HOMOGENIZATION AND APPLICATIONS TO MATERIAL SCIENCES

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Introduction.

These lecture notes are a brief introduction to the mathematical theory of homogenization and some of its applications to material sciences. For a more advanced presentation of homogenization (which is a huge and fascinating field since its beginning in the early seventies), the reader is referred to the classical books [12], [15], [19], [58], and [70]. Roughly speaking, homogenization is a rigorous version of what is known in physics or mechanics as averaging. In other words, homogenization extracts homogeneous effective parameters from disordered or heterogeneous media.

We shall work in the setting of linearized elasticity which is of paramount importance for applications. We could have exposed the same ideas in the conductivity setting which is simpler and for which stronger and deeper results hold true. We do not discuss the non-linear setting which, of course, is more relevant in the context of, e.g., phase transitions. The reason is that, in this case, the theory is less complete and uses different tools than those presented here.

The first chapter focus on the homogenization of periodic structures. The method of two-scale asymptotic expansions is presented, and its mathematical justification will be briefly discussed. The second chapter introduces the notion of G- or H-convergence which can be applied to any kind of disordered media (not necessarily periodic). The third chapter is devoted to the notion of H-measure, introduced by Gerard [27] and Tartar [65]. It is a default measure which characterizes the lack of compactness of a weakly converging sequence. When specialized to multiphase composite materials it appears as a two-point correlation function which plays a crucial role in estimating their effective properties. The fourth chapter is concerned with the mathematical modelling of two-phase composite materials. Bounds on their effective properties are established with the help of the Hashin-Shtrikman variational principle. Those bounds are optimal being attained by a special class of composites, the so-called sequential laminates. Since the set of all two-phase elastic composites is unknown (this is the so-called G-closure problem), we address its characterization up to second order terms with respect to the contrast between the phases. This so-called small amplitude homogenization is equivalent to a problem of characterizing all possible H-measures of the phases mixtures. Finally, the fifth chapter explores the so-called multiple wells problems in the calculus of variations. In the case of quadratic wells in the linearized elasticity setting, their solution is equivalent to finding all possible H-measures of phases mixtures, i.e. it is similar to characterize the small amplitude G-closure. Such problems are a crude model for phase transitions, but are already so difficults that a full answer is not yet available. Through these lectures notes, we want to emphasize the link between all these questions which turns out to be the notion of H-measure.

Chapter 1

Periodic homogenization.

Homogenization has first been developed for periodic structures. Indeed, in many fields of science and technology one has to solve boundary value problems in periodic media. Quite often the size of the period is small compared to the size of a sample of the medium, and, denoting by ϵ their ratio, an asymptotic analysis, as ϵ goes to zero, is called for. Starting from a microscopic description of a problem, we seek a macroscopic, or effective, description. This process of making an asymptotic analysis and seeking an averaged formulation is called homogenization.

We emphasize that homogenization is not restricted to the periodic case and can be applied to any kind of disordered media. This is the focus of the second chapter where the notion of G- or H-convergence is introduced. It allows to consider any possible geometrical situation without any specific assumptions like periodicity or randomness.

1.1 Setting of the problem.

We consider a model problem of linear elasticity in a periodic medium (for example, a composite material where stiff fibers are included in a matrix of a more compliant phase). To fix ideas, the periodic domain is called Ω (a bounded open set in $\mathbb{R}^N$ with $N \geq 1$), its period ϵ (a positive number which is assumed to be very small in comparison with the size of the domain), and the rescaled unit cell Y (i.e. $Y = (0,1)^N$). The Hooke's law in Ω is not constant but varies periodically with period ϵ in each direction. It is a fourth order tensor $A(y)$, where $y = x/\epsilon \in Y$ is the fast periodic variable, while $x \in \Omega$ is the slow variable. Equivalently, x is also called the macroscopic variable, and y the microscopic variable. If the Hooke's law A

is isotropic, with positive bulk and shear moduli κ and μ, we have

$$A(y) = (\kappa(y) - \frac{2\mu(y)}{N})I_2 \otimes I_2 + 2\mu(y)I_4,$$

but, A can be any fourth order tensor satisfying the usual symmetries of linear elasticity, $A_{ijkl} = A_{klij} = A_{jikl} = A_{ijlk}$ for $1 \leq i,j,k,l \leq N$, and the usual coerciveness assumption, i.e. there exist a positive constant $\alpha > 0$ such that, for any constant symmetric matrix ξ with entries $\xi_{ij} \in \mathbb{R}^N$ and at any point $y \in Y$,

$$\alpha|\xi|^2 \leq \sum_{i,j,k,l=1}^{N} A_{ijkl}(y)\xi_{ij}\xi_{kl}.$$

The tensor $A(y)$ is a periodic function of y, with period Y, and it may be discontinuous in y (to model the discontinuity of the elastic properties from one phase to the other).

