper sense by a sequence of gradients, then the bound is optimal. Using (3.2), this minimization problem can be written as:

$$\text{Minimize in } s_j, d_j : \int_\Omega [(k+t)(s_1^2 + s_2^2) + (k-t)(d_1^2 + d_2^2)]\, dx$$

subject to (3.5) and (3.8)

We can split the integral into a sum of integrals over Ω_i and minimize in each Ω_i independently, due to the fact that the differential constraint on the field is relaxed, hence the boundary conditions between the fields in neighboring domains may be omitted also. Introduce

$$S_{ij} = \frac{1}{m_i}\int_{\Omega_i} s_j(x)\,dx, \quad D_{ij} = \frac{1}{m_i}\int_{\Omega_i} d_j(x)dx,\ j = 1, 2, \tag{3.14}$$

and recall that the field in Ω_3 is zero

$$s_j(x) = d_j(x) = 0,\ \forall x \in \Omega_3 \ \Rightarrow\ S_{3j} = D_{3j} = 0. \tag{3.15}$$

Then the problem can be reformulated as:

$$\text{Minimize in } (S_{ij}, D_{ij}) : V_1 + V_2, \tag{3.16}$$

subject to

$$\begin{gathered} m_1 S_{11} + m_2 S_{21} = S_{01},\ m_1 S_{12} + m_2 S_{22} = 0, \\ m_1 D_{11} + m_2 D_{21} = D_{01},\ \ m_1 D_{12} + m_2 D_{22} = 0, \end{gathered} \tag{3.17}$$

where

$$V_i = \inf_{s^2 \geq d^2} \int_{\Omega_i} \left((k_i + t)s^2 + (k_i - t)d^2\right) dx \tag{3.18}$$

and

$$s^2 = s_1^2 + s_2^2, \quad d^2 = d_1^2 + d_2^2.$$

V_i are functions of S_{ij}, D_{ij}, which we show in the following section.

3.3.1 Structure of minimizers

Depending on the sign of $k_i - t$, expression V_i and corresponding $s(x), d(x)$ vary, and there are three situations:

1. $k_i - t > 0$ holds. All terms in the integrand of V_i are convex, hence applying Jensen's inequality to each of them, we have:

$$V_i = m_i(k_i + t)(S_{i1}^2 + S_{i2}^2) + m_i(k_i - t)(D_{i1}^2 + D_{i2}^2). \tag{3.19}$$

   The infimum is actually a minimum when fields s, d satisfy:

$$s_j(x) = S_{ij}\ , d_j(x) = D_{ij} \ \text{ a.e. } x \in \Omega_i, \quad j = 1, 2.$$

2. $k_i - t < 0$ holds. In this situation the d terms are concave, yet the inequality

$$(k_i - t)d^2 \geq (k_i - t)s^2$$

holds. Thus the replacement of the second term by $(k_i - t)s^2$ decreases the integral value. Consequently, we get:

$$V_i = \inf \int_{\Omega_i} 2k_i s^2 \, dx = 2k_i m_i (S_{i1}^2 + S_{i2}^2), \tag{3.20}$$

where the infimum becomes a minimum again, if s, d are:

$$s_j = S_{ij}, \ d^2 = s^2 \text{ a.e. } x \in \Omega_i \ \text{ or } \ s_j = S_{ij}, \ d^2 = S_{i1}^2 + S_{i2}^2 \text{ a.e. } x \in \Omega_i.$$

As a consequence,

$$\det(E) = s_1^2 + s_2^2 - (d_1^2 + d_2^2) = 0, \ \text{a.e. } x \in \Omega_i.$$

3. If $k_i - t = 0$ holds, the second term disappears, thus one has:

$$V_i = \inf \int_{\Omega} 2k_i s^2 = 2m_i k_i (S_{i1}^2 + S_{i2}^2), \tag{3.21}$$

which is the same as the previous case. However the minimum is achieved by different fields:

$$s_j = S_{ij}, \quad d^2 \leq s^2.$$

In the second situation, the constraint (3.8) comes to play a role because of the non-convexity of term $(k_i - t)d^2$, and this will lead us to new bounds.

3.4 Derivation of bounds

We will first solve the minimization problem (3.16) for fixed t, whose solution $Y(r,t)$ changes, depending on the range of t. There exist five cases, in each of which, after the solution $Y(r,t)$ of (3.16) is obtained, the bounds will be derived by solving the maximization problem with respect to t. The G-closure boundary is described after derivation of bounds.

3.4.1 Intermediate value $\mathbf{t} \in (\mathbf{k_1}, \mathbf{k_2})$

There will be two different situations when $t \in (k_1, k_2)$ because the solution of the minimization problem (3.16) varies depending on the average (or external) field $E_0(r)$.

3.4.1.1 Study of minimization problem (3.16)

If $t \in (k_1, k_2)$, we would have $k_2 - t > 0$ and $k_1 - t < 0$, $V = V_1 + V_2$ are as follows (see (3.19), (3.20))

$$V = 2m_1k_1(S_{11}^2 + S_{12}^2) + m_2(k_2 + t)(S_{21}^2 + S_{22}^2) + m_2(k_2 - t)(D_{21}^2 + D_{22}^2). \tag{3.22}$$

We will minimize V subject to (3.17). As stated in the previous section, the components d_i in Ω_1 are:

$$d_1^2 + d_2^2 = S_{11}^2 + S_{12}^2, \quad \text{a.e.} \quad x \in \Omega_1.$$

Applying Jensen's inequality, we get:

$$|\Omega_1|(S_{11}^2 + S_{12}^2) = \int_{\Omega_1} (d_1^2 + d_2^2)\, dx \geq |\Omega_1|(D_{11}^2 + D_{12}^2),$$

or equivalently,

$$S_{11}^2 + S_{12}^2 \geq D_{11}^2 + D_{12}^2. \tag{3.23}$$

We express S_{1j} in terms of S_{2j}, and D_{1j} in terms of D_{2j}, respectively, using the affine equality contraint in (3.17):

$$\begin{aligned} S_{11} &= \frac{S_{01} - m_2 S_{21}}{m_1}, \ S_{12} = \frac{-m_2 S_{22}}{m_1}, \\ D_{11} &= \frac{D_{01} - m_2 D_{21}}{m_1}, \ D_{12} = \frac{-m_2 D_{22}}{m_1}. \end{aligned} \tag{3.24}$$

Substituting (3.24) back into (3.23) and the expression of V, we get the minimization problem, where both the objective functional $\tilde{V}$ and the inequality constraint Ψ are quadratic functions:

$$\begin{aligned} \tilde{V} = \frac{2k_1((S_{01} - m_2 S_{21})^2 + m_2^2 S_{22}^2)}{m_1} + m_2(k_2 + t)(S_{21}^2 + S_{22}^2) + m_2(k_2 - t)(D_{21}^2 + D_{22}^2), \\ \Psi = (D_{01} - m_2 D_{21})^2 + (m_2 D_{22})^2 - (S_{01} - m_2 S_{21})^2 - (m_2 S_{22})^2 \leq 0. \end{aligned}$$

The necessary condition for $(S_{21}, S_{22}, D_{21}, D_{22})$ to be a minimum is the Karush-Kuhn-Tucker condition:

$$\nabla \tilde{V} + \lambda \nabla \Psi = 0, \tag{3.25}$$

$$\lambda \Psi = 0, \ \lambda \geq 0, \tag{3.26}$$

$$\Psi((S_{21}, S_{22}, D_{21}, D_{22}) \leq 0. \tag{3.27}$$

The solutions to (3.25) and (3.26) are as follows:

$$s_1 = \{D_{22}=0,\ D_{21}=0,\ S_{22}=0,\ S_{21}=\frac{2k_1S_{01}}{2k_1m_2+k_2m_1+m_1t}\},\ \lambda_1=0;$$

$$\begin{aligned}
s_2 &= \{D_{21}=\frac{m_1(k_2+t)S_{01}+D_{01}(m_1k_2+2k_1m_2+m_1t)}{2m_2\tilde{k}},\ D_{22}=0,\\
S_{22} &= 0,\ S_{21}=\frac{(m_1k_2+2k_1m_2-m_1t)S_{01}+m_1(k_2-t)D_{01}}{2m_2\tilde{k}}\},\\
\lambda_2 &= -\frac{(k_2^2-t^2)m_1S_{01}+((k_2^2-t^2)m_1+(k_2-t)k_1m_2)D_{01}}{(k_2(S_{01}-D_{01})+t(S_{01}+D_{01}))m_1m_2};
\end{aligned}$$

$$\begin{aligned}
s_3 &= \{S_{21}=\frac{S_{01}\left[(k_2-t)\,m_1+2k_1m_2\right]}{2m_2\tilde{k}}-\frac{D_{01}m_1\,(k_2-t)}{2m_2\tilde{k}},\ S_{22}=0,\\
D_{21} &= -\frac{S_{01}m_1\,(k_2+t)}{2m_2\tilde{k}}+\frac{D_{01}\left[(k_2+t)\,m_1+2k_1m_2\right]}{2m_2\tilde{k}},\ D_{22}=0\}\\
\lambda_3 &= -\frac{(k_2^2-t^2)m_1S_{01}-((k_2^2-t^2)m_1+(k_2-t)k_1m_2)D_{01}}{(k_2(S_{01}+D_{01})+t(S_{01}-D_{01}))m_1m_2},
\end{aligned} \tag{3.28}$$

where $\tilde{k}=k_1m_2+k_2m_1$. First, notice $\lambda_2<0$ under the condition $k_1<t<k_2$, therefore s_2 cannot be a minimum. Whether s_1 can be a minimum depends on whether $\Psi(s_1)\le 0$ is satisfied. Substitute s_1 into Ψ and get:

$$\Psi=\frac{(D_{01}-S_{01})m_1(t+k_2)+2k_1m_2D_{01}}{(2k_1m_2+m_1k_2+m_1t)m_1},$$

which can be simplified to:

$$\Psi=\frac{2k_1m_2-2(\tilde{k}+m_1t)r}{(2k_1m_2+m_1k_2+m_1t)m_1},$$

using $D_{01}=\frac{1-r}{\sqrt{2}}$ and $S_{01}=\frac{1+r}{\sqrt{2}}$. $\Psi\le 0$ holds if and only if

$$2k_1m_2-2(\tilde{k}+m_1t)r\le 0,\quad or\quad \frac{k_1m_2}{\tilde{k}+m_1t}\le r. \tag{3.29}$$

If (3.29) is true, it can be shown that $\lambda_3<0$. Therefore, in this situation, s_3 cannot be a minimum either. The only possible minimum is s_2. On the other hand, if (3.29) does not hold, then $\Psi(s_1)>0$, which eliminates s_1. Furthermore, we have $\lambda_3>0$ in this situation, thus s_3 becomes the possible minimum. The Karush-Kuhn-

Tucker conditions are sufficient as well in our specific problem, because of the positive definiteness of $\nabla^2(\tilde{V} + \lambda_i \Psi),\ i = 1\ or\ 3$, which is shown as follows:

$$\nabla^2(\tilde{V} + \lambda_i \Psi) = diag(a, a, b, b),$$

where

$$a \;=\; \frac{4k_1 m_2^2}{m_1} + 2m_2(k_2 + t) - 2\lambda_i m_2^2, \quad b = 2m_2(k_2 - t) + 2\lambda_i m_2^2.$$

By "*diag*", we mean diagonal matrices. Both a and b are positive for $\lambda_1 = 0$. Substituting λ_3 into a and b, we get:

$$a = 2m_2(1 + r)(k_2 + t)\tilde{k}, \quad b = 2m_2(1 - r)(k_2 - t)\tilde{k},$$

which are also positive under the assumption $r \leq 1$ and $t \in (k_1, k_2)$. Therefore, s_1 is a minimum of V if $\dfrac{k_1 m_2}{\tilde{k} + m_1 t} \leq r$ holds (case B), otherwise s_3 is the minimum (case C). We discuss those two cases successively.

3.4.1.2 Case B

When $\dfrac{k_1 m_2}{\tilde{k} + m_1 t} \leq r$ holds, substituting s_1 back into $\tilde{V}$, we find the minimum $Y_B(t, r)$:

$$Y_B(t, r) = H_0 S_{01}^2 = \frac{(1 + r)^2}{2} H_0, \tag{3.30}$$

where

$$H_0 = \left(\frac{m_1}{2k_1} + \frac{m_2}{k_2 + t} \right)^{-1}. \tag{3.31}$$

The corresponding average field in Ω_1 can be found as well, using (3.24),

$$D_{11} = \frac{D_{01}}{m_1}, D_{12} = 0, S_{12} = 0, S_{11} = \frac{(k_1 + t)S_{01}}{2k_1 m_2 + k_1 m_1 + t m_1} = \frac{H_0}{2k_1} S_{01},$$

and the point-wise minimizers are:

$$d_1 = D_{21} = 0, d_2 = D_{22} = 0, s_2 = S_{22} = 0, s_1 = S_{21},\ \text{a.e. in } \Omega_2, \tag{3.32}$$

$$d_1^2 + d_2^2 = S_{11}^2,\ s_1 = S_{11},\ s_2 = S_{12} = 0, \quad \text{a.e. in } \Omega_1, \tag{3.33}$$

which implies

$$E \;=\; \alpha I, \quad a.e.\ in\ \Omega_2, \tag{3.34}$$

$$Tr(E) \;=\; constant, \quad det(E) = 0 \;\; a.e.\ in\ \Omega_1, \tag{3.35}$$

taking into account (3.2). Notice that $S_{11} = Tr(E)$ and recall

$$det(E) = \frac{1}{2}(s_1^2 + s_2^2 - d_1^2 - d_2^2).$$

The computation shows another fact about the minimizing field:

$$\frac{S_{11}}{S_{21}} = \frac{Tr(E_1)}{Tr(E_2)} = \frac{k_2 + t}{2k_1}, \tag{3.36}$$

where $E_i, i = 1, 2$, represent the field in Ω_i. The relationship (3.36) is used to solve the field in structures that realize the bound. The corresponding bound B_B is found by solving:

$$B_B = \max_{t \in (k_1, k_2)} (Y_B(t, r) - 2tr).$$

Differentiating $Y_B(t, r) - 2tr$ with respect to t, two critical values of t are obtained:

$$\begin{aligned} t_{cr1} &= -\frac{r\, m_1 k_2 + 2r\, m_2 k_1 - k_1 \sqrt{r m_2}(1 + r)}{r\, m_1}, \\ t_{cr2} &= -\frac{r\, m_1 k_2 + 2r\, m_2 k_1 + k_1 \sqrt{r m_2}(1 + r)}{r\, m_1}. \end{aligned} \tag{3.37}$$

Using basic knowledge of calculus (study sign of derivative), it can be easily shown that the maximum is achieved at t_{cr1}, therefore $t_{opt} = t_{cr1}$. Substituting it back into $Y_B(t, r) - 2tr$, we get the energy bound:

$$B_B = \frac{k_1(1 + r - 2\sqrt{r m_2})^2}{2m_1} + r\, k_2. \tag{3.38}$$

3.4.1.2.1 G-closure boundary After the energy bound B_B is obtained, the parametric representation for k_{*1} and $k_{*2}(r)$ at the boundary of the G-closure are found using (2.8), if B_B is optimal:

$$k_{*1} = K(r) \quad \text{and} \quad k_{*2} = K\left(\frac{1}{r}\right), \tag{3.39}$$

where

$$K(r) = \frac{k_1\left(1 - \sqrt{r m_2}\right)\left(1 + r - 2\sqrt{r m_2}\right)}{m_1} + r k_2.$$

The eigenvalues $k_{*1}(r)$ and $k_{*2}(r)$ are correlated through the parametric equation

$$\frac{1}{k_{*1} - t_{cr1}(r)} + \frac{1}{k_{*2} - t_{cr1}(r)} = \frac{2}{H_0 - 2t_{cr1}(r)}. \tag{3.40}$$

3.4.1.3 Case C

If $\dfrac{k_1 m_2}{\tilde{k} + m_1 t} > r$ holds, s_3 is substituted into $\tilde{V}$ to find the minimum $Y_C(r,t)$:

$$Y_C = 2\frac{-m_1 r^2 t^2 + 2m_2\left(k_1 - \tilde{k}\right) r\, t + m_2 k_1 k_2 + \tilde{k} k_2 r^2}{2m_2 \tilde{k}}. \tag{3.41}$$

The average field inside Ω_1, in this case, is found by substitution of s_3 into (3.24):

$$D_{12} = S_{12} = 0,\ D_{11} = S_{11} = \frac{S_{01}\left(k_2 + t\right)}{2\tilde{k}} + \frac{D_{01}\left(k_2 - t\right)}{2\tilde{k}}. \tag{3.42}$$

Let us analyze the point-wise condition on the field in Ω_1. We know they should satisfy

$$d_1^2 + d_2^2 = S_{11}^2,\ s_1 = S_{11},\ s_2 = S_{12} = 0, \quad \text{a.e. in } \Omega_1,$$

as in case B, because $k_1 - t < 0$ holds in both cases (see "structure of minimizer" for details), which is equivalent to:

$$det(E) = 0,\ Tr(E) = constant.$$

On the other hand, we have $D_{11} = S_{11}$, which implies $d_1 = S_{11},\ d_2 = 0$ under the relation

$$d_1^2 + d_2^2 = S_{11}^2.$$

Therefore the point-wise fields are:

$$d_2 = s_2 = 0, \quad d_1 = s_1 = S_{11}. \tag{3.43}$$

In other words, the field E in Ω_1 is also constant. This is not necessary in case B where the field in Ω_1 can vary as long as (3.35) is satisfied. The point-wise fields in Ω_2 satisfy:

$$s_1 = S_{21},\ s_2 = S_{22} = 0,\ d_1 = D_{21},\ d_2 = D_{22} = 0. \tag{3.44}$$

This says that the field in Ω_2 is a constant diagonal matrix $E = diag(a,b)$, different from the multiple of the identity matrix in case B.

Differentiating $Y_C(r,t) - 2rt$ with respect to t, the optimal value t_{opt} can be found:

$$t_{opt} = \frac{\left(k_1 - \tilde{k}\right) m_2}{r m_1}, \tag{3.45}$$

and the bound in case C is:

$$B_C = \frac{\left(1 - m_2\right)^2 k_1 + m_1 m_2 k_2}{2m_1} + \frac{k_2}{2m_2} r^2. \tag{3.46}$$

3.4.1.3.2 G-closure boundary The calculation for the region C is similar. According to (2.8), we have:

$$k_{*1} = \frac{(1-m_2)^2 k_1 + m_1 m_2 k_2}{m_1}, \quad k_{*2} = \frac{k_2}{m_2}. \tag{3.47}$$

3.4.1.4 Description of regions B and C

The applicability of bounds will be described through systems of inequalities on r in terms of the conductivies k_i and volume fractions m_i. A part of the inequalities is obtained by solving the constraint:

$$k_1 < t_{opt} < k_2. \tag{3.48}$$

The rest is derived from the requirement:

$$\frac{k_1 m_2}{\tilde{k} + m_1 t} \leq r \quad \text{in case B,} \quad \text{or} \quad \frac{k_1 m_2}{\tilde{k} + m_1 t} > r \quad \text{in case C,} \tag{3.49}$$

and the assumption $r \in [0, 1]$. The plot of the solution to the system of inequalities (3.48) and (3.49), in the co-ordinate plane $r - m_1$ (taking m_2, k_i's as parameter), is named as region B and C, respectively. Region B is given by the following:

$$\psi_{AB} < r < \psi_{BD}, \quad 1 \geq r \geq m_2,$$

$$\psi_{AB} = m_2 \left(\frac{k_1}{\tilde{k} + \sqrt{\tilde{k}^2 - m_2 k_1^2}} \right)^2, \tag{3.50}$$

$$\psi_{BD} = m_2 \left(\frac{2k_1}{a + \sqrt{a^2 - 4 m_2 k_1^2}} \right)^2, \tag{3.51}$$

$$a = \tilde{k} + 2 m_2 k_1, \quad \tilde{k} = m_1 k_2 + m_2 k_1. \tag{3.52}$$

Region C is represented by:

$$\psi_{AC} < r < \psi_{CE}, \quad 0 \leq r < m_2,$$

$$\psi_{AC} = \frac{m_2(k_1 - \tilde{k})}{m_1 k_2}, \quad \psi_{CE} = \frac{m_2(k_1 - \tilde{k})}{m_1 k_1}. \tag{3.53}$$

ψ_{AB} and ψ_{AC} are solutions to $t_{opt} = k_2$ in case B and C, respectively. Similarly, ψ_{BD} and ψ_{CE} are solutions to $t_{opt} = k_1$. The boundary between Regions B and C is the line given by $r = \dfrac{k_1 m_2}{\tilde{k} + m_1 t}$. Substituting t_{opt} in either case B or C for t, leads to

$$r = m_2 \tag{3.54}$$

dividing regions B and C.