Denoting by $f(x)$ the external load (a vector function defined in Ω), and enforcing a Dirichlet boundary condition (for simplicity), our model problem of elasticity reads

$$\begin{cases} -\mathrm{div}\ \left(A\left(\frac{x}{\epsilon}\right)e(u_\epsilon)\right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega, \end{cases} \tag{1.1}$$

where u_ϵ is the unknown displacement, and $e(u_\epsilon)$ is the deformation tensor $1/2(\nabla u_\epsilon +^t \nabla u_\epsilon)$.

Remark 1.1.1 *From a mathematical point of view, problem (1.1) is well posed in the sense that, if the force $f(x)$ belongs to the space $L^2(\Omega)^N$ of square integrable vectors on Ω, then the Lax-Milgram lemma implies existence and uniqueness of the solution u_ϵ in the Sobolev space $H_0^1(\Omega)^N$ of vectors functions which belong to $L^2(\Omega)^N$ along with their first derivatives. More smoothness can be obtained for the solution u_ϵ, but it is not necessary in the sequel.*

From a mechanical point of view, the domain Ω with its material properties $A\left(\frac{x}{\epsilon}\right)$ is highly heterogeneous with periodic heterogeneities of length-size ϵ. Usually one does not need the full details of the elastic displacement, but rather some global of averaged behavior of the domain Ω submitted to the force f. From a numerical point of view, solving equation (1.1) by any method will require too much efforts if ϵ is small since the number of elements (or degrees of freedom) for a fixed level of accuracy grows like $1/\epsilon^N$. It is thus preferable to average or homogenize the properties of Ω and compute an approximation of u_ϵ on a coarse mesh. This process of averaging the displacement solution of (1.1) and finding the effective properties of the domain Ω is precisely what is called homogenization.

In order to find this homogenized or averaged behavior of Ω, we perform an asymptotic analysis of equation (1.1) as the period ϵ goes to 0. The solution u_ϵ is written as a series in power of ϵ

$$u_\epsilon = \sum_{i=0}^{+\infty} \epsilon^i u_i .$$

The first term u_0 of this series will be identified with the solution of the so-called homogenized equation whose Hooke's law A^* can be exactly computed. Note that A^* is a constant tensor describing a homogeneous medium. Numerical computations on the homogenized equation does not require a fine mesh since the heterogeneities of size ϵ have been averaged out. This homogenized tensor A^* is usually not a usual average (arithmetic or harmonic) of $A(y)$... Various estimates will confirm this asymptotic analysis by telling in which sense u_ϵ is close to u_0 as ϵ is small.

Remark 1.1.2 *From a mathematical point of view, homogenization can be interpreted as follows. Rather than studying equation (1.1) for the precise value ϵ which is the physical lengthscale of the heterogeneities, we embed this problem in a sequence of problems indexed by the period ϵ which is now regarded as a small parameter going to zero. Therefore, we now consider the sequence of solutions $(u_\epsilon)_{\epsilon>0}$ as a sequence in the Sobolev space $H_0^1(\Omega)^N$.*

Multiplying equation (1.1) by u_ϵ, integrating by parts, and using Poincaré inequality (i.e. the L^2 norm of u_ϵ is bounded by that of ∇u_ϵ) yields the following a priori estimate

$$\|u_\epsilon\|_{H_0^1(\Omega)^N} \leq C\|f\|_{L^2(\Omega)^N} \tag{1.2}$$

where C is a positive constant which does not depend on ϵ. It implies that the sequence u_ϵ is bounded in $H_0^1(\Omega)^N$. Therefore, up to extracting a subsequence, it converges weakly in $H_0^1(\Omega)^N$ to some limit u (and by Rellich' theorem it converges also strongly to u in $L^2(\Omega)^N$). Finally, the homogenization process amounts to find what is the equation satisfied by u. Of course, u will turn out to coincide with u_0, the first term in the series defined above, and it is therefore the solution of the homogenized equation.

1.2 Two-scale asymptotic expansions.

The method of two-scale asymptotic expansions is a formal method which allows to homogenize a great variety of models or equations posed in a periodic domain. There are many good reference books on this topic, see in particular [12], [15], and [58]. As already said, the starting point is to consider the following ansatz, or *two-scale asymptotic expansion*, for the solution u_ϵ of equation (1.1)

$$u_\epsilon(x) = \sum_{i=0}^{+\infty} u_i\left(x, \frac{x}{\epsilon}\right), \tag{1.3}$$

where each term $u_i(x,y)$ is a function of both variables x and y, periodic in y with period $Y = (0,1)^N$. This series is plugged in the equation, and the following derivation rule is used

$$\nabla\left(u_i\left(x, \frac{x}{\epsilon}\right)\right) = \left(\epsilon^{-1}\nabla_y u_i + \nabla_x u_i\right)\left(x, \frac{x}{\epsilon}\right),$$

where ∇_y and ∇_x denote the partial derivative with respect to the first and second variable of $u_i(x,y)$. For example, one has

$$\nabla u_\epsilon(x) = \epsilon^{-1}\nabla_y u_0\left(x, \frac{x}{\epsilon}\right) + \sum_{i=0}^{+\infty} \epsilon^i\left(\nabla_y u_{i+1} + \nabla_x u_i\right)\left(x, \frac{x}{\epsilon}\right).$$

Equation (1.1) becomes a series in ϵ

$$\begin{aligned}&-\epsilon^{-2}\left[\mathrm{div_y}\ (Ae_y(u_0))\right]\left(x, \tfrac{x}{\epsilon}\right)\\ &-\epsilon^{-1}\left[\mathrm{div_y}\ (A(e_x(u_0)+e_y(u_1))) + \mathrm{div_x}\ (Ae_y(u_0))\right]\left(x, \tfrac{x}{\epsilon}\right)\\ &-\textstyle\sum_{i=0}^{+\infty}\epsilon^i\left[\mathrm{div_x}\ (A(e_x(u_i)+e_y(u_{i+1}))) + \mathrm{div_y}\ (A(e_x(u_{i+1})+e_y(u_{i+2})))\right]\left(x, \tfrac{x}{\epsilon}\right) \quad = f(x).\end{aligned} \tag{1.4}$$

Identifying each coefficient of (1.4) as an individual equation yields a cascade of equations (a series of the variable ϵ is zero for all value of ϵ if each coefficient is zero). It turns out that the three first equations are enough for our purpose. The ϵ^{-2} equation is

$$-\mathrm{div_y}\ (A(y)e_y(u_0(x,y))) = 0,$$

which is nothing else than an equation in the unit cell Y with periodic boundary condition. In this equation, y is the variable, and x plays the role of a parameter. There exists a unique solution of this equation up to a constant (with respect to y). This implies that u_0 is a function which *does not depend on* y, i.e. there exists a function $u(x)$ which depends only on x such that

$$u_0(x,y) \equiv u(x).$$

Since $e_y(u_0) = 0$, the ϵ^{-1} equation is

$$-\mathrm{div_y}\ \left(A(y)e_y(u_1(x,y))\right) = \mathrm{div_y}\ \left(A(y)e_x(u(x))\right), \tag{1.5}$$

which is an equation for the unknown u_1 in the periodic unit cell Y. Again, it is a well-posed problem wich admits a unique solution, up to a constant, as soon as the right hand side is known. Equation (1.5) allows to compute u_1 in terms of u, and it is easily seen that $u_1(x,y)$ depends linearly on the first derivative $\nabla_x u(x)$.

Finally, the ϵ^0 equation is

$$-\mathrm{div_y}\ \left(A(y)e_y(u_2(x,y))\right) = \mathrm{div_y}\ \left(A(y)e_x(u_1)\right) + \mathrm{div_x}\ \left(A(y)(e_y(u_1) + e_x(u))\right) + f(x), \tag{1.6}$$

which is an equation for the unknown u_2 in the periodic unit cell Y. Equation (1.6) admits a solution (unique up to a constant) if a compatibility condition is satisfied (the so-called Fredholm alternative). Indeed, integrating the left hand side of (1.6) over Y, and using the periodic boundary condition for u_2, we obtain a zero mean value for equation (1.6). This implies that the right hand side *must have zero average over* Y

$$\int_Y \left[\mathrm{div_y}\ \left(A(y)e_x(u_1)\right) + \mathrm{div_x}\ \left(A(y)(e_y(u_1) + e_x(u))\right) + f(x)\right] dy = 0,$$

which simplifies in

$$-\mathrm{div_x} \int_Y A(y)\left(e_y(u_1) + e_x(u)\right) dy \ = \ f(x) \ \text{ in } \Omega. \tag{1.7}$$