3.4.2 Case $t = k_2$

We follow the same steps as in the previous section. First we find $V = V_1 + V_2$ by evaluating V_1, V_2 in this case (see (3.20), (3.21)):

$$V = 2k_1 m_1 (S_{11}^2 + S_{12}^2) + 2k_2 m_1 (S_{21}^2 + S_{22}^2). \tag{3.55}$$

V does not depend on D_{1j}, D_{2j}. Therefore we can minimize V only subject to the constraints

$$m_1 S_{1j} + m_2 S_{2j} = S_{0j},\ \ j = 1, 2$$

because the constraints

$$m_1 D_{1j} + m_1 D_{1j} = D_{0j}$$

can be satisfied by modifying point-wise $d_j, j = 1, 2$, in $\Omega_i, i = 1, 2$,

$$\begin{aligned} d_1^2 + d_2^2 &\le s_1^2 + s_2^2, \quad and \quad s_j = S_{2j}, && a.e\ in\ \ \Omega_2, \\ d_1^2 + d_2^2 &= s_1^2 + s_2^2, \quad and \quad s_j = S_{1j}, && a.e.\ in\ \ \Omega_1, \end{aligned} \tag{3.56}$$

due to the fact $D_{0j} \le S_{0j}$ for $r \in [0, 1]$. The minimum of V is found using the standard Lagrange multiplier procedure:

$$S_{1j} = \frac{H_2}{2k_1} S_{0j}, \quad S_{2j} = \frac{H_2}{2k_2} S_{0j}, \quad j = 1, 2, \tag{3.57}$$

or

$$S_{11} = \frac{H_2(1+r)}{2\sqrt{2}k_1},\ S_{21} = \frac{H_2(1+r)}{2\sqrt{2}k_2},\ S_{12} = S_{22} = 0,$$

if we take into account $S_{01} = \dfrac{1+r}{\sqrt{2}}$ and $S_{02} = 0$, where

$$H_2 = \left(\frac{m_1}{2k_1} + \frac{m_2}{2k_2} \right)^{-1},$$

and S_{11}, S_{21} satisfy

$$\frac{S_{11}}{S_{21}} = \frac{k_2}{k_1}. \tag{3.58}$$

(3.56) and (3.57) imply that point-wise fields in Ω_i satisfy:

$$\begin{aligned} Tr(E) &= constant, \quad a.e.\ in\ \Omega_i,\ i = 1, 2, \\ det(E) &= 0, \qquad\qquad a.e.\ in\ \Omega_1. \end{aligned} \tag{3.59}$$

The minimum $Y_A(r)$ is:

$$Y_A(r) \quad = \quad H_2 S_{01}^2 = \frac{H_2(1+r)^2}{2}. \tag{3.60}$$

The bound B_A is:

$$B_A = Y_A(r) - 2k_2 r = \frac{H_2(1+r)^2}{2} - 2k_2 r. \tag{3.61}$$

3.4.2.1 G-closure boundary

Find $k_{*1}(r)$ and $k_{*2}(r)$ again using (2.8) where

$$k_{*1} = K_A(r) = \frac{1}{2}(r+1)H_2 - rk_2, \quad k_{*2} = K_A(1/r). \tag{3.62}$$

Excluding r from (3.62), we find the equation describing the boundary. One can check that $k_{*1}(r)$ and $k_{*2}(r)$ are bounded as

$$\frac{2}{H_2 - 2k_2} = \frac{1}{k_{*1} - k_2} + \frac{1}{k_{*2} - k_2}. \tag{3.63}$$

This is similar to the Translation bound [25, 29, 39]. If the composite is isotropic, the bounds coincide with the ones found in [14, 32].

3.4.2.2 Description of region A

The region A where bound B_A is effective is defined similarly to regions B and C. We notice that when $t \in (k_2, \infty)$, the expression V is the same as in the case $t = k_2$, although the point wise $d_j,\ in\ \Omega_2$ is different (see the description of 'structure of minimizer' for details). Therefore the minimum of V will be Y_A as well and it is independent of t. Consequently, when maximizing $Y_A - 2tr$ with respect to t to find the bound, $t = k_2$ gives the maximum or the bound, because $Y_A - 2tr$ is linearly decreasing with respect to t. In conclusion, when $t \in (k_2, \infty)$, the bound is also B_A. We have pointed out that $r = \psi_{AB}$ and $r = \psi_{AC}$ are obtained by setting $t_{opt} = k_2$ in case B and C respectively. In addition, t_{opt} is a decreasing function of r in both case B and C; therefore any point below the curves ψ_{AB} and ψ_{AC} corresponds to some

$t > k_2$. As a consequence, the region below ψ_{AB} and ψ_{AC} occurs where the bound B_A is active. In the $r - m_1$ coordinate plane, it is given by the inequalities:

$$m_1 \geq 0, \quad 0 \leq r \leq 1, \tag{3.64}$$

$$r \leq \phi_{AB}, \; m_2 \leq r \leq 1, \tag{3.65}$$

$$r \leq \phi_{AC}, \quad 0 < r \leq m_2. \tag{3.66}$$

Curves ϕ_{AB} and ϕ_{AC} are described in (3.50) and (3.53).

3.4.3 Case $t = k_1$ (Translation bound)

This case can be viewed as a particular case of B, corresponding to some specific value $t = k_1$. The minimum Y_D of V and corresponding minimizers S_{ij}, D_{ij} can be obtained by substituting k_1 for t in s_1 (see (3.28)) and (3.30):

$$Y_D = H_1 \frac{(1+r)^2}{2}, \tag{3.67}$$

$$S_{21} = \frac{S_{01}}{k_1 + k_2} H_1, \; S_{22} = 0, D_{2j} = 0, \tag{3.68}$$

where

$$H_1 = \left(\frac{m_1}{2k_1} + \frac{m_2}{k_1 + k_2} \right)^{-1}.$$

Substituting (3.68) into thecorresponding affine equality in (3.24), the average in Ω_1 can be found as:

$$D_{12} = 0, \quad D_{11} = \frac{D_{01}}{m_1}, \quad S_{12} = 0, \quad S_{11} = \frac{S_{01}}{2k_1} H_1. \tag{3.69}$$

And the pointwise s_i, d_i in Ω_1 satisfy:

$$s_1 = S_{11}, \quad s_2 = S_{12}, \quad d_1^2 + d_2^2 \leq s_1^2 + s_2^2 \;\; a.e. \; in \; \Omega_1, \tag{3.70}$$

which is equivalent to:

$$d_1^2 + d_2^2 \leq S_{11}^2, \tag{3.71}$$

by (3.69). It is also true that $Tr(E(x)) = constant, \; x \in \Omega_1$. However $det(E) \neq 0$, which is different from case A, B and C. The bound B_D is:

$$B_D = H_1 \frac{(1+r)^2}{2} - 2r\, k_1 \tag{3.72}$$

and matches the classical Hashin-Shtrikman bound [20] if $r = 1$, and translation bounds [2, 18, 29], if $r \leq 1$.

3.4.3.1 G-closure Boundary

The calculations are similar to the previous case A. The effective conductivities are found using (3.62) with k_2 replaced by k_1 and H_2 by H_1. The parameter r can be excluded, and the boundary of the G-closure corresponding to the Translation bound is:

$$\frac{2}{H_1 - 2k_1} = \frac{1}{k_{*1} - k_1} + \frac{1}{k_{*2} - k_1}. \tag{3.73}$$

3.4.4 Small values $t \in (k_1, 0]$

In this case, both $k_2 - t > 0$ and $k_1 - t > 0$ are true; therefore V is:

$$\begin{aligned} V &= m_1(k_1 + t)(S_{11}^2 + S_{12}^2) + m_2(k_2 + t)(S_{21}^2 + S_{22}^2) \\ &+ m_1(k_1 - t)(D_{11}^2 + D_{12}^2) + m_2(k_2 - t)(D_{21}^2 + D_{22}^2). \end{aligned}$$

Differentiating V with respect to S_{ij}, D_{ij}, we get:

$$\begin{aligned} S_{i1} &= \frac{S_{01}}{k_i + t} H_+, \quad D_{i1} = \frac{D_{01}}{k_i - t} H_-., \quad S_{i2} = D_{i2} = 0. \\ H_+^{-1} &= \frac{m_1}{k_1 + t} + \frac{m_2}{k_2 + t}, \quad H_-^{-1} = \frac{m_1}{k_1 - t} + \frac{m_2}{k_2 - t}. \end{aligned}$$

Here H_+ and H_- are the Lagrange multipliers enforcing the constraint on S_{ij} and D_{ij} respectively in (3.17). This says that the fields E_i in each pure material component Ω_i are constant matrices with $rank(E_i - E_j) \neq 1$.

We compute the bound B_E as before:

$$\begin{aligned} B_E &= \max_{t \in [0, k_1)} (Y_E - 2tr), \\ Y_E &= \frac{1}{2} \left[H_+(1 + r)^2 + H_-(1 - r)^2 \right]. \end{aligned} \tag{3.74}$$

In principle, the optimal value t_{opt} could be found by solving the fourth-order equation:

$$\frac{d\,(Y_E - 2tr)}{d\,t} = 0.$$

After $t_{opt}(r)$ is found, B_E can be obtained by substituting $t_{opt}(r)$ into (3.74), then one can compute the G-closure boundary using (2.8), if this bound is optimal. The region E, where B_E is effective, could have also been obtained by solving $t_{opt} < k_1$. However, the complex nature of the fourth-order equation make an explicit algebraic expression unachievable. Although the general formula for the bound cannot be obtained, we do know that this bound is not realizable by laminate structures, because the optimality condition on the fields tells that such fields either are constant a.e. in Ω, or are approached by a sequence of gradients that are constant values in a proper sense [37]. Consequently, optimal laminates matching B_E will not exist. Under this circumstance, we can only conclude that B_E is a lower bound. Numerical experiments are performed to show how close B_E is to the optimal bound, by computing the relative difference between B_E and the energy of some particular structure, which is described and discussed in next chapter.

3.4.4.1 Region B_D and B_E

The region D is adjacent to the region B along the curve ϕ_{BD} (3.51) and E is adjacent to C along the curve ψ_{CE}, (3.53). These two regions are divided by the curve

$$\phi_{D2E} = -\frac{m_1 b - 2m_2 k_1 \tilde{k} + a\sqrt{m_1\left(m_1-1\right)b}}{2m_2 k_1 \tilde{k}}, \tag{3.75}$$

$$a = \tilde{k} + \left(m_1 + m_2\right) k_1,$$

$$b = a^2 - (k_1+k_2)^2 m_1 - 4m_2 {k_1}^2, \tag{3.76}$$

and are described as

$$\begin{aligned} \text{Region D} &: \quad \phi_{DB} < r, \quad \phi_{D2E} \le r \le 1, \quad m_1 \le 1 - m_2, \\ \text{Region E} &: \quad \max\{0, \phi_{CE}\} < r < \phi_{D2E}, \quad m_1 \le 1 - m_2. \end{aligned}$$

Note that ϕ_{D2E} is found by solving $\left.\dfrac{d\left(Y_E - 2tr\right)}{d\,t}\right|_{t=k_1} = 0$ for r.

CHAPTER 4

OPTIMAL STRUCTURES

In this chapter, we describe how to build structures that realize the bounds or optimal structures. The method used here follows closely the paper by [2]. The key is to join the pure material components whose fields comply with optimality conditions, derived in the last chapter, through rank-1 connections. A similar idea was used in [33].

All structures are orthogonal laminates of some rank, obtained by sequentially adding to the existing laminate a new one, along one of mutually orthogonal axes x_1 and x_2. The length scales in laminates are well separated. We choose to work with laminates because the field inside each layer can be treated as constant (see [10]) when well-separated length scales go to zero, thus making the computation of the energy easy. One can also show this by the use of gradient Young measures ([30, 34]). The fields in neighboring layers in a laminate have to satisfy rank-1 connections.

4.1 Rank-1 connections and optimality conditions on fields

The average field, prescribed by external loading, is assumed to be a diagonal matrix (see [28]) and eigenvectors are aligned with x_1 and x_2, hence fields in each layer are also diagonal matrices in $\mathbf{R}^{2\times 2}$ with eigenvectors codirected with the axes. Such matrices are denoted as $E = (\alpha, \beta)$ through their diagonal entries or eigenvalues. Two fields $E_1 = (\alpha_1, \beta_1)$ and $E_2 = (\alpha_2, \beta_2)$ are rank-1 connected if and only if

$$det(E_1 - E_2) = 0, \quad \text{or} \quad (\alpha_1 - \alpha_2)(\beta_1 - \beta_2) = 0. \tag{4.1}$$

In the eigenvalues plane, this means (α_1, β_1), (α_2, β_2) either lie in the same vertical line or horizontal line which are called rank-1 paths. Only materials whose fields form rank-1 paths can be joined together in laminates. On the other hand, the fields in optimal structures must satisfy the optimality conditions derived in Chapter 3. Hence, optimal structures can be created through rank-1 paths. Or more precisely, the materials whose fields agree with sufficient optimality conditions are joined together through rank-1 connections to generate laminates. The average field and volume fractions are computed while the construction carries on. The last rank-1 path must pass through the point $(1, r)$ in the plane prescribed by external loading E_0 and all materials are consumed in this last step. The created structures are optimal because we request that the optimality condition holds through the whole procedure. The optimal structures in regions A, B, C, D and best possible structure in region E are shown in Fig. 4.1. Note that region A is divided into two subregions A1 and A2 because of the difference of optimal structures realizing the bound B_A. And region D is divided into D1 and D2 according to the achievability of the bound. In D1, the optimal structures are found in [2], while in D2, no optimal laminates are obtained yet.

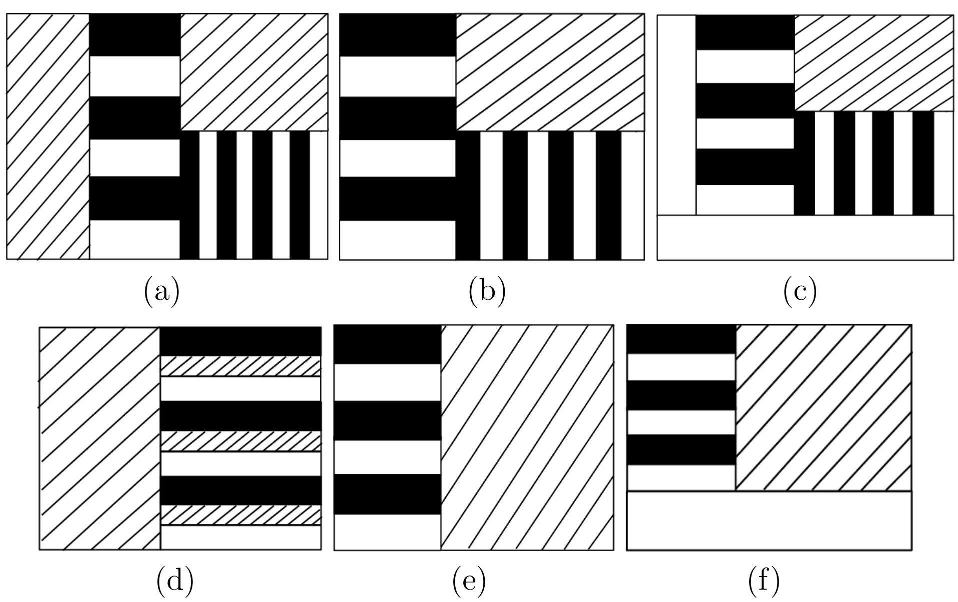

Figure 4.1 Cartoon of optimal structures in regions A -D1 and the presumed optimal structure in region E. (a) L(13,2,13,2) region A1 (b) L(13,2,13) region B (c) L(13,2,13,1,1) region D1 (d) L(123,2) region A2 (e) L(13,2,1) regions D2, E

4.2 Optimal structures in region B

In case B, the optimality condition (3.34) and (3.35) requests:

$$E_1 = (0, \beta) \text{ or } E_1 = (\beta, 0), \text{ in } \Omega_1, \quad E_2 = (\alpha, \alpha), \text{ in } \Omega_2.$$

Hence, material k_2 is never rank-1 connected to material k_3 whose fields are zero and material k_1 is used in layers to ensure compatibility. The optimal multiscale laminates in region B are T^2 structures (or $L(13, 2, 13)$-structure) and built through the following steps. The formation of rank-1 paths among optimal fields is illustrated in Fig. 4.2.

1. $L(13)$ substructure is formed. Materials k_1 and k_3 are laminated along the x_2 direction with relative volume fraction of material k_1 equal to μ_{11}. The fields in the materials are called E_{11} and E_{13}, and $E_{13} = (0, 0)$. The average field in the substructure is called E_{10}.

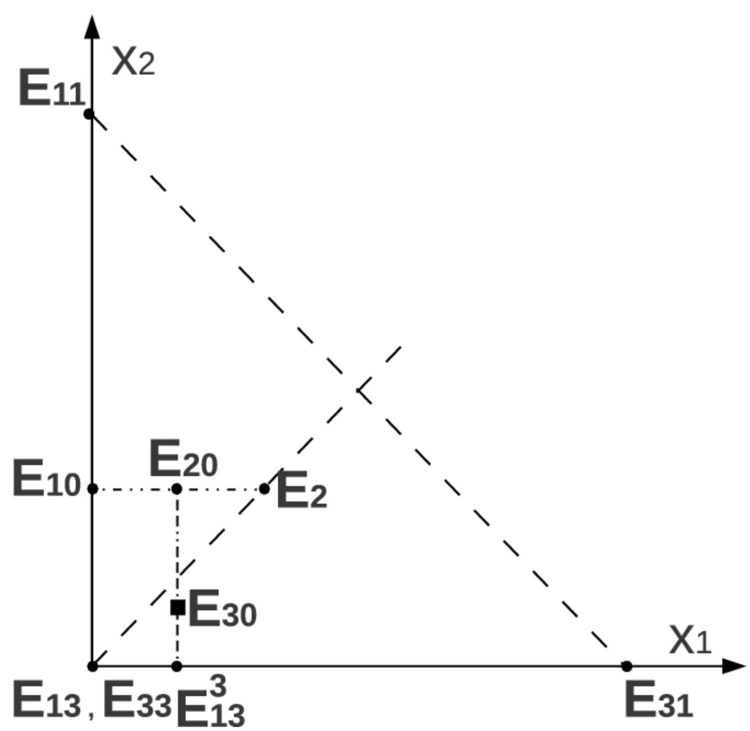

Figure 4.2 Fields in optimal laminates L(13,2,13) and formation of rank-1 path.

2. $L(13,2)$ substructure is formed. The obtained $L(13)$ structure is laminated with material k_2 (field $E_2 = (\alpha, \alpha)$) along the x_1 direction, with relative volume fraction of material k_2 equal to μ_2, to form a second rank laminate. The average field in the substructure is called E_{20}.