Since $u_1(x,y)$ depends linearly on $\nabla_x u(x)$, equation (1.7) is simply an equation for $u(x)$ involving only the second order derivatives of u. The next section is devoted to an interpretation of this equation as the homogenized equation.

Remark 1.2.1 *This method of two-scale asymptotic expansions is mathematically formal. In other words, it yields heuristically the homogenized equation, but it is not a rigorous proof of the homogenization process. The reason is that the ansatz (1.3) is not always correct. Indeed, it is usually false after the two first terms. For example, it does not include possible boundary layers in the vicinity of $\partial\Omega$ (for details, see e.g. [40]).*

1.3 Cell and homogenized problems.

The method of two-scale asymptotic expansions give rise to a couple of equations (1.5) (1.7) that have a mathematical, as well as physical, interpretation. Let us introduce the so-called *cell problems*. We denote by

$(e_i)_{1\leq i\leq N}$ the canonical basis of $\mathbb{R}^N$. Defining

$$e_{ij} = \frac{1}{2}\left(e_i \otimes e_j + e_j \otimes e_i\right),$$

we obtain a basis of the space of symmetric matrices. For each matrix e_{ij}, consider the following elasticity problem in the periodic unit cell

$$\left\{ \begin{array}{ll} -\mathrm{div_y}\ \left(A(y)\left(e_{ij} + e_y(w_{ij}(y))\right)\right) = 0 & \text{in } Y \\ y \to w_{ij}(y) & Y\text{-periodic,} \end{array} \right. \tag{1.8}$$

where $w_{ij}(y)$ is the displacement created by a mean deformation equal to e_{ij}.

By linearity, it is not difficult to compute $u_1(x,y)$, solution of (1.5), in terms of $u(x)$ and $w_{ij}(y)$

$$u_1(x,y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\partial u_i}{\partial x_j}(x) + \frac{\partial u_j}{\partial x_i}(x)\right) w_{ij}(y). \tag{1.9}$$

Inserting this expression in equation (1.7), we obtain the *homogenized equation* for u

$$-\mathrm{div_x}\ \left(A^* e_x(u(x))\right) = f(x) \text{ in } \Omega, \tag{1.10}$$

that we supplement with Dirichlet boundary condition on $\partial\Omega$. The homogenized Hooke's law A^* is defined by its entries

$$A^*_{ijkl} = \int_Y A(y)\left(e_{ij} + e(w_{ij})\right)\cdot\left(e_{kl} + e(w_{kl})\right) dy, \tag{1.11}$$

or equivalently, by a simple integration by parts in Y,

$$A^*_{ijkl} = \int_Y \left(A(y) e_y(w_{ij})_{kl} + A_{ijkl}(y)\right) dy.$$

The constant tensor A^* describes the effective or homogenized properties of the heterogeneous material $A\left(\frac{x}{\epsilon}\right)$. Remark that it does not depend on the choice of domain Ω, force f, or boundary condition on $\partial\Omega$.

Remark 1.3.1 *From a mathematical point of view, it is possible to rigorously justify the fact that equation (1.10) is the homogenized equation associated to the original equation (1.1). For example, in [12], [15], and [58], it is proved that the sequence $u_\epsilon(x)$ of solutions of (1.1) converges weakly in $H^1_0(\Omega)^N$ to a limit $u(x)$ which is the unique solution of the homogenized problem 1.10) . This justifies the first term in the ansatz of u_ϵ, but one can justify the two first terms and improve the weak convergence of*

u_ϵ. *More precisely,* $(u_\epsilon(x) - u(x) - \epsilon u_1\left(x, \frac{x}{\epsilon}\right))$ *converges strongly to 0 in* $H_0^1(\Omega)^N$ *(one can even estimate the speed of convergence in terms of* ϵ*).*

Technically, the most general and powerful method for proving such an homogenization theorem is the so-called energy method *of Tartar [62]. Another method (which is simpler but restricted to the periodic setting) is the two-scale convergence introduced by Nguetseng [51] and Allaire [2].*

1.4 Variational characterization of the homogenized coefficients.

The homogenized Hooke's law A^* is defined in terms of the solutions of the cell problems by equation (1.11). It is convenient to give another definition of A^* involving standard variational principles. Recall that both the original and the homogenized Hooke's law $A(y)$ and A^* are symmetric fourth order tensors. Therefore, A^* is completely determined by the knowledge of the quadratic form $A^*\xi \cdot \xi$ where ξ is any symmetric matrix. From definition (1.11) it is not difficult to check that

$$A^*\xi \cdot \xi = \int_Y A(y)\,(\xi + e(w_\xi)) \cdot (\xi + e(w_\xi))\,dy, \tag{1.12}$$

where w_ξ is the solution of

$$\begin{cases} -\mathrm{div_y}\ (A(y)\,(\xi + e_y(w_\xi(y)))) = 0 & \text{in } Y \\ y \to w_\xi(y) & Y\text{-periodic.} \end{cases} \tag{1.13}$$

It is well-known that equation (1.13) is the Euler-Lagrange equation of the following variational principle : find w which minimizes

$$\int_Y A(y)\,(\xi + e(w)) \cdot (\xi + e(w))\,dy$$

over all periodic displacement fields w. In other words, $A^*\xi \cdot \xi$ is given by the minimization of the elastic energy (primal formulation)

$$A^*\xi \cdot \xi = \min_{w \in H^1_\#(Y)^N} \int_Y A(y)\,(\xi + e(w)) \cdot (\xi + e(w))\,dy \tag{1.14}$$

where $H^1_\#(Y)^N$ is the Sobolev space of periodic displacements in Y.

There is also a dual formulation for the elastic energy, in terms of stresses rather than deformations. For any symmetric matrix σ, this yields a definition of A^{*-1}

$$A^{*-1}\sigma \cdot \sigma = \min_{\substack{\tau(y) \in L^2_\#(Y)^{N^2} \\ \mathrm{div}\ \tau = 0 \text{ and } \int_Y \tau\,dy = 0}} \int_Y A^{-1}(y)\,(\sigma + \tau(y)) \cdot (\sigma + \tau(y))\,dy \tag{1.15}$$

where $L^2_\#(Y)^{N^2}$ is the space of periodic square integrable admissible stresses in Y.

Remark that all the above equivalent definitions of A^* are not simple algebraic formulae, but rather deliver the value of A^* at the price of a non-explicit computation of the solutions of the cell problems. However, in practice one is not always interested in the precise value of A^* but rather in lower or upper estimates of its value. In this respect, the above variational characterization of A^* is useful since it provides an upper bound by choosing a specific test function $w(y)$. The most simple choice is to take $w(y) = 0$, and it yields the so-called arithmetic mean upper bound

$$A^*\xi \cdot \xi \leq \left(\int_Y A(y)dy \right) \xi \cdot \xi. \tag{1.16}$$

Similarly, a lower bound on A^* can be derived from (1.15), by taking $\tau = 0$

$$A^{*-1}\sigma \cdot \sigma \leq \left(\int_Y A^{-1}(y)dy \right) \sigma \cdot \sigma.$$

This lower bound can also be obtained from (1.14) if the space of admissible fields in the minimization is enlarged. Indeed, remarking that the strain tensor $e(w)$ has zero-average over Y because of the periodicity of $w(y)$, this strain can be replaced by any zero-average symmetric matrix field

$$A^*\xi \cdot \xi \geq \min_{\substack{\zeta(y) \in L^2_\#(Y)^{N^2} \\ \int_Y \zeta(y)dy = 0}} \int_Y A(y)\left(\xi + \zeta(y)\right) \cdot \left(\xi + \zeta(y)\right) dy. \tag{1.17}$$

The minimum in the right hand side of (1.17) is easy to compute : the optimal $\zeta_\xi(y)$ satisfies the following Euler-Lagrange equation

$$A(y)\left(\xi + \zeta_\xi(y)\right) = C,$$

where C is a constant (a Lagrange multiplier for the constraint $\int_Y \zeta_\xi(y)dy = 0$. After some algebra, one can compute explicitly the optimal ζ_ξ as well as the minimal value which delivers the so-called harmonic mean lower bound

$$A^*\xi \cdot \xi \geq \left(\int_Y A^{-1}(y)dy \right)^{-1} \xi \cdot \xi. \tag{1.18}$$

The bounds (1.16) and (1.18) are sometimes called the Voigt and Reuss bounds [56], [67], or Paul bounds [54]. These estimates hold true in great generality (i.e. in a non-periodic setting too), but are usually not optimal and can be improved. Actually, improving the harmonic and arithmetic mean bounds is one of the main problem of homogenization theory applied to the modelling of composite materials. It turns out to have also many applications to optimal design problems.