3. $L(13,2,13)$ structure is formed. The obtained $L(13,2)$ structure is laminated, along x_2 direction, with another laminate $L(13)$ which is formed by laminating material k_1 (field E_{31}) with k_3 (field $E_{33} = (0,0)$) along x_1 direction. The relative volume fraction of the second rank laminate $L(13,2)$ is μ_4. The average field of $L(13)$ is represented as E_{13}^3 and the relative volume fraction of material k_1 equals to μ_{31}. The average field in the final structure is called E_{30}.

4.2.1 Constraints

The average fields in the described substructures are:

$$E_{10} = E_{11}\mu_{11}, \quad E_{20} = E_{10}(1-\mu_2) + E_2\mu_2, \tag{4.2}$$

$$E_{13}^3 = E_{31}\mu_{31}, \quad E_{30} = E_{31}^3(1-\mu_4) + E_{20}\mu_4. \tag{4.3}$$

The laminate's volume fractions satisfy the geometric constraints:

$$\mu_{11}(1-\mu_2)\mu_4 + \mu_{31}(1-\mu_4) = m_1, \quad \mu_4\mu_2 = m_2. \tag{4.4}$$

There are four interfaces between layers in $L(13,2,13)$, which impose four rank-1 connection conditions or continuity conditions along the tangential direction of the interfaces on fields. The design variables μ's in the sequential structures are properly chosen to ensure these continuity conditions are satisfied, hence the following relations hold

$$E_{11} = (0,\beta), \; E_{31} = (\beta, 0), \tag{4.5}$$

$$E_{10}[2] = E_2[2] \;\rightarrow\; \beta\mu_{11} = \alpha, \tag{4.6}$$

$$E_{20}[1] = E_{13}^3[1] \;\rightarrow\; \alpha\mu_2 = \beta\mu_{31}. \tag{4.7}$$

The average field of the mixture equaling to the external field results in

$$e_{30} = (1, r),$$

hence:

$$1 = \alpha\mu_2(1-\mu_4) + \beta\mu_{31}\mu_4, \quad (\beta\mu_{11}(1-\mu_2) + \alpha\mu_2)\mu_4 = r. \tag{4.8}$$

4.2.2 Calculations of constants

Solving (4.4) and (4.6)-(4.8), we obtain:

$$\begin{aligned}
\beta &= \frac{(1+r) - 2\sqrt{m_2 r}}{m_1}, \quad \alpha = \sqrt{\frac{r}{m_2}}, \\
\mu_{11} &= \frac{r m_1}{(1+r)\sqrt{r m_2} - 2r\, m_2}, \quad \mu_4 = \sqrt{r m_2}, \\
\mu_{31} &= \frac{m_1}{(1+r) - 2\sqrt{r m_2}}, \quad \mu_2 = \sqrt{\frac{m_2}{r}}.
\end{aligned}$$

A straight calculation confirms that the fields coincide with the fields computed for the bounds; thus the energy matches the bound B_B.

4.2.3 Region of applicability

Requiring all volume fractions fall into the interval (0,1) and also enforcing $0 < r \le 1$, we obtain a system of inequalities of r:

$$\begin{aligned}
0 < \frac{r m_1}{(1+r)\sqrt{r m_2} - 2r\, m_2} < 1, \\
0 < \frac{m_1}{(1+r) - 2\sqrt{r\, m_2}} < 1, \\
0 < \sqrt{\frac{m_2}{r}} < 1, \quad 0 < \sqrt{r m_2} < 1.
\end{aligned}$$

The solution of the above inequalities varies depending on the relationship between m_1 and m_2:

$$\begin{cases} m_2 < r < 1 & \text{if } \; m_1 < 2\left(\sqrt{m_2} - m_2\right), \\ m_2 < r < \dfrac{1 - a_5 - \sqrt{1 - 2a_5}}{a_5}, & \text{otherwise }, \end{cases} \tag{4.9}$$

where

$$a_5 = \frac{2m_2}{(m_1 + 2m_2)^2}.$$

The region represented by (4.9) contains the region of applicability of the bound B_B.

4.3 Optimal structures in region C

Note that if $r = m_2$, then $\mu_2 = 1$, which implies that the substructure $L(13)$ formed in the first step of constructing $L(13, 2, 13)$ disappears or the composite degenerates into the T structure - second-rank laminate $L(13, 2)$ (see Fig. 4.1, region C). And one can show that L(13,2) matches the bound B_C that is effective in region C and therefore is optimal. The fields inside each component of the T structure comply with the optimality condition for this region. This structure plays the same role as the laminates in two-phase problem, in which an optimal structure of higher rank degenerates into a laminate if r is small enough.

4.4 Optimal structures in region A

In this region, two structures are found independently. Each of them is optimal in one of two mutually disjoint subregions A1, A2 of region A. The difference of the structures arises because the field in material k_2, prescribed by optimality conditions (3.59), allows for the multiple existence of rank-1 paths and hence multiple optimal structures (see Fig. 4.3 and Fig. 4.4 for the difference). In Fig. 4.3 and 4.4, the admissible range of fields in k_2 is represented by 45° solid line l.

4.4.1 Optimal structures in region A_1

Laminate L(13,2,13,2) is optimal in A1 (Fig. 4.1). It is built by adding a layer of material k_2 with field E_{42} along direction x_1 to the laminate $L(13, 2, 13)$ described in the previous section. The relative volume fraction of $L(13, 2, 13)$ is defined as μ_5. The field in material k_1 in region A is the same as that in region B; therefore the fields E_{11} and E_{31} are as in (4.5).

$$E_{11} = (0, \quad \beta), E_{31} = (\beta, \quad 0).$$

The construction of structure and rank-1 connectedness tell that E_{42} is in the form:

$$E_{42} = (\alpha_2, \quad r),$$

and the field E_{22} is assumed to be:

$$E_{22} = (\alpha_1, \quad \beta_1).$$

Also the optimality condition (3.59) on the field and relationship (3.58) lead to

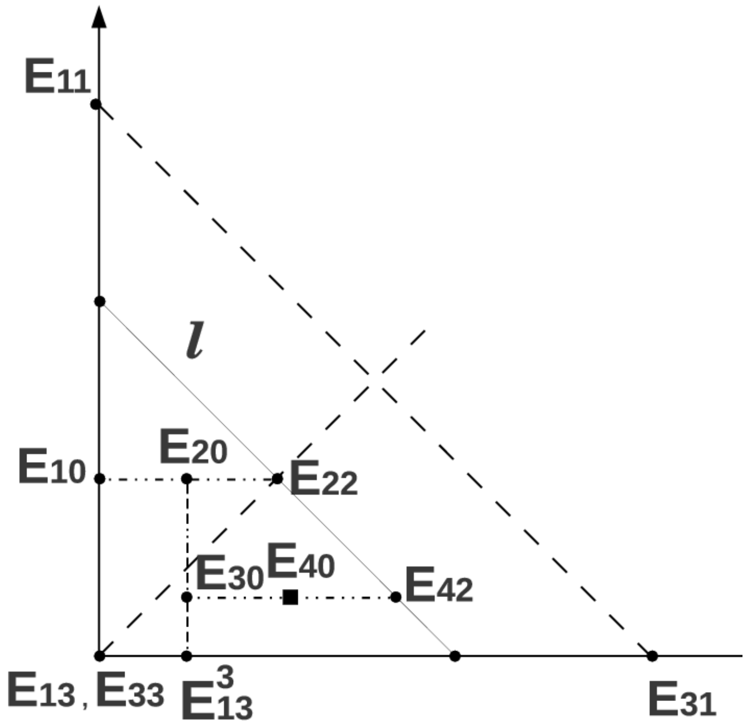

Figure 4.3 Fields in optimal laminate L(13,2,13,2) and formation of rank-1 path.

$$\beta_1 + \alpha_1 = \alpha_2 + r, \quad k_1\beta = k_2(\alpha_1 + \beta_1). \tag{4.10}$$

The average fields in the sequential substructures are as in (4.2), (4.3) and the average field in the whole laminate is computed as:

$$E_{40} = E_{30}\mu_5 + E_{42}(1 - \mu_5)$$

It has to match the external field $E_0 = (1, r)$. Continuity conditions along the interfaces in the substructures request:

$$E_{10}[2] \;=\; E_{22}[2], \quad E_{20}[1] = E_{13}^3[1]\mu_{31}, \quad E_{30}[2] = e_{42}[2],$$

and yield:

$$\mu_{11}\beta = \beta_1, \quad \mu_2\alpha_1 = \mu_{31}\beta, \quad \mu_{11}\mu_4(1 - \mu_2)\beta + \mu_2\mu_4\beta_1 = r. \tag{4.11}$$

The average field $E_{40} = (1, r)$ leads to:

$$1 = \alpha_2(1 - \mu_5) + \beta\mu_{31}\mu_5. \tag{4.12}$$

The volume fractions (relative and absolute) satisfy:

$$m_1 \;=\; \mu_{11}(1-\mu_2)\mu_4\mu_5 + \mu_{31}(1-\mu_4)\mu_5, \quad m_2 = \mu_2\mu_4\mu_5 + (1-\mu_5). \tag{4.13}$$

There are nine variables and eight conditions. To deal with the uncertainty, we assume

$$\alpha_1 = \beta_1, \tag{4.14}$$

which significantly simplifies the calculation.

Remark 4.1 *The assumption* (4.14) *is based on the observation that the bound in region A is a continuation of the bound in region B where the optimal structure is* $L(13,2,13)$ *and the field in material* k_2 *is a multiple of the identity matrix. Therefore it is reasonable to keep such a property in the core part* k_2 *in* $L(13,2,13,2)$*.*

4.4.1.1 Calculation of the constants

Solving equations (4.10)- (4.14), we find the volume fractions and fields inside each material:

$$\begin{aligned}
\mu_{11} &= \frac{k_1}{2k_2}, \quad \mu_{31} = \frac{a_2\, k_1^2}{r\, k_2 a_1}, \quad \mu_2 = \frac{2a_2k_1}{r\, a_1}, \\
\mu_4 &= \frac{2r\tilde{k}}{k_1(r+1)}, \quad \mu_5 = \frac{r(1+r)a_1}{(2\tilde{k}-k_1(1+r))^2}. \\
e_{11} &= \frac{k_2(r+1)}{\tilde{k}}\,[0,\,1]\,, \quad e_{31} = \frac{k_2(r+1)}{\tilde{k}}\,[1,\,0]\,, \\
e_{22} &= \frac{k_1(r+1)}{2\tilde{k}}\,[1,\,1]\,, \quad e_{42} = \frac{k_1(r+1)}{\tilde{k}}[1,\,0] + r[-1,1],
\end{aligned} \tag{4.15}$$

where

$$\begin{aligned}
a_1 &= -5rm_2{k_1}^2 - 4rk_1m_1k_2 + 4r\tilde{k}^2 + (1+r-m_2){k_1}^2, \\
a_2 &= k_1m_2(m_2-1) + m_1k_2(m_2+r).
\end{aligned}$$

Notice that $\mu_{31} = \mu_2\mu_{11}$ holds and $\mu_{11} \neq 0$, which tells us that μ_{31} and μ_2 vanish simultaneously. Such degeneration brings the $L(13,2,13,2)$ structure into the $L(13,2)$-structure.

4.4.1.2 Region of applicability

All the volume fractions have to be in the interval (0,1); therefore we have the following inequalities:

$$0 < \frac{(m_2\tilde{k} - k_1 m_2 + r m_1 k_2){k_1}^2}{r\,k_2 a_2} < 1, \tag{4.16}$$
$$0 < \frac{2(m_2\tilde{k} - k_1 m_2 + r m_1 k_2)k_1}{r\,a_2} < 1,$$
$$0 < \frac{2\tilde{k}}{k_1(r+1)} < 1, \quad 0 < \frac{r(1+r)a_2}{(-r\,k_1 - k_1 + 2\tilde{k})^2} < 1. \tag{4.17}$$

The above system of inequalities has solutions :

$$\psi_{A1A2} < r < \psi_{A1B}, \tag{4.18}$$
$$\text{where} \quad \psi_{A1A2} = \frac{(k_1 - \tilde{k})m_2}{m_1 k_2}, \quad \psi_{A1B} = m_2\left(\frac{k_1}{\tilde{k} + \sqrt{\tilde{k}^2 - m_2 k_1^2}}\right)^2, \tag{4.19}$$

only if $k_i,\ m_i, i = 1, 2$, satisfy:

$$m_1 < \frac{k_1(1 - m_2)}{2k_2}.$$

At the boundary of the applicability domain where $r = \psi_{A1B}$, by calculation, we have $\mu_5 = 1$. This means the last layer k_2 disappears and the structure degenerates into $L(13, 2, 13)$-laminate. At the other boundary, when $r = \psi_{A1A2}$, we have $\mu_2 = 0, \mu_{31} = 0$, which means that the composite degenerates into $L(13, 2)$-structure.

4.4.2 Optimal structure in region A2

In this region, the second-rank laminate $L(123, 2)$ (Fig. 4.1 region A2) is shown to be optimal. The formation of rank-1 paths is presented in Fig. 4.4. It is built in two steps:

1. $L(123)$ substructure is formed. Material k_1, k_2, and k_3 are laminated along the x_1 direction, with relative volume fraction of materials k_1 and k_2 equaling to μ_{11} and μ_{12}, respectively. The fields in the materials are represented by $E_{11} = (\alpha_1, 0)$ in Ω_1, $E_{12} = (\alpha_2, 0)$ in Ω_2^1, and $E_3 = (0, 0)$ in Ω_3. The average field in the substructure is E_{10}.

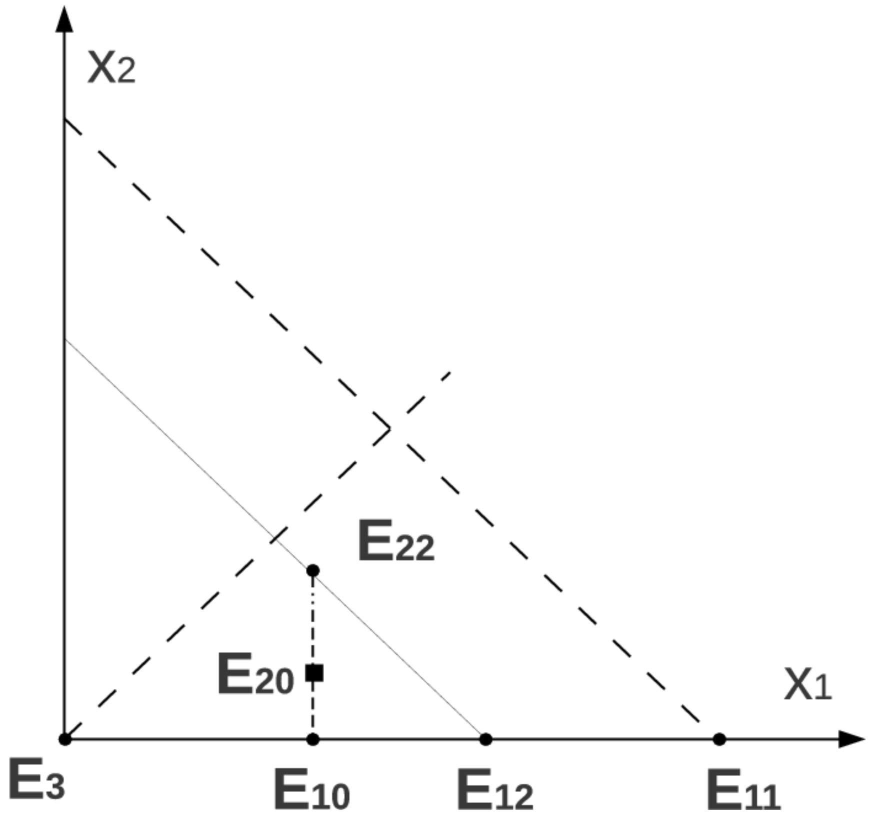

Figure 4.4 Fields in optimal laminates L(123,2) and formation of rank-1 path.

2. $L(123,2)$ structure is formed. The obtained $L(123)$ structure is laminated with material k_2 (field $E_{22} = (\alpha_{22},\ \beta_{22})$ in Ω_2^2) along x_2 direction, with relative volume fraction of material k_2 equaling to μ_2, to form a second rank laminate. The average field in the substructure is called E_{20}.

Here Ω_2^1 and Ω_2^2 are the subdivisions of Ω_2, $\Omega_2 = \Omega_2^1 \cup \Omega_2^2$.

The optimality condition requires that

$$\alpha_2 = \alpha_{22} + \beta_{22},$$

and the compatibility requires that

$$k_1\alpha_1 = k_2\alpha_2.$$

The computation of the constants is similar to the previous case. They are:

$$\alpha_1 = \frac{k_2(1+r)}{\tilde{k}}, \quad \alpha_2 = \frac{k_1(1+r)}{\tilde{k}}, \quad \alpha_{22} = r,$$
$$\beta_{22} = \frac{k_1(1+r)}{\tilde{k}} - r, \quad \mu_2 = \frac{r\tilde{k}}{k_1(1+r)-\tilde{k}},$$
$$\mu_{11} = \frac{m_1}{1+r} - \frac{rm_1k_1}{(\tilde{k}-k_1)(1+r)}, \; \mu_{12} = \frac{m_2}{1+r} + \frac{rm_1k_2}{(\tilde{k}-k_1)(1+r)}.$$

The region is bounded by the lines,

$$r = 0. \;\; r = 1, \quad m_1 = 0, \quad r = \psi_{A1A2}, \quad r = \psi_{AC}.$$

When $r \to 0$, $\mu_2 \to 0$, and the optimal L(123,2)-structure degenerates into a laminate.

4.5 Optimal structures in region D

Laminate L(13,2,13,1,1) is shown in [2] to be optimal in a subregion D1 of region D, using a method similar to the one presented above. The most anisotropic structure of this type is L(13,2,1) with the parameters:

$$p = \frac{k_1(1-m_2-m_1)}{m_1k_2}, \quad e_{11} = \left[0, \frac{r(k_1+k_2)(k_1+k_2-\tilde{k}-m_1k_1)}{m_2k_2k_1}\right],$$
$$e_2 = \left[\frac{r(k_1+k_2-\tilde{k}-m_1k_1)}{m_2k_2}, \frac{r(k_1+k_2-\tilde{k}-m_1k_1)}{m_2k_2}\right],$$
$$e_{31} = \left[r, \frac{r(1-m_1)(k_1+k_2)^2}{m_2k_1k_2} - \frac{r(k_1+2k_2)}{k_2}\right], \tag{4.20}$$

and pm_1 is the volume fraction of material k_1 that is rank-1 connected with material k_3. L(13,2,1) is optimal when

$$r = \psi_{D1D2} = \frac{m_2k_1k_2}{a_6+a_7}, \tag{4.21}$$

where

$$a_6 = (k_1+k_2)m_1((k_1+k_2)(1-m_1) - 3m_2k_1), \quad a_7 = m_2k_1(2k_1+k_2-2m_2k_1),$$

and region $D1$ is described as

$$m_1 \geq \frac{k_1(1-m_2)}{k_1+k_2}, \quad \psi_{D1D2} \leq r \leq 1, \quad r \geq \psi_{BD}. \tag{4.22}$$

In region D2 where $\psi_{D2E} < r < \psi_{D1D2}$, optimal structures cannot be found even if the optimality conditions obtained in Chapter 3 are applied. The possible reason is either that the pointwise description of the field in material k_1 is too rough and could not provide a definite rank-1 path used to build structures, or the bound is not optimal. Our best guess is that $L(13, 2, 1)$ is probably the structure closest to the G-closure boundary.

4.6 Estimate of the bound in region E and D2

The bound (3.74) in region E is not attainable by laminates and might not be exact. We conjecture that an exact bound probably would require more constraints on the field other than (3.8) or the constraints in [14]. It is desired that new constraints will reveal more information on the relationship among the mean field in each material, and this might help one to find the optimal structure in the region D2 as well.