Chapter 2

G- or H-convergence.

The first chapter was devoted to a brief presentation of homogenization in a periodic setting. This second chapter focus on the general setting of homogenization when no geometric assumptions are available (like periodicity, or ergodicity in a probabilistic framework) . It turns out that homogenization can be applied to any kind of disordered media, and is definitely not restricted to the periodic case (although the nice "explicit" formulae of the periodic setting for the homogenized Hooke's law have no analogue). We introduce the notion of G- or H-convergence which is due to Spagnolo [60], [61], and has been further generalized by Murat and Tartar [49], [50], [62] (see also the textbooks [52], [70]). It allows to consider any possible geometrical situation without any specific assumptions like periodicity or randomness. The G- or H-convergence turns out to be the adequate notion of convergence for effective properties that will be the key tool in the study of optimal shape design problems.

To conclude this introduction, let us mention that there is also a stochastic theory of homogenization (see [39], [20], [53]) and a variational theory of homogenization (the Γ-convergence of De Giorgi, [21], [22], see also the book [19]) that will not be described below.

2.1 Definition of G-, or H-convergence.

The G-convergence is a notion of convergence associated to sequences of symmetric operators (typically, these operators are applications giving the solution of a partial differential equation in terms of the right hand side). The G means Green since this type of convergence corresponds roughly to the convergence of the associated Green functions. The H-convergence is a generalization of the G-convergence to the case of non-symmetric operators (it provides also an easier mathematical framework, but we shall not dwell on that). The H stands for Homogenization since it is an important tool of that theory. Since the elasticity equations have symmetric coefficients, the underlying operators are symmetric too. Therefore in the sequel, we use only the notation G-convergence for simplicity.

The main result of the G-convergence is a compactness theorem in the homogenization theory which states that, for any bounded and uniformly coercive sequence of coefficients of a symmetric second order elliptic equation, there exist a subsequence and a *G-limit* (i.e. homogenized coefficients) such that, for any source term, the corresponding subsequence of solutions converges to the solution of the homogenized equation. In practical terms, it means that the mechanical properties of an heterogeneous medium (like its conductivity, or elastic moduli) can be well approximated by the properties of a homogeneous or homogenized medium if the size of the heterogeneities are small compared to the overall size of the medium.

The G-convergence can be seen as a mathematically rigorous version of the so-called *representative volume element* method for computing effective or averaged parameters of heterogeneous media.

We introduce the notion of G-convergence for the specific case of the elasticity system with a Dirichlet boundary condition, but all the results hold for a larger class of second order elliptic operators and boundary conditions. Let Ω be a bounded open set in $\mathbb{R}^N$, and let α, β be two positive constants such that $0 < \alpha \leq \beta$. We introduce the set $\mathcal{M}(\alpha, \beta, \Omega)$ of all possible symmetric fourth order tensors defined on Ω with uniform coercivity constant α and $L^\infty(\Omega)$-bound β. Furthermore, $A \in \mathcal{M}(\alpha, \beta, \Omega)$ satisfies the usual symmetries of a Hooke's law, $A_{ijkl} = A_{klij} = A_{jikl} = A_{ijlk}$ for $1 \leq i, j, k, l \leq N$. The coerciveness and boundedness of $A(x)$ is equivalent to

$$\alpha|\xi|^2 \leq \sum_{i,j,k,l=1}^{N} A_{ijkl}(x)\xi_{ij}\xi_{kl} \leq \beta|\xi|^2.$$

We consider a sequence $A_\epsilon(x)$ of Hooke's law in $\mathcal{M}(\alpha, \beta, \Omega)$, indexed by a sequence of positive numbers ϵ going to 0. Here, ϵ is not associated to any specific lengthscale or statistical property of the elastic medium. In other words, no special assumptions (like periodicity or stationarity) are placed on the sequence A_ϵ.

For a given force $f(x) \in L^2(\Omega)^N$, there exists a unique displacement u_ϵ, solution in the Sobolev space $H_0^1(\Omega)^N$ of the following elasticity equation

$$\begin{cases} -\text{div } (A_\epsilon(x)e(u_\epsilon)) = f(x) & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega, \end{cases} \tag{2.1}$$

where $e(u_\epsilon)$ is the deformation tensor $1/2(\nabla u_\epsilon + {}^t\nabla u_\epsilon)$. The G-convergence of the sequence A_ϵ is defined below as the convergence of the corresponding solutions u_ϵ.

Definition 2.1.1 *The sequence of tensors $A_\epsilon(x)$ is said to G-converge to a limit $A^*(x)$, as ϵ goes to 0, if, for any force $f \in L^2(\Omega)^N$ in (2.1), the sequence of solutions u_ϵ converges weakly in $H_0^1(\Omega)$ to a limit u which is the unique solution of the homogenized equation associated to A^*:*

$$\begin{cases} -\text{div }(A^*(x)e(u)) = f(x) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega. \end{cases} \tag{2.2}$$

Remark that, by definition, the homogenized tensor A^* is independent of the applied force f. We shall see that it is also independent of the boundary condition and of the domain.

This definition makes sense because of the compactness of the set $\mathcal{M}(\alpha, \beta, \Omega)$ with respect to the G-convergence, as stated in the following theorem.

Theorem 2.1.2 *For any sequence A_ϵ in $\mathcal{M}(\alpha, \beta, \Omega)$, there exist a subsequence (still denoted by ϵ) and a homogenized limit A^*, belonging to $\mathcal{M}(\alpha, \beta, \Omega)$, such that A_ϵ G-converges to A^*.*

The G-convergence of a general sequence A_ϵ is always stated *up to a subsequence* since A_ϵ can be the union of two sequences converging to two different limits. The G-convergence of A_ϵ is not equivalent to any other "classical" convergence. For example, if A_ϵ converges strongly in $L^\infty(\Omega)$ to a limit A (i.e. the convergence is pointwise), then its G-limit A^* coincides with A. But the converse is not true ! On the same token, the G-convergence has nothing to do with the usual weak convergence. Indeed, the G-limit A^* of a sequence A_ϵ is usually different of its weak-* $L^\infty(\Omega)$-limit. For example, a straightforward computation in one dimension ($N = 1$) shows that the G-limit of a sequence A_ϵ is given as the inverse of the weak-* $L^\infty(\Omega)$-limit of A_ϵ^{-1} (the so-called harmonic limit). However, this last result holds true only in 1-D, and no such explicit formula is available in higher dimensions.

The G-convergence enjoys a few useful properties as enumerated in the following proposition.

Proposition 2.1.3 *Properties of G-convergence.*

1. *If a sequence A_ϵ G-converges, its G-limit is unique.*

2. *Let A_ϵ and B_ϵ be two sequences which G-converge to A^* and B^* respectively. Let $\omega \subset \Omega$ be a subset strictly included in Ω such that $A_\epsilon = B_\epsilon$ in ω. Then $A^* = B^*$ in ω (this property is called the locality of G-convergence).*

3. *The G-limit of a sequence A_ϵ is independent of the source term f and of the boundary condition on $\partial\Omega$.*

4. *Let A_ϵ be a sequence which G-converges to A^*. Then, the associated density of energy $A_\epsilon e(u_\epsilon) \cdot e(u_\epsilon)$ also converges to the homogenized density of energy $A^* e(u) \cdot e(u)$ in the sense of distributions in Ω.*

5. *If a sequence A_ϵ G-converges to a limit A^*, then the sequence of stresses $A_\epsilon e(u_\epsilon)$ converges weakly in $L^2(\Omega)^{N^2}$ to the homogenized stress $A^* e(u)$.*

These properties of the G-convergence implies that the homogenized medium A^* approximates the heterogeneous medium A_ϵ in many different ways. First of all, by definition of G-convergence, the displacements and the deformation tensors are closed (this is the sense of the convergence of u_ϵ to u in the Sobolev space $H_0^1(\Omega)^N$). Then, by application of the above proposition, the stresses and the energy densities are also closed.