4.6.1 Arguments for presumptive structures

Since bound B_E cannot be realized by laminates, the method that succeeds in other regions does not apply in region E. As pointed out, optimal structures in D2, neighboring with region E, were not found. So we try to guess the best structures in both D2 and E regions.

We notice that at the boundary of neighboring region $D1$, optimal structures $L(13, 2, 13, 1)$ degenerate on the boundary into the structures $L(13, 2, 1)$, Fig. 4.1. In another neighboring region C, optimal structures $L(13, 2)$ can be viewed as a degeneration of $L(13, 2, 1)$, when the volume fraction of the exterior layer k_1 in $L(13, 2, 1)$ goes to zero. Also, laminates $L(12)$ are optimal two-material ($m_3 \to 0$) structures that correspond to anisotropic loading $r < r_{tr} < 1$, ([25]). These laminates are a degeneration of laminates $L(13, 2, 1)$, as $m_3 \to 0$. Finally, the optimal structures for the limits, when $r \to 0$, were conjectured in [13] to be $L(13, 2, 1)$, because this structure, being different from simple laminates, has a conductivity in the x_1 direction that equals to the harmonic mean, while the conductivity in the orthogonal direction is finite (smaller than the arithmetic mean).

Base on these observations, we presume that structures $L(13, 2, 1)$ with the proper distribution of k_1 between the layers, stay optimal in the whole region $D2 \cup E$. In those structures, the fields in the second and third materials are constant everywhere, as the bound predicts. However, the field in the first material takes two different values in different layers; this contradicts the assumption of the bound but makes the structure compatible: the field E_{11} in the inner layer is rank-1 connected with E_3.

4.6.2 Numerical results

The numerical experiments are performed to see how well the suggested bounds approximate an optimal bound. In all the numerical experiments, the conductivity k_i of each material is fixed. So is the volume fraction m_i of each material. The relative difference between the bound B_E and energy $W_L(13,2,1)$ of L(13,2,1) structures (Fig. 4.1, region E)

$$\delta W_{rel} = \left(\frac{\min_{\alpha \in [0,1]} W_{L(13,2,1)}(\alpha) - B_E}{B_E} \right) \tag{4.23}$$

is calculated for $r \in [0, r_0]$, where r_0 is the threshold value where the t_{opt} in case E becomes k_1. Energy $W_{L(13,2,1)}$ depends on one parameter α - the relative amount of material k_1 used in the inner layer. We choose the value α_{opt} of α to minimize the energy stored in the structure. α_{opt} changes with respect to the anisotropy level r of the external field, as does $W_{L(13,2,1)}$. The results of one numerical experiment are shown in Fig. 4.5. The parameters are $m_1 = 0.2, m_2 = 0.5, m_3 = 0.3, k_1 = 1, k_2 = 3$. As we can see, the relative differences are rather small, of the order 10^{-4}, and even of order of 10^{-7} as r is very close to 0. This is true for all fixed m_1 values which fall

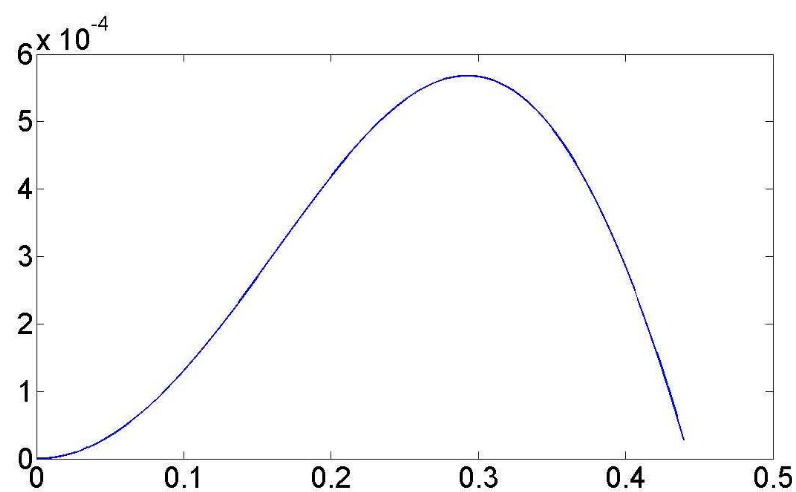

Figure 4.5 δW_{rel} **relative gap between the energy of the bounds and conjected structure in region E.**

inside region E in $r - m_1$ plane, and δW_{rel} also changes in the same way with respect to r for each fixed m_1.

4.7 Summary

4.7.1 Bounds on energy and minimizers

The optimal bound is a piecewise analytic function of the G-closure problem parameters k_i, m_i and the anisotropic level r of the external loading. It turns out that there are five distinct regions A, B, C, D, and E, where the bound takes different expressions and each of them corresponds to different values of $t_{opt}(k_1, k_2, m_1, m_2)$, a critical parameter in the derivation of the bounds. Those regions are conveniently presented in the rectangle

$$\{(m_1, r) : 0 \leq m_1 \leq (1 - m_2 - m_3), 0 \leq r \leq 1\}$$

in the $r - m_1$ plane while keeping the parameters k_i and m_2 fixed. The line $r = 1$ corresponds to isotropic external fields, i.e., the magnitude of fields in two orthogonal directions is equal,and hence refers to isotropic composites. $r = 0$ means single external loading. Fig. 4.6 is one of the plots of those regions where the parameters were set as $k_1 = 1, k_2 = 2, m_2 = 0.36, m_3 = 0.24$. The dependence on m_2 is not shown in the figure. A change of m_2 leads to a variation of the shape of those regions but not their topology. Region D corresponds to the known translation bound [29]. Optimal structures in part (D1) of region D have been found in [2]. The isotropic structures in this region were also found in [18]. On the line $r = 1$ outside region D, the bound has been derived in [32] and optimal structures have been found in [14]. The bounds and structures in the remaining regions are new results of this work.

4.7.2 Three special points

There are three points where several regions meet, as shown in Fig. 4.6.

The four regions A1, A2, B, and C meet in the point P_1:

$$r = m_2, \quad m_1 = \frac{k_1(1 - m_2)}{2k_2}. \tag{4.24}$$

The four regions B, C, D, and E meet at the point P_2:

$$r = m_2, \quad m_1 = \frac{k_1(1 - m_2)}{k_1 + k_2}. \tag{4.25}$$

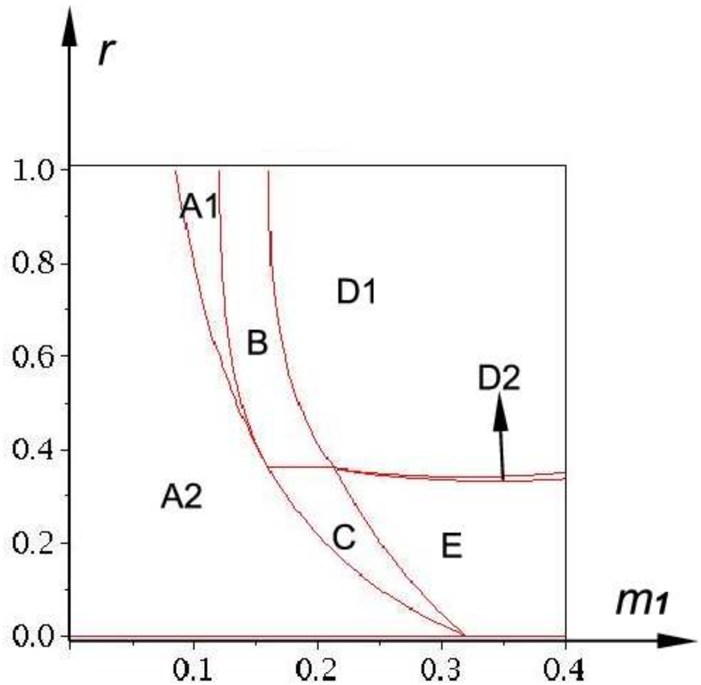

Figure 4.6 The graph of regions A-E where expression of energy bounds change.

Above the interval (P_1, P_2) the field E_2 is constant and proportional to the identity matrix, and below this line the proportionality is lost.

The three regions A2, C and E meet at the point P_3:

$$r = 0, \quad m_1 = \frac{k_1(1 - m_2)}{k_2}. \tag{4.26}$$

At this point, the L(12,3) structure has the same conductivity in the x_1 direction, as that of a simple laminate, see [13].

The boundaries between regions in Fig. 4.6 are calculated. The expressions are shown in Table 4.1. The division between A1 and A2, and between D1 and D2 are based on structural attainability, and the bounds are the same. In Table 4.2 the expressions of energy bounds in different regions and corresponding expressions for

Table 4.1 Boundaries between regions

Boundary	A1A2	A2B	BD	A1C,	CE	BC	D1D2	D2E
Formula	(4.18)	(3.50)	(3.51)	(3.53)	(3.53)	(3.54)	(4.21)	(3.75)

Table 4.2 Formulas for energy bounds and G-closure, and type of optimal structure or the best approximate

Region	Energy	G-closure	Structure	Exact?
A1	(3.61)	(3.63)	L(13,2,13,2)	yes
A2	(3.61)	(3.63)	L(123,2)	yes
B	(3.38)	(3.39)	L(13,2,13)	yes
C	(3.46)	(3.47)	L(13,2)	yes
D1	(3.72)	(3.73)	L(13,2,13,1,1)	yes
D2	(3.72)	(3.73)	L(13,2,1)	not known
E	(3.74)		L(13,2,1)	no

the G-closure boundary are listed. Optimal laminates that realize the bounds and the best structure that approximates the bound in the regions where the bound is not exact are also included in the table. Table 4.3 and Fig. 4.7 show the details of optimal parameters and minimizers in different regions assuming that $E_0 = (1, r)$.

4.7.3 G-closure boundaries

The results for the G-closure boundary follow from the energy bounds. The expression for the G-closure boundary is summarized in Table 4.2.

In Fig. 4.8, the eigenvalues $k_{*1}(r),\ k_{*2}(r)$ of points on the G-closure boundary are plotted separately as a function of r with parameter k_i, m_i fixed

$$k_1 = 1,\ k_2 = 2,\ m_1 = 0.15,\ m_2 = 0.5.$$

The horizontal line in the graph represents region C, because both eigenvalues are constant independent of r. In Fig. 4.9, the G-closure boundary represented by (k_{*1}, k_{*2}) and its symmetric image with respect to the 45° line are plotted with r excluded. To show the improvement of new bounds, the graphs of the G-closure

Table 4.3 Character of minimizers

Region	t_{opt}	$E(x)$ in Ω_1	$E(x)$ in Ω_2
A	$t = k_2$	$Tr(E) = constant,\ det(E) = 0$	$Tr(E) = constant$
B	$t \in (k_1, k_2)$	$Tr(E) = constant,\ det(E) = 0$	$E(x) = \alpha I$
C	$t \in (k_1, k_2)$	$E(x) = constant,\ det(E) = 0$	$E(x) = diag(\alpha, \beta)$
D	$t = k_1$	$Tr(E(x)) = constant$	$E(x) = \alpha I$
E	$t \in (0, k_1)$	$E(x) = constant$	$E(x) = constant$

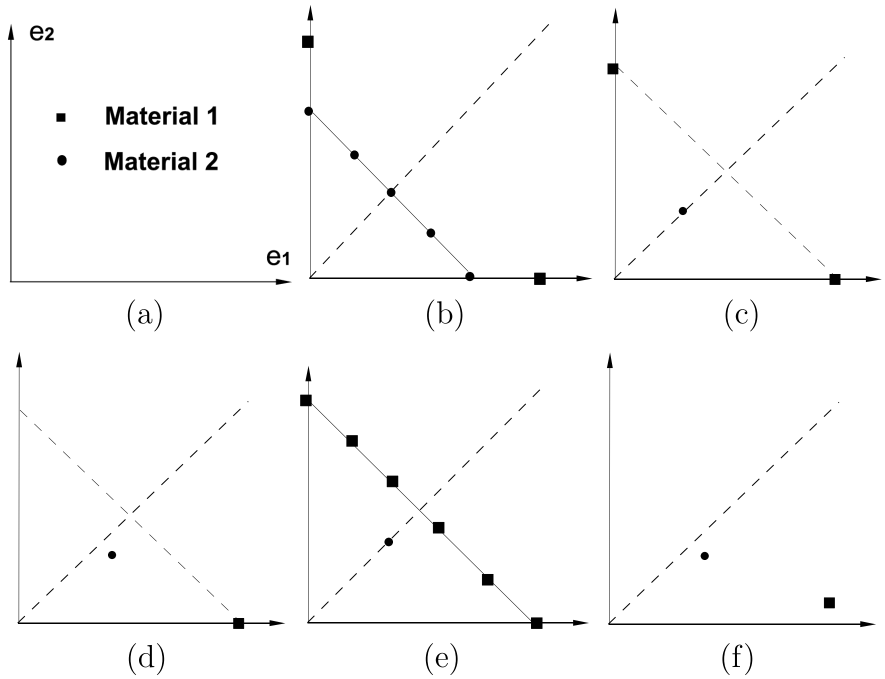

Figure 4.7 The eigenvalues of optimal fields- minimizers. (a) Axes (b) $t = k_2$ Case A (c) $k_1 < t < k_2$ Case B (d) $k_1 < t < k_2$ Case C (e) $t = k_1$ Case D (f) $t < k_1$ Case E

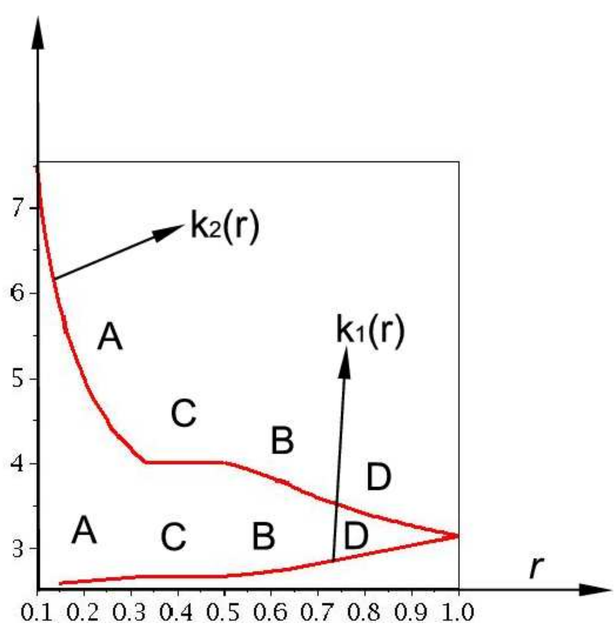

Figure 4.8 The eigenvalues of effective tensor K_* at the G-closure boundary as functions of r.

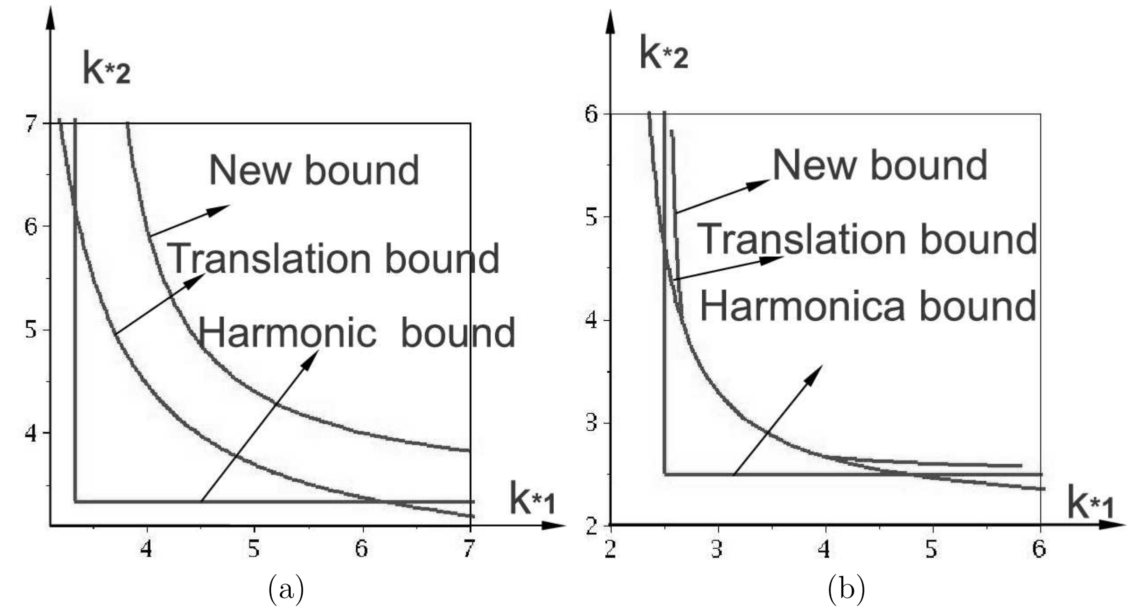

Figure 4.9 The G-closure boundaries of harmonic bounds, translation bounds and new bounds. Parameter: $k_1 = 1, k_2 = 2,\ m_2 = 0.5$ **(a)** $m_1 = 0.15$ **(In the** $r - m_1$ **plane, parameters chosen represent a vertical line that passes through regions D, B, C (two sharp bend points), A). (b)** $m_1 = 0.05$ **(Region A)**

boundaries corresponding to harmonic mean bounds, the translation bounds and new bounds are presented for two different values of m_1 while keeping the other parameters the same. Fig. 4.9(a) corresponds to one vertical line in the $r - m_1$ plane with k_1, k_2, m_1, m_2 fixed, which crosses the regions D, B, C and A as r decreases. As shown in the figure, in the region D, the new boundary of the G-closure matches the one given by the Translation bound. In the remaining region, the new bound is optimal while the Translation bound is not; therefore, the new bound is tighter than the Translation bound. Fig. 4.9(b) corresponds to a vertical line that lies in the region A only, as pointed out before, the new bound is optimal and the Translation bound isn't, as a consequence, the new bound lies above both the Translation bound and the Harmonic bound.

CHAPTER 5

PROBLEM DESCRIPTION AND PRELIMINARIES

In this chapter, we provide some preliminary knowledge of the technique that is used to solve the problem, or to be more specific, recall some important features of div-curl Young measures that will be used in our analysis, and review our variational method in terms of Young measures.

5.1 Problem description

We consider a typical optimal design problem in conductivity for the optimal layout of the distribution of $n \geq 3$ different conducting materials with conductivity A_i in a domain Ω, so that a certain cost functional depending on the underlying field is minimized. Precisely, we aim to minimize

$$(P): \quad I(\chi) = \int_\Omega \Psi(x, \nabla u(x))\, dx$$

under the constraints

$$\chi = (\chi_1, \chi_2, \dots, \chi_n) \in \{0,1\}^n, \int_\Omega \chi(x)\, dx = |\Omega|\mathbf{r},$$

and

$$\operatorname{div}\left[\sum_i \chi_i(x) A_i \nabla u(x)\right] = 0 \text{ in } \Omega, \quad u = u_0 \text{ on } \partial\Omega.$$

Here $\Omega \subset \mathbf{R}^N$ is a regular, bounded domain, $\mathbf{r} \in (0,1)^n$, $\mathbf{r} \cdot \mathbf{1} = 1$, $\mathbf{1} = (1, 1, \dots, 1)$. The matrices A_i for the constituents are assumed to be positive definite and such that $A_i - A_j$ is invertible for every pair $i \neq j$. Concerning the cost functional

$$\Psi : \Omega \times \mathbf{R}^N \to \mathbf{R},$$

we distinguish two cases:

1. the linear case: $\Psi(x,\xi) = G(x)\cdot\xi$, for some fixed field G;

2. a non-linear case: $\Psi(x,\xi) = (1/2)|\xi|^2$.

It is well-known that in general, such a problem does not admit optimal solutions because the oscillating behavior of minimizing sequences of characteristic functions persists to a degree that relaxation is needed. These relaxed versions might provide some insight in understanding optimal microstructures, and eventually lay down the foundation for setting up suitable numerical simulations. The main tool in the analysis is an appropriate reformulation of the optimal design problem as a nonconvex, vector variational problem for which, due to the underlying structure carried by the conductivity law, a relaxation can be either fully computed, or appropriately estimated. This procedure leads one to work with div-curl Young measures as introduced in [36]. This program has been carried out for two materials in [9]. The objective of the current work is to understand the differences in the more complex situations of multimaterials, and how the various ingredients and computations change for three or more materials. For simplicity, as a starting point, we will deal with the three-material situation.

5.2 Div-curl Young measures

In this section we will briefly recall some facts about div-curl Young measures. The main reference for this section is [36] and most materials are taken from it. We first give the definition of a div-curl Young measure.

Definition 5.1 *A family of probability measures $\nu = \{\nu_x\}_{x\in\Omega}$ is called a (L^2)* div-curl *Young measure if there exists a sequence of pairs of vector fields F_j in $L^2(\Omega;\mathbf{M}^{m\times N})$, and u_j in $H^1(\Omega,\mathbf{R}^m)$ such that*

$$\operatorname{div} F_j \to 0 \text{ in } H^{-1}(\Omega;\mathbf{R}^m), \quad \{|F_j|^2\}, \{|\nabla u_j|^2\} \text{ are equiintegrable in } \Omega,$$

and the Young measure associated with $\{(F_j, \nabla u_j)\}$ is precisely ν.

Such a measure ν has the property: that whenever the sequence of functions

$$\{\phi(x, F_j(x), \nabla u_j(x))\}$$

weakly converges in $L^1(\Omega)$ for some Caratheodory integrand ϕ, the weak limit is given by

$$\bar{\phi}(x) = \int_{\mathbf{M}^{m\times N}\times\mathbf{M}^{m\times N}} \phi(x,\rho,\lambda)\,d\nu_x(\rho,\lambda).$$

Even if $\{\phi(x, F_j(x), \nabla u_j(x))\}$ fails to converge weakly in $L^1(\Omega)$, the right inequality for lower semicontinuity still holds:

$$\liminf_{j\to\infty} \int_\Omega \phi(x, F_j(x), \nabla u_j(x))\,dx \geq \int_\Omega \int_{\mathbf{M}^{m\times N}\times\mathbf{M}^{m\times N}} \phi(x,\rho,\lambda)\,d\nu_x(\rho,\lambda) \tag{5.1}$$

and strict inequality occurs when concentrations develop in the sequence

$$\{\phi(x, F_j(x), \nabla u_j(x))\}.$$

One important feature of this class of measures associated with div-curl pairs is the direct consequence of the classic and well-known div-curl lemma ([31], [38], [41]), which says:

Lemma 5.1 *Let $\{F_j\}$ be a sequence of bounded fields in $L^2(\Omega;\mathbf{M}^{m\times N})$ converging weakly to F, such that $\{\operatorname{div} F_j\}$ is bounded in $L^2(\Omega,\mathbf{R}^m)$, and let $\{\nabla u_j\}$ be a bounded sequence of gradients in $H^1(\Omega,\mathbf{R}^m)$ converging weakly to ∇u. Then*

$$F_j(\nabla u_j)^T \rightharpoonup F\nabla u^T.$$

If we rewrite the limits $F,\ \nabla u,\ F\nabla u^T$ in terms of the div-curl Young measure associated with $(F_j, \nabla u_j)$, we obtain the fundamental commutation property of div-curl Young measures.

Lemma 5.2 *If $\{\nu_x\}_{x\in\Omega}$ is a* div-curl *Young measure, then for a.e. $x\in\Omega$,*

$$\int_{\mathbf{M}^{m\times N}\times\mathbf{M}^{m\times N}} \rho\lambda^T\,d\nu_x(\rho,\lambda) = \int_{\mathbf{M}^{m\times N}} \rho\,d\nu_x^{(1)}(\rho) \int_{\mathbf{M}^{m\times N}} \lambda^T\,d\nu_x^{(2)}(\lambda) \tag{5.2}$$

where $\nu_x^{(i)},\ i=1,2$ are the marginals on the two components, respectively.

Note that

$$F(x) = \int_{\mathbf{M}^{m\times N}} \rho\,d\nu_x(\rho,\lambda) = \int_{\mathbf{M}^{m\times N}} \rho\,d\nu_x^{(1)}(\rho)$$

is a divergence free matrix in $L^2(\Omega;\mathbf{M}^{m\times N})$, and

$$\nabla u(x) = \int_{\mathbf{M}^{m\times N}} \lambda^T\,d\nu_x(\rho,\lambda) = \int_{\mathbf{M}^{m\times N}} \lambda^T\,d\nu_x^{(2)}(\lambda)$$

holds for some $u\in H^1(\Omega,\mathbf{R}^m)$. We will call $(F,\nabla u)$ the barycenter or the first moment of the Young measure ν. Another crucial question to be discussed is how to build a div-curl Young measure in a general and explicit way. The answer is the following lemma.

Lemma 5.3 *Suppose that $\rho_i, \lambda_i,\ i = 1, 2$ are four $m \times N$ matrices such that*

$$(\rho_2 - \rho_1)(\lambda_2^T - \lambda_1^T) = 0 \tag{5.3}$$

as $m \times m$ matrices. Then the probability measure

$$\mu = t\delta_{(\rho_1,\lambda_1)} + (1-t)\delta_{(\rho_2,\lambda_2)}$$

is a div-curl Young measure for all $t \in [0, 1]$. If ν_1 and ν_2 are two div-curl *Young measures with barycenters (ρ_1, λ_1) and (ρ_2, λ_2), respectively, such that (5.3) holds, then*

$$\mu = t\nu_1 + (1-t)\nu_2 \tag{5.4}$$

is a div-curl *Young measure, too, for any $t \in [0, 1]$.*

Div-curl Young measures constructed in this way are called "laminate" div-curl Young measures. (5.3) and (5.4) can be recursively used to build higher or multirank laminate div-curl Young measures.

5.3 Reformulation of the problem and relaxation

We introduce the field

$$V(x) = \sum_i \chi_i(x) A_i \nabla u(x),$$

and reformulate the problem in terms of new design variables $(\nabla u(x), V(x))$. The cost functional stays the same as introduced in Section 5.1 in terms of $\nabla u(x)$. The variable pairs $(\nabla u(x), V(x))$ are subjected to the following constraints:

$$V \in L^2(\Omega; \mathbf{R}^N), \quad u \in H^1(\Omega),$$
$$\operatorname{div} V = 0 \text{ weakly in } \Omega, \quad u = u_0 \text{ on } \partial\Omega.$$

In addition, for a.e. $x \in \Omega$, feasible pairs should belong to the subset $\Lambda \subset \mathbf{R}^N \times \mathbf{R}^N$ determined by

$$\Lambda = \cup_i \Lambda_i, \quad \Lambda_i = \{(\lambda, \rho) \in \mathbf{R}^N \times \mathbf{R}^N : \rho = A_i \lambda\}; \tag{5.5}$$

and the subset Ω_i of Ω prescribed by

$$\Omega_i = \{x \in \Omega : (\nabla u(x), V(x)) \in \Lambda_i\}$$

has relative measure r_i. Let $\mathcal{A}$ stand for the class of feasible pairs. It is clear that this reformulation is equivalent to the original problem (P). However, it has some advantages from the perspective of relaxation. First, one is led to deal with pairs of usual vector fields instead of characteristic functions. Second, the reformulation enables us to use Young measures associated with feasible pairs and perform an analysis based on manipulation and calculations of such class of measures. The Young measures generated by admissible pairs in $\mathcal{A}$ are div-curl Young measures due to the differential constraints imposed on those pairs. Let $\nu = \{\nu_x\}_{x\in\Omega}$ be a div-curl Young measure corresponding to a sequence of feasible pairs $(\nabla u_j, V_j) \in \mathcal{A}$ with first moment $F = (F^{(1)}, F^{(2)}) \in \mathbf{M}^{2\times N}$. The relationship between the two components in admissible vector fields leads to the following fact:

$$\text{supp}(\nu_x) \subset \Lambda = \cup_i \Lambda_i,$$

and as a consequence, if

$$\nu_x = \sum_i t_i(x)\nu_{x,i}, \quad \text{supp}(\nu_{x,i}) \subset \Lambda_i, \mathbf{t} = (t_1(x), \dots t_n(x)) \in (0,1)^n, \mathbf{t}(x)\cdot \mathbf{1} = 1,$$

holds, then we should have

$$\int_\Omega t_i(x)\,dx = |\Omega| r_i.$$

The cost functionals can be expressed through feasible ν's as

$$I_1(\nu) = \int_\Omega G(x)\cdot F^{(1)}(x)\,dx, \quad I_2(\nu) = \int_\Omega \sum_i t_i(x) q_i(x)\,dx$$

where

$$F^{(1)} = \int_\Lambda X\,d\nu_x(X,Y), \quad q_i = \int_{\Lambda_i} |X|^2\,d\nu_{x,i}(X,Y).$$

The local feature of div-curl Young measure enables the compuation to be carried out locally for a.e. $x \in \Omega$. Therefore, we can treat x as an index, and even drop it for simplicity. Now one is allowed to work with a homogeneous div-curl Young measure ν such that:

$$\nu = \sum_i t_i \nu_i, \quad \mathrm{supp}(\nu_i) \subset \Lambda_i, t_i \in [0,1], \sum_i t_i = 1,$$

and the first moment of ν is given by

$$F = (F^{(1)}, F^{(2)}) = \int_\Lambda (X, Y)\, d\nu(X, Y).$$

Let $\overline{\mathcal{A}}(t, F)$ denote the class of such families of probability measures. The local version of the cost functionals is:

$$I_1(\nu) = g \cdot F^{(1)}, \quad I_2(\nu) = \sum_i t_i q_i,$$

where as before

$$F^{(1)} = \int_\Lambda X\, d\nu(X, Y), \quad q_i = \int_{\Lambda_i} |X|^2\, d\nu_i(X, Y).$$

In these terms, relaxation amounts to calculating (or estimating) the minimum of the optimization problem

$$(QP) \quad \text{Minimize in } \nu \in \overline{\mathcal{A}}(t, F): \quad I(\nu)$$

as a map of (t, F), for $I = I_j$, $j = 1, 2$. Let us call such a function $\Phi(t, F)$. This $\Phi(t, F)$ is actually the quasiconvex envelope of a certain intergrand in the original problem (P) expressing the interaction between Ψ and the state law [34]. Furthermore, if we can verify that the integrand Ψ enjoys a typical coercivity property and satisfies proper growth conditions, then by a standard relaxation theorem in ([15]), we have a relaxed version of the original optimal design problem as follows:

$$\text{Minimize in } (\nabla u, V): \quad \int_\Omega \Phi(t(x), \nabla u(x), V(x))\, dx,$$

where minimization is performed over the set of all weak limits $(\nabla u, V)$ of sequences from $\mathcal{A}$.

CHAPTER 6

LINEAR COST FUNCTIONAL

Situations where two constituents are at disposal have been thoroughly investigated using the parametrized measure or Young measure approach before, in particular, one can find in [9] the case of a linear cost functional; and in [17], a quadratic cost functional. We focus on the case where three isotropic phases

$$A_i = a_i I,\ i = 1, 2, 3 \quad \text{with } a_i > 0,$$

are present; furthermore, it is assumed $a_3 > a_2 > a_1$. Such simplification allows the algebra to be fully explicit. In this chapter, we deal with the linear cost functional, precisely,

$$(P) \qquad \text{Minimize in } \chi : \quad \int_\Omega G(x) \cdot \nabla u(x)\, dx$$

subject to

$$\operatorname{div}\left[\sum_{i=1}^{3} \chi_i a_i \nabla u\right] = 0 \text{ in } \Omega, \quad u = u_0 \text{ on } \partial\Omega,$$

and

$$\chi = (\chi_i) \in \{0, 1\}^3, \chi \cdot \mathbf{1} = 1, \int_\Omega \chi(x)\, dx = \mathbf{r}|\Omega|,$$

where $\Omega \subset \mathbf{R}^N$, $\mathbf{1} = (1, 1, 1)$, $\mathbf{r} \in [0, 1]^3$ with $\mathbf{r} \cdot \mathbf{1} = 1$, and $G \in L^2(\Omega; \mathbf{R}^N)$. We leave the quardratic cost for the next chapter, which requires a different strategy.

6.1 Quasiconvex hull of admissible set $\mathcal{A}$

Any sequence $\{\nabla u_j, V_j\} \in \mathcal{A}$ is equiintegrable because they are solutions of a sequence of uniformly elliptic problems (see [6]), thus generates a div-curl Young measure ν. In addition, we have the following:

$$\nabla u_j \rightharpoonup \nabla u = \int_{\mathbf{R}^N \times \mathbf{R}^N} X\, d\nu(X, Y), \quad V_j \rightharpoonup V = \int_{\mathbf{R}^N \times \mathbf{R}^N} Y\, d\nu(X, Y) \text{ in } L^2(\Omega, \mathbf{R}^N)$$

because of equiintegrability of ∇u_j and V_j, and the representation of weak limit in terms of Young measure. Recall $(\nabla u, V)$ is the first moment of ν. Hence for any $G \in L^2(\Omega, \mathbf{R}^N)$, it is true that:

$$\int_\Omega G(x) \cdot \nabla u_j \, dx \to \int_\Omega G(x) \cdot \nabla u \, dx, \text{ as } j \to \infty$$

and consequently relaxation in such a situation is just a matter of finding all the weak limits of sequences in $\mathcal{A}$ or obtaining the set of all div-curl Young measures generated by sequences in $\mathcal{A}$. This set is the quasiconvex hull of $\mathcal{A}$ which is the union of three linear manifold Λ_i at given proportion. Now our attention is brought to finding the quasiconvex hull itself. It will be shown that, as in the two-material situation [9], this quasiconvex hull $Q_t\mathcal{A}$ or envelope is given by the set

$$\{(t, F) : P_{\mathbf{t}}(F) \leq 0\}$$

for a specific homogeneous-of-degree-two polynomial $P_{\mathbf{t}}$. Here

$$\mathcal{A} = \cup_i \Lambda_i, \quad \Lambda_i = \{(\lambda, \rho) \in \mathbf{R}^N \times \mathbf{R}^N : \rho = a_i \lambda\},$$

and $Q_t\mathcal{A}$ is described as:

$$\begin{aligned} Q_t\mathcal{A} = \{F = (F^{(1)}, F^{(2)}) \in \mathbf{R}^N \times \mathbf{R}^N : \text{ there is a div-curl Young measure } \nu \\ \text{supported in } S \text{ with mass } t_i \text{ in } \Lambda_i, \text{ and barycenter } F\}. \end{aligned}$$

Note that $\mathbf{t} = (t_1, t_2, t_3)$ is a collection of proportions

$$1 = t_1 + t_2 + t_3, \quad t_i \geq 0.$$

6.1.1 Necessary conditions on an admissible ν for given t

Feasible div-curl Young measures ν admit the decomposition:

$$\nu = t_1\nu_1 + t_2\nu_2 + t_2\nu_3, \quad supp(\nu_i) \subset \Lambda_i, t_1 + t_2 + t_3 = 1, t_i \geq 0.$$

If we define

$$x_i = \int_{\Lambda_i} X \, d\nu_i(X, Y) = \int_{\mathbf{R}^N} X \, d\nu_i^{(1)}(X)$$

where $\nu_i^{(1)}$ is the projection of ν_i onto the λ-component, then due to the structure of the manifolds Λ_i, we have

$$F^{(1)} = t_1x_1 + t_2x_2 + t_3x_3 \in \mathbf{R}^N, \quad F^{(2)} = t_1a_1x_1 + t_2a_2x_2 + t_3a_3x_3 \in \mathbf{R}^N. \tag{6.1}$$

Furthermore, the commutation property of div-curl Young measure (Lemma 5.2) provides

$$F^{(1)} \cdot F^{(2)} = t_1q_1 + t_2q_2 + t_3q_3 \tag{6.2}$$

where

$$q_i = \int_{\Lambda_i} |X|^2 \; d\nu_i^{(1)}(X) \in \mathbf{R}.$$

Finally, by Jensen's inequality we have the following relationship:

$$q_i \geq |x_i|^2,$$

$$F^{(1)} \cdot F^{(2)} \geq t_1a_1|x_1|^2 + t_2a_2|x_2|^2 + t_3a_3|x_3|^2. \tag{6.3}$$

These conditions will be used to prove part of the central result of this chapter stated in the following theorem

Theorem 6.1 *For each* $t \in [0,1]^3, t \cdot \mathbf{1} = 1,\ \mathbf{1} = (1,1,1)$, *the quasiconvexification of the union of the three manifolds*

$$\mathcal{A} = \cup_{i=1}^3 \Lambda_i$$

at volume t_i *in* Λ_i *is given by the pairs* $(F^{(1)}, F^{(2)}) \in \mathbf{R}^N \times \mathbf{R}^N$ *for which*

$$((a_1t_1 + a_2t_2 + a_3t_3)F^{(1)} - F^{(2)}) \cdot (a_1a_2a_3F^{(1)} - (a_1a_3t_2 + a_1a_2t_3 + a_2a_3t_1)F^{(2)}) \leq 0.$$

Proof. The proof is carried out in two steps. First, we derive constraints on (t, F), which are represented as $\{P_t(F) \leq 0\}$, such that conditions (6.1)-(6.3) can be satisfied by some x_i's. We therefore have $Q_t\mathcal{A} \subset \{P_t(F) \leq 0\}$. In the second step, we show that every $F \in \{P_t \leq 0\}$ is the first moment of a laminate div-curl Young measure supported in $\mathcal{A}$ with mass t_i at Λ_i, using Lemma 5.3. Hence we also have $\{P_t(F) \leq 0\} \subset Q_t\mathcal{A}$.

Step1: find those constraints on (t, F). Unlike the two-material case, where F takes form

$$F^{(1)} = t_1 x_1 + t_2 x_2 \in \mathbf{R}^N, \quad F^{(2)} = t_1 a_1 x_1 + t_2 a_2 x_2 \in \mathbf{R}^N, \tag{6.4}$$

which enables $x_i, i = 1, 2$ to be uniquely determined, (6.1) is underdetermined and leaves us one free variable. It also makes the problem a lot more complicated. We take x_3, for example, as the free variable. Express x_1, x_2 in terms of x_3 using (6.1)

$$\begin{aligned} x_1 &= \frac{a_2 t_3 x_3 - a_3 t_3 x_3 - a_2 F^{(1)} + F^{(2)}}{t_1(a_1 - a_2)}, \\ x_2 &= \frac{a_3 t_3 x_3 - a_1 t_3 x_3 + a_1 F^{(1)} - F^{(2)}}{t_2(a_1 - a_2)}. \end{aligned} \tag{6.5}$$

Substituting it into the inequality (6.3), we get a quadratic form in x_3

$$\begin{aligned} &\left(\frac{a_1(a_3 t_3 - a_2 t_3)^2}{t_1(a_1 - a_2)^2} + \frac{a_2(a_3 t_3 - a_1 t_3)^2}{t_2(a_1 - a_2)^2} + a_3 t_3 \right) |x_3|^2 \\ &+2 \left(\frac{a_1(a_3 t_3 - a_2 t_3)(a_2 F^{(1)} - F^{(2)})}{t_1(a_1 - a_2)^2} + \frac{a_2(a_3 t_3 - a_1 t_3)(a_1 F^{(1)} - F^{(2)})}{t_2(a_1 - a_2)^2} \right) \cdot x_3 \\ &+ \frac{a_1(a_2 F^{(1)} - F^{(2)}) \cdot (a_2 F^{(1)} - F^{(2)})}{t_1(a_1 - a_2)^2} + \\ &\frac{a_2(a_1 F^{(1)} - F^{(2)}) \cdot (a_1 F^{(1)} - F^{(2)})}{t_2(a_1 - a_2)^2} - F^{(1)} \cdot F^{(2)} \leq 0. \end{aligned} \tag{6.6}$$

This inequality can have solutions only if the minimum of the left-hand side, let us call it $G(a_i, t_i, F, x_3)$, is less than or equal to 0. We will derive restrictions on F associated with t_i, based on this condition. Standard procedure shows that the minimum of G is achieved at

$$x_{30} = \frac{\rho_1 F^{(1)} + \rho_2 F^{(2)}}{a_1 t_2 t_3 (a_2 - a_3)^2 + a_2 t_1 t_3 (a_1 - a_3)^2 + a_3 t_1 t_2 (a_1 - a_2)^2} \tag{6.7}$$

where

$$\rho_1 = a_1 a_2 (a_1 t_1 + a_2 t_2) - a_1 a_2 a_3 (t_1 + t_2), \quad \rho_2 = a_3 (a_1 t_2 + a_2 t_1) - a_1 a_2 (t_1 + t_2),$$

and the minimum itself equals to:

$$G(x_{30}) = \frac{P_{\mathbf{t}}(F)}{a_1 t_2 t_3 (a_2 - a_3)^2 + a_2 t_1 t_3 (a_1 - a_3)^2 + a_3 t_1 t_2 (a_1 - a_2)^2},$$

where

$$P_{\mathbf{t}}(F) = (a_1a_2a_3F^{(1)} - (a_1a_3t_2 + a_1a_2t_3 + a_2a_3t_1)F^{(2)}) \cdot ((a_1t_1 + a_2t_2 + a_3t_3)F^{(1)} - F^{(2)}). \tag{6.8}$$

Hence $(\mathbf{t}, F)$ must satisfy $P_{\mathbf{t}}(F) \leq 0$.

Remark 6.1 *Note that $P_{\mathbf{t}} = 0$ can only hold when $G(a_i, t_i, F, x_{30}) = 0$, and then inequality (6.6) becomes equality. This forces ν_i to be Dirac masses based at (x_i, a_ix_i). As a matter of fact, x_{30} is the only point satisfying $G(a_i, t_i, F, x_3) \leq 0$ when $P_{\mathbf{t}}(F) = 0$. However, there exist $x_3 \neq x_{30}$ such that $G(a_i, t_i, F, x_3) = 0$ while $P_{\mathbf{t}}(F) < 0$ is true, which will also leads to ν_i being a Dirac mass, and there exist many x_3 such that $G(a_i, t_i, F, x_3) \leq 0$.*

Step 2. We would like to show that every F with $P_{\mathbf{t}}(F) \leq 0$ is achievable as a second-order laminate div-curl Young measure. This requires that every ν_i is a Dirac mass based at (x_i, a_ix_i), and, in addition, (x_i, a_ix_i) satisfy (see Lemma 5.3),

$$(x_i - x_j) \cdot (a_ix_i - a_jx_j) = 0, \tag{6.9}$$

$$R(t_i, x_i, a_i) \equiv (z - x_k) \cdot (Z - a_kx_k) = 0 \tag{6.10}$$

where

$$z = \frac{t_ix_i}{t_i + t_j} + \frac{t_jx_j}{t_i + t_j}, \quad Z = \frac{t_ia_ix_i}{t_i + t_j} + \frac{t_ja_jx_j}{t_i + t_j},$$

and (6.10) can be rewritten as:

$$R(t_i, x_i, a_i) \equiv (t_ix_i + t_jx_j - (t_i + t_j)x_k) \cdot (a_it_ix_i + a_jt_jx_j - a_k(t_i + t_j)x_k) = 0.$$

As pointed out in Remark 6.1, we know that if $G(a_i, t_i, F, x_3) = 0$, we will have Dirac masses supported in each manifold Λ_i. The following lemma is to prove that having (6.9) and (6.10) satisfied, automatically, ensures that ν_i supported in Λ_i is a Dirac mass.

Lemma 6.1 *Suppose* (6.1), (6.2), *and* (6.3) *hold. If $(x_i - x_j) \cdot (a_ix_i - a_jx_j) = 0$, then $R(t_i, x_i, a_i) = 0$ if and only if $G(a_i, t_i, F, x_3) = 0$ or, equivalently, if and only if*

$$F^{(1)} \cdot F^{(2)} - a_1t_1x_1^2 - a_2t_2x_2^2 - a_3t_3x_3^2 = 0. \tag{6.11}$$

The proof is straightforward. We can assume, without loss of generality, $i = 1, j = 2, k = 3$ (the other cases are similar). We may rewrite $R(a_i, t_i, x_i)$ in the form

$$\begin{aligned} R(a_i, t_i, x_i) &= (t_1+t_2)(t_1(x_1-x_3)\cdot(a_1x_1-a_3x_3)+t_2(x_2-x_3)\cdot(a_2x_2-a_3x_3)) \\ &\quad -t_1t_2(x_1-x_2)\cdot(a_1x_1-a_2x_2). \end{aligned} \tag{6.12}$$

Let us denote by $D(x_i, a_i, t_i)$, the left hand side of (6.11). Direct algebra shows that

$$D - R = -(t_1(x_1-x_3)\cdot(a_1x_1-a_3x_3)+t_2(x_2-x_3)\cdot(a_2x_2-a_3x_3)).$$

If $(x_1 - x_2)\cdot(a_1x_1 - a_2x_2) = 0$ holds, we will have

$$D - R = \frac{-1}{t_1+t_2}R \quad \text{or} \quad D = \frac{t_1+t_2-1}{t_1+t_2}R,$$

which finishes the proof of the lemma.

As a consequence of Lemma 6.1, if we can find x_3 satisfying (6.9) and (6.10), so that $G(a_i, t_i, F, x_3) = 0$, by the remark above, each ν_i will be a Dirac mass supported in Λ_i, and, in addition, they will form a second rank-laminate as desired. Therefore $\nu = \sum_i t_i\nu_i$ will be a div-curl Young measure. Our goal is then to prove that such x_3 can be found for all $F = (F^{(1)}, F^{(2)})$ such that $P_{\mathbf{t}}(F) \le 0$. Using (6.1), we can rewrite both equations in (6.9)-(6.10) as quadratic forms of x_3

$$(x_3 - v_1)\cdot(x_3 - v_2) = 0, \tag{6.13}$$

$$(x_3 - F^{(1)})\cdot(x_3 - \frac{F^{(2)}}{a_3}) = 0, \tag{6.14}$$

where

$$\begin{aligned} v_1 &= \frac{a_1a_2(t_1+t_2)F^{(1)} - (a_1t_2+a_2t_1)F^{(2)}}{t_3(a_1a_2t_1+a_1a_2t_2-a_1t_2a_3-a_2t_1a_3)}, \\ v_2 &= \frac{(a_1t_1+a_2t_2)F^{(1)} - (t_1+t_2)F^{(2)}}{t_3(a_1t_1+a_2t_2-t_1a_3-t_2a_3)}. \end{aligned}$$

Equations (6.13) and (6.14) represent two N-1 spheres in $\mathbf{R}^N$ centered at

$$\frac{v_1+v_2}{2}, \quad \frac{F^{(1)}+\frac{F^{(2)}}{a_3}}{2}$$

respectively, with corresponding radii

$$r_1 = \left\|\frac{v_1-v_2}{2}\right\|, \quad r_2 = \left\|\frac{F^{(1)}-\frac{F^{(2)}}{a_3}}{2}\right\|.$$

We need to show that these two spheres intersect with or touch each other. By elementary geometry, this is equivalent to showing that the distance d between the centers and radii $r_i,\ i=1,2$ of the spheres satisfy $d \le (r_1+r_2)$. One can find, by direct calculation, that

$$\begin{aligned} r_1 &= \frac{t_1t_2(a_1-a_2)^2\|a_3F^{(1)}-F^{(2)}\|}{t_3(a_1t_1+a_2t_2-t_1a_3-t_2a_3)(a_1a_2t_1+a_1a_2t_2-a_1t_2a_3-a_2t_1a_3)}, \\ r_2 &= \frac{\|a_3F^{(1)}-F^{(2)}\|}{2a_3}. \end{aligned}$$

The computation of $d^2-(r_1+r_2)^2$ will be much easier than that of $d-(r_1+r_2)$ due to these last formulae. The result is

$$d^2-(r_1+r_2)^2 = \frac{C_1\cdot C_2}{\rho},$$

where

$$\begin{aligned} \rho &= t_3^2a_3(a_1t_1+a_2t_2-t_1a_3-t_2a_3)(a_1a_2t_1+a_1a_2t_2-a_1t_2a_3-a_2t_1a_3), \\ C_1 &= (a_1t_3t_1+t_3a_2t_2-a_1t_1-a_2t_2-t_2t_3a_3-t_3a_3t_1)F^{(1)}+(t_1+t_2)F^{(2)}, \\ C_2 &= (a_1a_2t_2t_3+a_1t_3t_1a_2+a_1t_2a_3+a_2t_1a_3-a_2a_3t_1t_3-a_1t_2t_3a_3)F^{(2)} \\ &\quad -a_1a_2a_3(t_1+t_2)F^{(1)}. \end{aligned}$$

Use the fact $t_1+t_2+t_3=1$, to rewrite C_1 and C_2 as

$$\begin{aligned} C_1 &= (t_1+t_2)(F^{(2)}-(a_1t_1+a_2t_2+a_3t_3)F^{(1)}), \\ C_2 &= (t_1+t_2)((a_1a_3t_2+a_1a_2t_3+a_2a_3t_1)F^{(2)}-a_1a_2a_3F^{(1)}). \end{aligned}$$

Thus, we have

$$d^2-(r_1+r_2)^2 = \frac{(t_1+t_2)^2}{\rho}P_{\mathbf{t}}.$$

Since $\rho > 0$ holds under the assumption $a_3 > a_2 > a_1$, $d^2-(r_1+r_2)^2 \le 0$ on $\{P_{\mathbf{t}} \le 0\}$. Hence the spheres (6.13) and (6.14) intersect with or touch each other. We conclude that every $F=(F^{(1)},F^{(2)})$ with $P_{\mathbf{t}}(F)\le 0$, is the barycenter of a div-curl Young measure (a second order laminate in fact) supported in the union of the three manifolds Λ_i, and with mass t_i over each one, thus finishing the proof of Theorem 6.1.

6.2 Relaxation of the problem (P)

The relaxation result is contained in the following theorem whose proof follows immediately after the quasiconvex hull $\overline{\mathcal{A}}$ is obtained, by simply noticing that the cost functional, being linear with respect to ∇u, is weakly continuous with respect to weak convergence in $H^1(\Omega)$.

Theorem 6.2 *The variational problem* $(\overline{P})$ *below is a full relaxation of the problem* P*:*

$$(\overline{P}) \qquad \text{Minimize in } (\mathbf{t}, \nabla u, V) \in \overline{\mathcal{A}} : \quad \int_\Omega G(x) \cdot \nabla u(x)\, dx$$

subject to

$$u = u_0 \text{ on } \partial\Omega, \quad \operatorname{div} V = 0 \text{ in } \Omega, \quad \mathbf{t} \in [0,1]^3, \mathbf{t} \cdot \mathbf{1} = 1, \int_\Omega \mathbf{t}(x)\, dx = \mathbf{r}|\Omega|,$$

where

$$\overline{\mathcal{A}} = \{(\mathbf{t}, (F^{(1)}, F^{(2)})) : P_{\mathbf{t}}(F) \le 0\}$$

and

$$P_{\mathbf{t}}(F) = (F^{(2)} - (a_1 t_1 + a_2 t_2 + a_3 t_3) F^{(1)}) \cdot ((a_1 a_3 t_2 + a_1 a_2 t_3 + a_2 a_3 t_1) F^{(2)} - a_1 a_2 a_3 F^{(1)}).$$

Actually, such relaxation becomes more transparent if we rephrase the main result in this chapter, Theorem 6.1, as follows.

Theorem 6.3 *A pair of fields* $(\nabla u, V)$ *with* $u \in H^1(\Omega)$*,* $u = u_0$ *on* $\partial\Omega$*,* $V \in L^2(\Omega; \mathbf{R}^N)$*,* $\operatorname{div} V = 0$*, is the weak limit of a sequence of pairs* $(\nabla u^{(j)}, V^{(j)})$ *with*

$$\operatorname{div}\left[(\chi_1^{(j)} a_1 + \chi_2^{(j)} a_2 + \chi_3^{(j)} a_3)\nabla u^{(j)}\right] = 0 \text{ in } \Omega, \quad u^{(j)} = u_0 \text{ on } \partial\Omega,$$

and

$$V^{(j)} = (\chi_1^{(j)} a_1 + \chi_2^{(j)} a_2 + \chi_3^{(j)} a_3)\nabla u^{(j)}, \quad t_i|\Omega| = \int_\Omega \chi_i^{(j)}\, dx, i = 1, 2, 3,$$

if and only if

$$P_{\mathbf{t}}(\nabla u(x), V(x)) \le 0.$$

CHAPTER 7

QUADRATIC COST FUNCTIONAL

In this chapter, we deal with the quadratic cost functional, namely

$$\text{Minimize in } \chi : \quad \int_\Omega \frac{1}{2}|\nabla u(x)|^2\, dx$$

subject to

$$\operatorname{div}\left[\sum \chi_i a_i \nabla u\right] = 0 \text{ in } \Omega, \quad u = u_0 \text{ on } \partial\Omega,$$

and

$$\chi = (\chi_i) \in \{0,1\}^3, \chi \cdot \mathbf{1} = 1, \int_\Omega \chi(x)\, dx = \mathbf{r}|\Omega|,$$

where $\mathbf{1} = (1,1,1)$, $\mathbf{r} \in [0,1]^3$ with $\mathbf{r} \cdot \mathbf{1} = 1$, and $a_i > 0$. According to the discussion in the end of Section 5.3, and similar to the two-material case, a lower bound for the appropriate relaxed integrand amounts to finding the minimum for the optimization problem

$$(PP) \quad \text{Minimize in } (x_i, q_i) : \ \sum_i t_i q_i$$

subject to

$$F^{(1)} \cdot F^{(2)} = \sum_i a_i t_i q_i, \ F^{(1)} = \sum_i t_i x_i, \ F^{(2)} = \sum_i a_i t_i x_i, \ q_i \geq |x_i|^2.$$

It has been proved in the previous chapter that the feasible set for the minimization problem is non-empty if $P_{\mathbf{t}}(F) \leq 0$ holds, where $\mathbf{t} = (t_1, t_2, t_3)$, and

$$P_{\mathbf{t}} = ((a_1t_1 + a_2t_2 + a_3t_3)F^{(1)} - F^{(2)}-) \cdot (a_1a_2a_3F^{(1)} - (a_1a_3t_2 + a_1a_2t_3 + a_2a_3t_1)F^{(2)}).$$

Let $\overline{\mathcal{A}}^*(\mathbf{t}, F)$ stand for the set of $(\mathbf{t}, F)$ satisfying this last constraint. For each such fixed $(\mathbf{t}, F)$, and for fixed vector x_i, the feasible set in the variables q_i actually is a triangle in $\mathbf{R}^3$. Therefore the optimal solution will be achieved at one of its three vertices depending on the relationship among the a_i's. Under our assumption $a_3 > a_i,\ i = 1, 2$, elementary algebra shows that the optimal solution will occur at $q_i = |x_i|^2,\ i = 1, 2$, by comparing

$$J = (\sum t_i q_i)\Big|_{q_i = x_i^2, q_j = x_j^2},\ i, j = 1, 2, 3,\ \text{and } i \neq j.$$

We can rewrite J, by using the linear constraints (6.2), as

$$J = t_1|x_1|^2 + t_2|x_2|^2 + \frac{F^{(1)} \cdot F^{(2)} - a_1 t_1 |x_1|^2 - a_2 t_2 |x_2|^2}{a_3},$$

and then, after the inner optimization in the variables q_i's, we are left with

$$\text{Minimize in } x_i: \quad t_1\left(1 - \frac{a_1}{a_3}\right)|x_1|^2 + t_2\left(1 - \frac{a_2}{a_3}\right)|x_2|^2 + \frac{F^{(1)} \cdot F^{(2)}}{a_3}$$

subject to

$$F^{(1)} \cdot F^{(2)} \geq a_1 t_1 |x_1|^2 + a_2 t_2 |x_2|^2 + a_3 t_3 |x_3|^2,$$
$$F^{(1)} = t_1 x_1 + t_2 x_2 + t_3 x_3, \quad F^{(2)} = t_1 a_1 x_1 + t_2 a_2 x_2 + t_3 a_3 x_3. \tag{7.1}$$

Call the minimum of this problem $\Phi(\mathbf{t}, (F^{(1)}, F^{(2)}))$ and we have a lower bound on the relaxation as stated in the following theorem.

Theorem 7.1 *Consider the variational problem*

$$\textit{Minimize in } (\mathbf{t}, \nabla u, V) \in \overline{\mathcal{A}}: \quad \int_\Omega \Phi(\mathbf{t}, (\nabla u, V))\, dx$$

subject to

$$u = u_0 \text{ on } \partial\Omega, \quad \operatorname{div} V = 0 \text{ in } \Omega, \quad \mathbf{t} \in [0,1]^3, \mathbf{t} \cdot \mathbf{1} = 1, \int_\Omega \mathbf{t}(x)\, dx = \mathbf{r}|\Omega|,$$

where

$$\overline{\mathcal{A}} = \{(\mathbf{t}, (F^{(1)}, F^{(2)})) : P_{\mathbf{t}}(F) \leq 0\}$$

and

$$P_{\mathbf{t}}(F) = (F^{(2)} - (a_1 t_1 + a_2 t_2 + a_3 t_3) F^{(1)}) \cdot ((a_1 a_3 t_2 + a_1 a_2 t_3 + a_2 a_3 t_1) F^{(2)} - a_1 a_2 a_3 F^{(1)}).$$

The optimal value for this problem is a lower bound for the relaxation of the quadratic problem considered above.

One can use the two identities in (7.1) to express x_1 and x_2, as an affine quantity in terms of x_3 as in (6.5), and substitute this into the inequality constraint and the cost functional. That will result in a quadratic cost in x_3 subject to a quadratic inequality constraint. The algebra involved is rather tedious, and certainly leads to a lower bound for our relaxed problem. However, we do not have any means to show that such an optimal value for the lower bound could possibly be achieved by lamination. Sometimes the inequality constraint is inactive, so that we cannot even be sure about the structure of the third probability measure ν_3. But even if the optimal value would be attained with that inequality being active, so that it is an equality, all we can be sure about is that the third probability measure is also a delta measure because

$$F^{(1)} \cdot F^{(2)} = a_1 t_1 |x_1|^2 + a_2 t_2 |x_2|^2 + a_3 t_3 |x_3|^2$$

implies $q_3 = |x_3|^2$. Yet, one cannot show that the three delta measures, one in each manifold, is a second-order laminate. If they turn out to be a laminate, then we achieved the quasiconvexification of the original integrand; hence we have a relaxation. Otherwise one gets only a lower bound of the quasiconvexification. Therefore, even if it were possible to provide an explicit form for this subrelaxation, all we can get is a lower bound as stated in Theorem 7.1.

One can make a further attempt based on the JBOC (see section 7.1) introduced in [35]. By focusing on optimality conditions, it may be possible to provide a more explicit form of the subrelaxation which surprisingly may turn out to be, as a matter of fact, a full relaxation! The explanation for such a remarkable situation is clear: one may not be able to compute exactly the values of a certain integrand for all potential values of its arguments, but sometime it might be possible to provide those exact values for part of the admissible values of the arguments related to a specific optimization problem.

7.1 The JBOC condition

In this section, we follow closely the material in Section 3 of [35], although we will adapt those ideas to our div-curl situation in arbitrary spatial dimension N.

Assume we have found a (sub)relaxation, of a certain optimal design problem, in the form

$$\text{Minimize in } (\mathbf{t}, u, V): \quad \int_\Omega \Phi(x, \mathbf{t}(x), \nabla u(x), V(x))\, dx$$

subject to

$$u \in H^1(\Omega), \quad u = u_0 \text{ on } \partial\Omega, \quad V \in L^2(\Omega; \mathbf{R}^N),$$
$$\operatorname{div} V = 0 \text{ in } \Omega, \quad 0 \leq \mathbf{t} \leq 1, \quad \int_\Omega \mathbf{t}(x)\, dx = \mathbf{r}|\Omega|,$$

and

$$\Psi(x, \mathbf{t}(x), \nabla u(x), V(x)) \leq 0 \text{ a.e. } x \in \Omega,$$

for certain functions $\Psi, \Phi : \Omega \times [0,1]^3 \times \mathbf{R}^N \times \mathbf{R}^N \to \mathbf{R}$. Let us introduce the JBOC condition that bounds Φ and Ψ.

Definition 7.1 *Two functions $\Phi(F)$ and $\Psi(F)$ defined for $F = (F^{(1)}, F^{(2)}) \in \mathbf{R}^N \times \mathbf{R}^N$ are said to satisfy the JBOC (joint boundary optimality condition) if there is a map $\mathbf{M} : \mathbf{R}^N \to \mathbf{R}^N$ with $\Psi(F^{(1)}, \mathbf{M}(F^{(1)})) = 0$ so that an optimal solution of the (nonlinear) mathematical programming problem*

$$\textit{Minimize in } F^{(2)}: \quad \Phi(F) \quad \textit{subject to } \Psi(F) \leq 0$$

is given when $F^{(2)} = \mathbf{M}(F^{(1)})$, and, in addition, an optimal solution of the optimization problem

$$\textit{Minimize in } F^{(1)}: \quad \Phi(F^{(1)}, \mathbf{M}(F^{(1)})) \quad \textit{subject to } \Psi(F) \leq 0$$

is also provided when $F^{(2)} = \mathbf{M}(F^{(1)})$.

Such a definition is tailored to help in the following sense: even if the integrand Φ is not explicitly known, we can still focus on optimality in an appropriate way, and be led to a new, simpler, equivalent optimization problem which may even be a full relaxation of the original problem. Suppose that for a.e. $x \in \Omega$ and $\mathbf{t} \in [0,1]^3$, the functions $\Psi(x, \mathbf{t}, \cdot, \cdot)$ and $\Phi(x, \mathbf{t}, \cdot, \cdot)$ verify the JBOC condition so that there is a map $\mathbf{M} : \Omega \times [0,1]^3 \times \mathbf{R}^N \mapsto \mathbf{R}^N$ in such a way that the identity $V = \mathbf{M}(x, \mathbf{t}, U)$

furnishes the optimal relationship between the two variables V and U as indicated in the definition. We furthermore assume that

$$\Psi(x, \mathbf{t}, U, \mathbf{M}(x, \mathbf{t}, U)) = 0,$$

and the problem

$$\mathrm{div}\,[\mathbf{M}(x, \mathbf{t}(x), \nabla u(x))] = 0 \text{ in } \Omega, \quad u = u_0 \text{ on } \partial\Omega,$$

always has a unique solution in $H^1(\Omega)$. Through this mapping, we can consider two additional variational problems intimately related to our (sub)relaxation, namely:

- Problem (P^*):

$$\text{Minimize in } (\mathbf{t}, u, V): \quad \int_\Omega \tilde{\Phi}(x, \mathbf{t}(x), \nabla u(x))\,dx$$

  subject to

$$u \in H^1(\Omega), \quad u = u_0 \text{ on } \partial\Omega, \quad 0 \le \mathbf{t} \le 1,$$
$$\int_\Omega \mathbf{t}(x)\,dx = \mathbf{r}|\Omega|, \quad \Psi(x, \mathbf{t}(x), \nabla u(x), V(x)) \le 0,$$

  where

$$\tilde{\Phi}(x, \mathbf{t}, U) = \Phi(x, \mathbf{t}, U, \mathbf{M}(x, \mathbf{t}, U)).$$

- Problem $(\tilde{P})$:

$$\text{Minimize in } \mathbf{t}: \quad \int_\Omega \tilde{\Phi}(x, \mathbf{t}(x), \nabla u(x))\,dx$$

  subject to

$$\mathrm{div}\,[\mathbf{M}(x, \mathbf{t}(x), \nabla u(x))] = 0 \text{ in } \Omega,$$
$$u = u_0 \text{ on } \partial\Omega, \quad 0 \le \mathbf{t} \le 1, \quad \int_\Omega \mathbf{t}(x)\,dx = \mathbf{r}|\Omega|.$$

Let us identify as $(\overline{P})$ the initial problem in this section. The key lemma to relate all of these optimization problems is the following.

Lemma 7.1 *If for every non-negative function $p(x)$ (multiplier) and volume fractions $\mathbf{t}(x)$, the combination*

$$\tilde{\Phi}(x, \mathbf{t}(x), U) + p(x)\Psi(x, \mathbf{t}(x), U, V)$$

is an integrand with the property that the integral functional

$$\int_\Omega \left[\tilde{\Phi}(x, \mathbf{t}(x), \nabla u(x)) + p(x)\Psi(x, \mathbf{t}(x), \nabla u(x), V(x))\right] dx \tag{7.2}$$

under a Dirichlet boundary condition for u, and the div-free condition for V, cannot have local minima which are not global, then the pair determined by

$$\operatorname{div}\left[\mathbf{M}(x, \mathbf{t}(x), \nabla u(x))\right] = 0 \text{ in } \Omega, \quad u = u_0 \text{ on } \partial\Omega, \quad V(x) = \mathbf{M}(x, \mathbf{t}(x), \nabla u(x)) \tag{7.3}$$

is optimal for (P^*) for each admissible volume fraction $t(x)$, and the three optimization problems $(\overline{P})$, (P^*), and $(\tilde{P})$ are equivalent.

This lemma implies that when we are interested in finding optimal solutions for $(\overline{P})$. We can find them by treating $(\tilde{P})$ as well. When an explicit form for Φ is not available, if, however, we are able to obtain the optimal map $\mathbf{M}$, we turn to problem $(\tilde{P})$ that is much more explicit and easier to handle than $(\overline{P})$. In addition, if $(\overline{P})$ comes from an original nonconvex problem, it may happen that $(\tilde{P})$ is a relaxation for that nonconvex problem, even if $(\overline{P})$ is not.

Proof. Let $\mathbf{t}$ be given, and let u and V be uniquely determined by (7.3). Because of the JBOC condition, there is no better mate for ∇u, among those complying with $\Psi(x, \mathbf{t}(x), \nabla u(x), \tilde{V}(x)) \leq 0$, than V itself, and no better mate for V, among those verifying $\Psi(x, \mathbf{t}(x), \nabla \tilde{u}(x), V(x)) \leq 0$ than ∇u. This double assertion implies that the pair $(\nabla u, V)$ is a local minimizer for (P^*), and so there is a multiplier $p(x) \geq 0$ such that the same pair $(\nabla u, V)$ is a local minimizer for the augmented functional in (7.2). By our main hypothesis in the statement, that same pair is in fact a global minimizer for (7.2) under (7.4). Take any other pair $(\tilde{u}, \tilde{V})$ admissible for (P^*), such that

$$\tilde{u} \in H^1(\Omega), \quad \tilde{u} = u_0 \text{ on } \partial\Omega, \quad \Psi(x, \mathbf{t}(x), \nabla \tilde{u}(x), \tilde{V}(x)) \leq 0. \tag{7.4}$$

It is immediate to check that

$$\begin{aligned}
&\int_\Omega \tilde{\Phi}(x, \mathbf{t}(x), \nabla u(x))\, dx = \\
&\int_\Omega \tilde{\Phi}(x, \mathbf{t}(x), \nabla u(x))\, dx + \int_\Omega p(x)\Psi(x, \mathbf{t}(x), \nabla u(x), V(x))\, dx \\
&\leq \int_\Omega \tilde{\Phi}(x, \mathbf{t}(x), \nabla \tilde{u}(x))\, dx + \int_\Omega p(x)\Psi(x, \mathbf{t}(x), \nabla \tilde{u}(x), \tilde{V}(x))\, dx \\
&\leq \int_\Omega \tilde{\Phi}(x, \mathbf{t}(x), \nabla \tilde{u}(x))\, dx,
\end{aligned}$$

because

$$\int_\Omega p(x)\Psi(x, \mathbf{t}(x), \nabla u(x), V(x))\, dx = 0$$

but

$$\int_\Omega p(x)\Psi(x, \mathbf{t}(x), \nabla \tilde{u}(x), \tilde{V}(x))\, dx \leq 0.$$

The pair $(\nabla u, V)$ is then optimal for (P^*) for each feasible $\mathbf{t}$. Denote by m^*, $\tilde{m}$ and $\overline{m}$ the infima of the associated optimization problems. Notice that problem $\overline{P}$ contains $(\tilde{P})$ because the admissible fields for $(\tilde{P})$ come from the ones for $\overline{P}$. Furthermore m^* is the lower bound for all infima because $\tilde{\Phi}$ is defined as a result of minimizing Φ over $F^{(2)}$. Hence we have:

$$m^* \leq \bar{m} \leq \tilde{m}.$$

On the other hand, the optimal solution $(\nabla u, V)$ of (P^*) for each feasible $\mathbf{t}$ is admissible for $(\tilde{P})$, which implies:

$$\tilde{m} \leq m^*.$$

Combining those two inequalities, one gets:

$$m^* = \bar{m} = \tilde{m}.$$

7.2 Application of JBOC to our quadratic cost

We found a (sub)relaxation or lower bound for the relaxation of the original optimal design problem (see Theorem 7.1), where $\Phi(t, F)$ is the minimum of the minimization problem:

$$\text{Minimize in } x_i: \quad t_1\left(1 - \frac{a_1}{a_3}\right)|x_1|^2 + t_2\left(1 - \frac{a_2}{a_3}\right)|x_2|^2 + \frac{F^{(1)} \cdot F^{(2)}}{a_3}$$

subject to

$$F^{(1)} \cdot F^{(2)} \geq a_1 t_1 |x_1|^2 + a_2 t_2 |x_2|^2 + a_3 t_3 |x_3|^2,$$
$$F^{(1)} = t_1 x_1 + t_2 x_2 + t_3 x_3, \quad F^{(2)} = t_1 a_1 x_1 + t_2 a_2 x_2 + t_3 a_3 x_3.$$

Even though we do not have an explicit form for it, we show that this $\Phi(t, F)$ and

$$\Psi(t, F) = (F^{(2)} - (a_1 t_1 + a_2 t_2 + a_3 t_3) F^{(1)}) \cdot ((a_1 a_3 t_2 + a_1 a_2 t_3 + a_2 a_3 t_1) F^{(2)} - a_1 a_2 a_3 F^{(1)}) \tag{7.5}$$

comply with the JBOC condition for any given $\mathbf{t} \in [0, 1]^3$. In particular, we are able to determine the optimal map $\mathbf{M}$ in the surprisingly simple form

$$V = \mathbf{M}(\mathbf{t}, U), \quad V = (a_1 t_1 + a_2 t_2 + a_3 t_3) U.$$

In addition, Φ and Ψ are verified to fulfill Lemma 7.1.

We turn our attention first to the JBOC condition. Two optimization problems are solved to show the applicability of JBOC to Φ and Ψ. First, we find an optimal solution $F^{(2)} = \mathbf{M}(F^{(1)})$ of

$$(P_2) \qquad \text{Minimize in } F^{(2)}: \quad \Phi(F) \quad \text{subject to } \Psi(F) \leq 0$$

for fixed $(\mathbf{t}, F^{(1)})$. Afterwards, for given $(\mathbf{t}, F^{(2)})$ we obtain an optimal solution of the second optimization problem

$$(P_1/P_2) \qquad \text{Minimize in } F^{(1)}: \quad \Phi(F^{(1)}, \mathbf{M}(F^{(1)})) \quad \text{subject to } \Psi(F) \leq 0$$

which can be written $F^{(2)} = \mathbf{M}(F^{(1)})$, as well; besides

$$\Psi(x, \mathbf{t}, F^{(1)}, \mathbf{M}(F^{(1)}) = 0$$

holds, too.

- Solve problem (P_2) for fixed $\mathbf{t}$ and $F^{(1)}$:

$$\min_{F^{(2)}} \min_{x_i} \Phi(\mathbf{t}, F, x)$$

subject to

$$F^{(1)} \cdot F^{(2)} \geq a_1 t_1 |x_1|^2 + a_2 t_2 |x_2|^2 + a_3 t_3 |x_3|^2,$$
$$F^{(1)} = t_1 x_1 + t_2 x_2 + t_3 x_3, \quad F^{(2)} = t_1 a_1 x_1 + t_2 a_2 x_2 + t_3 a_3 x_3. \tag{7.6}$$

Note that the set of values of x_i varies depending on the $(\mathbf{t}, F)$ such that

$$\Psi(\mathbf{t}, F) \leq 0.$$

We can switch the order of the two minimizations without changing the solution, and end up with the optimization problem

$$\min_{x \in \{G(x_i, t_i, F) \leq 0,\ (7.6)\ holds\}} \ \min_{F^{(2)} \in \mathcal{A}(F^{(1)}, \mathbf{t})} \Phi(\mathbf{t}, F, x)$$

where

$$\begin{aligned}
\mathcal{A}(F^{(1)}, \mathbf{t}) &= \{F^{(2)} : \Psi(\mathbf{t}, F^{(1)}, F^{(2)}) \leq 0 \text{ for given } \mathbf{t} \text{ and } F^{(1)}\}, \\
G(a_i, t_i, x_i, F) &= a_1 t_1 |x_1|^2 + a_2 t_2 |x_2|^2 + a_3 t_3 |x_3|^2 - F^{(1)} \cdot F^{(2)}.
\end{aligned}$$

We first deal with inner constrained minimization problem using the standard Karush-Kuhn-Tucker conditions due to the convexity of both the cost functional Φ and the constraints on $F^{(2)}$, which can be easily checked:

$$\frac{\partial \Phi(x_i)}{\partial F^{(2)}} + s \frac{\partial \Psi}{\partial F^{(2)}} = 0, \;\; s\Psi = 0, s \geq 0, \Psi \leq 0. \tag{7.7}$$

The solutions to (7.7) are:

$$\begin{aligned}
F^{(2)} &= f(\mathbf{t}, x_i, F^{(1)}), \;\; s = 0, \\
F^{(2)} &= (a_1 t_1 + a_2 t_2 + a_3 t_3) F^{(1)}, \;\; s_1 = S_1(x, F^{(1)}), \\
F^{(2)} &= \frac{a_1 a_2 a_3 F^{(1)}}{a_1 a_2 t_3 + a_1 a_3 t_2 + a_2 a_3 t_1}, \;\; s_2 = S_2(x, F^{(1)}).
\end{aligned}$$

It is not hard to find that $\Psi(\mathbf{t}, F) = 0$, if

$$F^{(2)} = F^{(1)}(a_1 t_1 + a_2 t_2 + a_3 t_3), \quad \text{or} \quad F^{(2)} = \frac{a_1 a_2 a_3 F^{(1)}}{a_1 a_2 t_3 + a_1 a_3 t_2 + a_2 a_3 t_1}$$

is true. And as pointed out in Remark 6.1, there is only one value $x_3 = x_{30}$ (see (6.7)) such that $G(\mathbf{t}, x, F) \leq 0$ holds. Substitute it into S_1 and S_2, and after some tedious algebra, we get

$$s_1 = \frac{1}{a_3}, \quad s_2 = \frac{a_1 a_2 t_3 + a_1 a_3 t_2 + a_2 a_3 t_1 - 2a_3^2}{a_3}.$$

The fact that the constraints on the x's depend on $(F^{(1)}, F^{(2)})$ plays a crucial role here. One can check that $s_2 < 0$ under the condition $\mathbf{t} \cdot \mathbf{1} = 1$ and the assumption

$a_1 < a_2 < a_3$. The Karush-Kuhn-Tucker conditions are also sufficient, if the cost functional and constraints are convex differentiable functions, which is true in our particular problem. Therefore

$$F^{(2)} = (a_1t_1 + a_2t_2 + a_3t_3)F^{(1)}$$

is a minimum. Furthermore, this minimum is unique because of the strict convexity of objective function Φ. As a conclusion,

$$F^{(2)} = (a_1t_1 + a_2t_2 + a_3t_3)F^{(1)}$$

is the optimal solution of P_2.

Remark 7.1 *It is worth pointing out that it is really hard to verify whether the first stationary point $F^{(2)} = f(t, x_i, F^{(1)})$ satifies $\Psi \leq 0$ due to the complex form of $f(\mathbf{t}, x_i, F^{(1)})$. However, this is not necessary because*

$$F^{(2)} = (a_1t_1 + a_2t_2 + a_3t_3)F^{(1)},$$

being the unique minimum, eliminates that possibility.

- Solving problem (P_1/P_2)

  We have found out that

$$F^{(2)} = (a_1t_1 + a_2t_2 + a_3t_3)F^{(1)} = \mathbf{M}(t, F^{(1)}) \tag{7.8}$$

is an optimal solution of P_2. Substituting this into function Φ and take into account the fact that $x_3 = x_{30}$ when (7.8) holds, we obtain a surpringly neat expression

$$\tilde{\Phi} = \Phi(t, F^{(1)}, \mathbf{M}(F^{(1)}) = |F^{(1)}|^2.$$

The optimization problem we are looking at now is:

$$\text{Minimize in } F^{(1)} : \tilde{\Phi} + \rho\Psi(t, x, , F^{(1)}, F^{(2)})$$

subject to

$$\Psi \leq 0.$$

Notice how the outer minimization disappeared automatically by virtue of the fact that there exists only one value of x_3 satisfying the constraint $G(t, x, F) \leq 0$. Then following the same idea, we find out that if $F^{(2)} \neq 0$

$$\begin{aligned} F^{(1)} &= \frac{F^{(2)}}{a_1t_1 + a_2t_2 + a_3t_3}, \quad \rho_3 = \frac{2}{B_aC}, \\ F^{(1)} &= \frac{(a_1a_2t_3 + a_1a_3t_2 + a_2a_3t_1)F^{(2)}}{a_1a_2a_3}, \quad \rho_4 = \frac{-2}{B_hC}, \end{aligned}$$

where

$$B_a = a_1t_1 + a_2t_2 + a_3t_3,\ B_h = \frac{a_1a_2a_3}{a_1a_2t_3 + a_1a_3t_2 + a_2a_3t_1} = \frac{1}{\frac{t_1}{a_1} + \frac{t_2}{a_2} + \frac{t_3}{a_3}},$$
$$C = a_1t_2t_3(a_2 - a_3)^2 + a_2t_1t_3(a_2 - a_3)^2 + a_3t_1t_2(a_1 - a_2)^2.$$

Therefore

$$F^{(1)} = \frac{F^{(2)}}{a_1t_1 + a_2t_2 + a_3t_3}, \quad \rho_3 = \frac{2}{B_aC},$$

is the optimal solution to (P_1/P_2). Otherwise

$$F^{(1)} = 0, \quad \rho = 0$$

is the optimal solution to (P_1/P_2). We still can interpret it as

$$F^{(1)} = \frac{F^{(2)}}{B_a}, \quad \text{or} \quad F^{(2)} = \mathbf{M}(t, F^{(1)}) = B_aF^{(1)}.$$

We can conclude now that Φ and Ψ verifies JBOC with

$$F^{(2)} = \mathbf{M}(\mathbf{t}, F^{(1)}) = B_aF^{(1)}.$$

Next, once the map $\mathbf{M}$ is obtained, we check the validity of Lemma 7.1. Note that we also have

$$\tilde{\Phi}(x, \mathbf{t}, U) = \frac{1}{2}|U|^2.$$

Lemma 7.2 *Let $p(x)$ be a non-negative function defined in Ω, and consider the functional*

$$\int_\Omega \left[\frac{1}{2}|\nabla u(x)|^2 + p(x)\Psi(\mathbf{t}(x), \nabla u(x), V(x))\right] dx, \tag{7.9}$$

for a fixed volume fraction $\mathbf{t}$, and

$$u \in H^1(\Omega), \quad u = u_0 \text{ on } \partial\Omega, \quad V \in L^2(\Omega; \mathbf{R}^N), \quad \operatorname{div} V = 0 \text{ in } \Omega,$$

where Ψ is given by (7.5). Every local minimizer for this variational problem is also a global minimizer.

The proof of this lemma is elementary using the classical div-curl lemma. Notice that the integrand in (7.9) can be written as the sum of two terms: one which is strictly convex in the pair $(\nabla u, V)$ and another one which is a multiple of the inner product $\nabla u \cdot V$. By the div-curl lemma, the latter contribution is weakly continuous, and so it does not play a role regarding the issue local/global minimizer. The strict convexity of the first term, however, implies that local minimizers are global.

As a direct consequence of Lemma 7.2, we have the following relaxation theorem, which is a particular case of a conjecture of Tartar [40] for multimaterials.

Theorem 7.2 *The optimization problem*

$$\textit{Minimize in } \mathbf{t}: \quad \tilde{I}(\mathbf{t}, u) = \int_\Omega |\nabla u(x)|^2 \; dx$$

subject to

$$\begin{aligned} \operatorname{div}\left[(a_1 t_1 + a_2 t_2 + a_3 t_3)\nabla u(x)\right] &= f \;\; \textit{in } \Omega, \\ u &= u_0 \;\; \textit{on } \partial\Omega, \\ \mathbf{t} \in [0,1]^3, \;\; \mathbf{t} \cdot \mathbf{1} = 1, \;\; \int_\Omega \mathbf{t}(x)\, dx &= \mathbf{r}|\Omega|, \end{aligned}$$

is a relaxation of the original optimal design problem in the following sense:

1. *the infima for both problems are the same;*

2. *the second optimization problem always has an optimal solution* $(\tilde{\mathbf{t}}, \tilde{u})$.

CHAPTER 8

OPTIMAL STRUCTURES

In this chapter, we would like to shed some light on the optimal layout of the three materials optimal design problem. It has been shown in the previous chapter that optimal solutions are given by

$$F^{(2)} = (a_1t_1 + a_2t_2 + a_3t_3)F^{(1)},$$

which lie in the set $\{P_{\mathbf{t}} = 0\}$. Recall, in Remark 6.1, it is pointed out that the ν_i's are Dirac masses based at (x_i, a_ix_i) on the set $\{P_{\mathbf{t}} = 0\}$. Furthermore, the x_i's are uniquely determined: $x_3 = x_{30}$ (see (6.7)), x_1 and x_2 are found by substituting x_{30} into (6.5). We now find optimal structures that can be formed by these three mass points, one on each manifold Λ_i.

Lemma 8.1 *On the set $(F, t) \in \{P_t = 0\}$, any pair (x_i, a_ix_i) and (x_j, a_jx_j) supported in Λ_i and Λ_j respectively, is rank-1 connected for $i, j = 1, 2, 3, i \neq j$.*

The proof of the lemma is tedious, but straightforward. We check whether

$$(x_i - x_j) \cdot (a_ix_i - a_jx_j) = 0, i \neq j$$

is true on $\{P_t = 0\}$. Here we show only the case $i = 1, j = 2$. Direct calculation of $(x_1 - x_2) \cdot (a_1x_1 - a_2x_2)$ yields:

$$\begin{aligned} (x_1 - x_2) \cdot (a_1x_1 - a_2x_2) &= \frac{c_1c_2|x_3|^2 + (c_2A_1 + c_1A_2) \cdot x_3 + A_1 \cdot A_2}{t_1^2t_2^2(a_1 - a_2)^2} \\ &= \frac{(c_1x_3 + A_1) \cdot (c_2x_3 + A_2)}{t_1^2t_2^2(a_1 - a_2)^2} \end{aligned} \tag{8.1}$$

where

$$\begin{aligned}
c_1 &= (a_3t_2t_3 - a_1t_3t_1 + a_3t_1t_3 - a_2t_2t_3),\\
c_2 &= (a_1t_3t_2a_3 - t_2a_1a_2t_3 - t_3a_2t_1a_1 + t_3a_2t_1a_3),\\
A_1 &= (a_2t_2F^{(1)} - t_2F^{(2)} + a_1t_1F(1) - t_1F^{(2)}),\\
A_2 &= (t_2a_2a_1F^{(1)} - a_1t_2F^{(2)} + a_2t_1a_1F^{(1)} - a_2t_1F^{(2)}).
\end{aligned}$$

Evaluating $c_1x_3 + A_1$ at $x_3 = x_{30}$, we get:

$$c_1x_3 + A_1 = \frac{-(a_1-a_2)^2[(a_1t_1 + a_2t_2 + a_3t_3)F^{(1)} - (t_3+t_1+t_2)F^{(2)}]}{a_1t_2t_3(a_2-a_3)^2 + a_2t_1t_3(a_1-a_3)^2 + a_3t_1t_2(a_1-a_2)^2}.$$

Evaluation of $c_2x_3 + A_2$ at $x_3 = x_{30}$ results in:

$$c_2x_3 + A_2 = \frac{(a_1-a_2)^2[a_1a_2a_3(t_1+t_2+t_3)F^{(1)} - (a_1a_3t_2 + a_1a_2t_3 + a_2a_3t_1)F^{(2)}]}{a_1t_2t_3(a_2-a_3)^2 + a_2t_1t_3(a_1-a_3)^2 + a_3t_1t_2(a_1-a_2)^2}.$$

Taking into account the fact $t_1 + t_2 + t_3 = 1$, the last two equations can be simplified to:

$$\begin{aligned}
c_1x_3 + A_1 &= \frac{-(a_1-a_2)^2[(a_1t_1 + a_2t_2 + a_3t_3)F^{(1)} - F^{(2)}]}{a_1t_2t_3(a_2-a_3)^2 + a_2t_1t_3(a_1-a_3)^2 + a_3t_1t_2(a_1-a_2)^2},\\
c_2x_3 + A_2 &= \frac{(a_1-a_2)^2[a_1a_2a_3F^{(1)} - (a_1a_3t_2 + a_1a_2t_3 + a_2a_3t_1)F^{(2)}]}{a_1t_2t_3(a_2-a_3)^2 + a_2t_1t_3(a_1-a_3)^2 + a_3t_1t_2(a_1-a_2)^2}.
\end{aligned} \tag{8.2}$$

Therefore (see (6.8))

$$(x_1 - x_2)\cdot(a_1x_1 - a_2x_2) = \rho_1 P_t \tag{8.3}$$

where

$$\rho_1 = \frac{-(a_1-a_2)^2}{t_1^2t_2^2\left(a_1t_2t_3(a_2-a_3)^2 + a_2t_1t_3(a_1-a_3)^2 + a_3t_1t_2(a_1-a_2)^2\right)^2}.$$

Hence, (x_1, a_1x_1) and (x_2, a_2x_2) are rank-1 connected if

$$(F^{(1)}, F^{(2)}) \in \{(X,Y) \in \mathbf{R}^2 \times \mathbf{R}^2 : P_t(X,Y) = 0\}.$$

Similarly, it can be shown that:

$$\begin{aligned}
(x_1 - x_3)\cdot(a_1x_1 - a_3x_3) &= \rho_2 P_t,\\
(x_2 - x_3)\cdot(a_2x_2 - a_3x_3) &= \rho_3 P_t,
\end{aligned} \tag{8.4}$$

and

$$\begin{aligned}
\rho_2 &= \frac{-(a_1-a_3)^2}{t_1^2t_2^2\left(a_1t_2t_3(a_2-a_3)^2 + a_2t_1t_3(a_1-a_3)^2 + a_3t_1t_2(a_1-a_2)^2\right)^2},\\
\rho_3 &= \frac{-(a_2-a_3)^2}{t_1^2t_2^2\left(a_1t_2t_3(a_2-a_3)^2 + a_2t_1t_3(a_1-a_3)^2 + a_3t_1t_2(a_1-a_2)^2\right)^2},
\end{aligned}$$

which tells that both $\{(x_2, a_2x_2), (x_3, a_3x_3)\}$ and $\{(x_1, a_1x_1), (x_3, a_3x_3)\}$ are rank-1 connected when

$$(F^{(1)}, F^{(2)}) \in \{(X, Y) \in \mathbf{R}^2 \times \mathbf{R}^2 : P_t(X, Y) = 0\}.$$

Based on these calculations, we have the following theorem.

Theorem 8.1 *Let (t, u) be an optimal solution for the optimal design problem in Theorem 7.2. Put*

$$V(x) = (a_1t_1(x) + a_2t_2(x) + a_3t_3(x))\nabla u(x) \text{ for a.e. } x \in \Omega,$$

and,

$$\begin{aligned}
W_3(x) =& \frac{(a_1a_2(a_1t_1(x) + a_2t_2(x)) - a_1a_2a_3(t_1(x) + t_2(x)))\,\nabla u(x)}{a_1t_2(x)t_3(x)(a_2 - a_3)^2 + a_2t_1(x)t_3(x)(a_1 - a_3)^2 + a_3t_1(x)t_2(x)(a_1 - a_2)^2},\\
&+ \frac{(a_3(a_1t_2(x) + a_2t_1(x)) - a_1a_2(t_1(x) + t_2(x)))V(x)}{a_1t_2(x)t_3(x)(a_2 - a_3)^2 + a_2t_1(x)t_3(x)(a_1 - a_3)^2 + a_3t_1(x)t_2(x)(a_1 - a_2)^2},\\
W_1(x) =& \frac{a_2t_3(x)W_3(x) - a_3t_3(x)W_3(x) - a_2\nabla u(x) + V(x)}{t_1(x)(a_1 - a_2)},\\
W_2(x) =& \frac{a_3t_3(x)W_3(x) - a_1t_3(x)W_3(x) + a_1\nabla u(x) - V(x)}{t_2(x)(a_1 - a_2)}.
\end{aligned}$$

Then every local laminate of arbitrary finite order supported in the three mass points

$$(W_i(x), a_iW_i(x)), i = 1, 2, 3,$$

with corresponding weights $t_i(x)$ is an optimal microstructure for the original optimal design problem.

In fact, this theorem is a natural consequence of the following general fact and Lemma 8.1.

Lemma 8.2 *If in a two-dimensional linear manifold, three linearly independent directions are rank-1, then every direction in that manifold is rank-1, and every probability measure supported in such a manifold can be decomposed as a laminate of arbitrary order.*

This is exactly our situation with the three mass points, one on each manifold. The simplest optimal structures among all those diverse optimal structures, are the three second-rank laminates formed by the three mass points

$$\{(x_1, a_1x_1), (x_2, a_2x_2), (x_3, a_3x_3)\}$$

sitting over each manifold Λ_i, at the given proportion.

CHAPTER 9

SUMMARY

In this chapter, we describe the difference between the situation of two materials optimal design and that of three materials. In addition, we discuss the possibility of solving G-closure problem using Young measures, or the connection between the two parts of this dissertation.

9.1 Difference of three materials from two materials

The main differences are present in two aspects: (1) formation of the quasiconvex hull; (2) obtainability of the quasiconvexification of the integrand.

In the two-material situation, the system (6.4) has unique solutions $x_i, i = 1, 2$, hence corresponding to a $(F^{(1)}, F^{(2)})$-the first moment of some Young measure, the mass points $(x_i, a_i x_i)$ on each $\Lambda_i, i = 1, 2$ is uniquely determined. This is the main difference of the two-material situation from the three materials, and it simplifies the analysis and algebra involved. As a consequence, an explicit quasiconvexification is available. On the contrary, in the three-materials situation, (6.1) is underdetermined and has many solutions. Therefore, for fixed $\mathbf{t}$, corresponding to some F (see the proof of Theorem 6.1 and Remark 6.1):

$$F \in \{P_{\mathbf{t}}(F) \leq 0\},$$

there exist multiple vectors (x_1, x_2, x_3) that satisfy the necessary conditions (6.1), (6.2) and (6.3). Let us denote this set of vectors by S. Each vector leads to an admissible Young measure ν of the problem (PP) (polyconvexfication problem). However, only a subset of S can be recovered by a div-curl Young measure and forms the quasiconvex hull, which is the admissible set of the problem (QP) (quasiconvexification problem).

Each element of this subset satisfies (6.9) and (6.10). When one deals with the quadratic cost functional, the optimal solution of the problem (PP) can lie anywhere in S, not only in the quasiconvex hull. If it falls outside the quasiconvex hull, there is no way to find the explicit quasiconvexification of the original integrand, and in this situation, one has a lower bound of the relaxation (subrelaxation). As a consequence, we turn to the JBOC condition as discussed in Chapter 7. By focusing on such optimality conditions, we found the fully relaxation from which the minimizing sequences can be constructed explicitly.

9.2 Solving the G-closure problem using Young measures

The G-closure problem is actually a problem of finding the quasiconvexification of the multiwell energy [21]. So the two approaches presented in this dissertation embody some common ideas: due to the limited knowledge of quasiconvex functions, in both approaches, actually the polyconvexification is first obtained. This corresponds to the lower bound of energy in the first part, and the subrelaxation in the second part. Such a polyconvexfication is found by using the weak continuity of the determinant of fields. However, in the G-closure problem, it is incorporated in the integral through some lagrange multiplier t to form the augmented integrand; while in the context of Young measures, this property is enforced directly on the fields or the generalized fields-Young measures (the commutation property of determinant against Young measures). Once the polyconvexification is obtained, in both parts, it is shown that this polyconvexification is also a rank-1 convexification by presenting laminates structures that realized the lower bound on the energy in the G-closure problem; and showing that the optimal Young measures are laminate Young measures in the second part; thus this polyconvexification is a quasiconvexification, too. Note that the optimal Young measures are the weak limits of the laminate fields in the optimal structures (structures realizing the energy bound) in the first part.

It is possible to solve the G-closure problem using the Young measures. One needs to deal with two gradient fields in the G-closure problem; therefore, we introduce the new design variable V, as in the second part of the dissertation, however, corresponding to two gradient fields:

$$V = \sum_{i=1}^{3} a_i \chi_i \nabla U, \quad \text{where} \quad \nabla U = (\nabla u_1, \nabla u_2),$$

and consider the two-dimensional three-materials G-closure problem in terms of the new design variables $(\nabla U, V) \in \mathbf{M}^{2\times 4}$, subjected to the constraints:

$$V \in L^2(\Omega; \mathbf{M}^{2\times 2}), \quad U \in H^1(\Omega; \mathbf{M}^{2\times 2}),$$
$$\operatorname{div} V = 0 \text{ weakly in } \Omega, \quad U = U_0 \text{ on } \partial\Omega.$$

Furthermore, if we write $V = (V_1, V_2)$, then $(\nabla u_1, V_1) \times (\nabla u_2, V_2)$ should belong to $\Lambda \subset \mathbf{M}^{2\times 2} \times \mathbf{M}^{2\times 2}$, where

$$\Lambda = \bigcup_{i=1}^{3} \Lambda_i \times \Lambda_i, \quad \text{and} \quad \Lambda_i = \{(\lambda, \rho) \subset \mathbf{R}^2 \times \mathbf{R}^2 : \rho = a_i \lambda\}.$$

and the subset Ω_i of Ω prescribed by

$$\Omega_i = \{x \in \Omega : (\nabla u_1(x), V_1(x)) \times (\nabla u_2(x), V_2(x)) \in \Lambda_i \times \Lambda_i\}$$

has relative measure r_i. The Young measures $\nu = \{\nu_x\}_{x\in\Omega}$ associated with the sequences $\{(\nabla U_j, V^j)\}$ from the admissible set of the G-closure problem satisfy:

$$\operatorname{supp}(\nu_x) \subset \Lambda = \bigcup_i \Lambda_i \times \Lambda_i,$$

and as a consequence, if

$$\nu_x = \sum_i t_i(x) \nu_{x,i}, \quad \operatorname{supp}(\nu_{x,i}) \subset \Lambda_i \times \Lambda_i, \quad t_i(x) \in (0,1), \quad \sum_{i=1}^{3} t_i(x) = 1,$$

holds, then we should have

$$\int_\Omega t_i(x)\, dx = |\Omega| r_i.$$

Note that the integrand, in terms of the new design variables, is:

$$\Psi(x) = \nabla U(x) \cdot V(x),$$

where the inner product is defined over two by two matrices; therefore the G-closure problem is a case of the linear cost functionals. As pointed out in Chapter 6, in such a situation, all that matters is to find the quasiconvex hull of the admissible set, or the weak limits of the sequences $\{(\nabla U_j,\ V^j)\} \in \mathbf{M}^{2\times 4}$ coming from the G-closure problem, and they are the first moment of the associated Young measures.

In order to obtain the quasiconvex hull, we have to first find the constraints on the first moments $F \in \mathbf{M}^{2\times 4}$ of the admissible Young measures ν associated with the sequences $\{(\nabla U_j,\ V^j)\}$, which is expected to be described through polynomials of F as before. However, the situation is much more complicated, because we are dealing with Young measures associated with two divergence free vectors and two gradient vectors. The commutation property is satisfied by any pair of divergence free and gradient vectors against the Young measure, by div-curl lemma. In addition, due to the weak continuity of the determinant of a gradient matrix, the commutation property also holds for the determinant of the matrix formed of two gradient vectors and the determinant of the matrix of the two divergence free vectors, recalling that in $\mathbf{R}^2$, a divergence free vector is the 90° rotation of a gradient vector. To be more precise, if we let:

$$
\begin{aligned}
F^{(1)} &= \int_{\mathbf{M}^{2\times 4}} \lambda_1\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2), \quad F^{(2)} = \int_{\mathbf{M}^{2\times 4}} \lambda_2\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2),\\
F^{(3)} &= \int_{\mathbf{M}^{2\times 4}} \rho_1\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2), \quad F^{(4)} = \int_{\mathbf{M}^{2\times 4}} \rho_2\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2),
\end{aligned}
$$

we have:

$$
\begin{aligned}
F^{(1)}\cdot F^{(3)} &= \int_{\mathbf{M}^{2\times 4}} \lambda_1\cdot\rho_1\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2),\\
F^{(1)}\cdot F^{(4)} &= \int_{\mathbf{M}^{2\times 4}} \lambda_1\cdot\rho_2\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2),\\
F^{(2)}\cdot F^{(3)} &= \int_{\mathbf{M}^{2\times 4}} \lambda_2\cdot\rho_1\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2),\\
F^{(2)}\cdot F^{(4)} &= \int_{\mathbf{M}^{2\times 4}} \lambda_2\cdot\rho_2\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2),\\
\det(F^{(1)},F^{(2)}) &= \int_{\mathbf{M}^{2\times 4}} \det(\lambda_1,\lambda_2)\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2),\\
\det(F^{(3)},F^{(4)}) &= \int_{\mathbf{M}^{2\times 4}} \det(\rho_1,\rho_2)\, d\nu(\lambda_1,\lambda_2,\rho_1,\rho_2).
\end{aligned}
$$

Different from the situation where one gradient field is involved, we have more than one polynomials, each of which is related to the commutation property given by one of the above equations, describing the constraints on F. It is the main challenge to integrate all those polynomials into a proper framework and being able to show that, in this framework, every admissible F is the first moment of a laminate Young measure. Once this goal is achieved, we will find the quasiconvex hull of the set of matrices $(\nabla U, V)$ and thus obtain the G-closure.

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