Remark also that, by locality of the G-convergence, the homogenized tensor is defined at each point of the domain Ω independently of what may happen in other regions of Ω.

Of course, a particular example of G-convergent sequences A_ϵ is given by periodic media of the type $A\left(\frac{x}{\epsilon}\right)$ as in the previous chapter.

2.2 The G-closure problem.

A crucial problem in the theory of G-convergence is the following. Assume that we constrain the sequence of Hooke's law $A_\epsilon(x)$ to take only two values A and B, corresponding to two given elastic materials, at each point $x \in \Omega$. Then, what is the possible set of G-limits $A^*(x)$ that can be attained by such sequences ? In other words, what kind of composite materials can be achieved by mixing A and B in any possible manner ? This problem is known as *the G-closure problem.* A variant of this problem is to fix the overall volume fraction of A and B in Ω to be θ and $1-\theta$, with $0 \leq \theta \leq 1$. This problem is called the G_θ-closure problem.

Surprisingly enough, these two questions have not yet been solved in the context of elasticity (even if A and B are assumed to be isotropic), although the answer is known in the context of conductivity (see [50], [64], [41]). However, there are a few useful results in this direction that indicates that there is no loss of generality in considering only periodic composite materials (i.e. homogenized tensors A^* obtained by periodic homogenization). The following result is attributed to Dal Maso and Kohn.

Theorem 2.2.1 *Let $A^*(x)$ be any homogenized Hooke's law (or composite material) obtained by mixing the two constituents A and B in proportions $\theta(x)$ and $(1-\theta(x))$ in a domain Ω (in other words $A^*(x)$ is any element of the so-called G-closure). Then, at each point $x \in \Omega$, the proportion $\theta(x)$ can take any value between 0 and 1, while $A^*(x)$ can take any value in the set $G_{\theta(x)}$, defined as the closure of the set of all periodic homogenized Hooke's law (i.e., obtained by homogenization of a periodic mixture of A and B in proportions $\theta(x)$ and $(1-\theta(x))$).*

This theorem states that any homogenized material A^* (obtained with any possible mixing procedure) can locally be attained by a periodic mixture in the same proportions. This feature is, of course, not so surprising, since we already claimed that the G-convergence is local.

Although we do not have an explicit characterization of the set G_θ for $0 \leq \theta \leq 1$, we know part of the boundary of this set. In other words we know some "optimal composites" which live on ∂G_θ and are therefore extremal. For example, if A^* is isotropic, the celebrated Hashin-Shtrikman bounds hold for its bulk and shear moduli [33]. These bounds are known to be attained by optimal composites which are sequential laminates (see [25] and chapter 4 for details).

We conclude this chapter by referring to the classical book [17] for more informations on the theory of composite materials.

Chapter 3

H-measures.

The notion of H-measure has been introduced by Gerard [27] and Tartar [65]. It is a default measure which quantifies, in the phase space, the lack of compactness of weakly converging sequences in $L^2(\Omega)$. In other words, it indicates where in the physical space, and at which frequency in the Fourier space, are the obstructions to strong convergence. As recognized by Tartar [65], this abstract tool has many important applications in the mathematical theory of composite materials. We therefore give a brief survey on this notion of H-measure.

3.1 General definition.

Let u_ϵ be a sequence of functions defined in $\mathbb{R}^N$ with values in $\mathbb{R}^p$. The components of the vector-valued function u_ϵ are denoted by $(u_\epsilon^i)_{1\leq i\leq p}$. We assume that u_ϵ converges weakly to 0 in $L^2(\mathbb{R}^N)^p$.

Theorem 3.1.1 *There exist a subsequence (still denoted by ϵ) and a family of complex-valued Radon measures $(\mu_{ij})_{1\leq i,j\leq p}$ on $\mathbb{R}^N\times S_{N-1}$ such that, for every functions $\phi_1(x)$, $\phi_2(x)$ in $C_0(\mathbb{R}^N)$, and $\psi(\xi)$ in $C(S_{N-1})$, it satisfies*

$$\int_{\mathbb{R}^N}\int_{S_{N-1}} \phi_1(x)\overline{\phi}_2(x)\psi\left(\frac{\xi}{|\xi|}\right)\mu_{ij}(dx,d\xi) = \lim_{\epsilon\to 0}\int_{\mathbb{R}^N} \mathcal{F}\left(\phi_1 u_\epsilon^i\right)(\xi)\overline{\mathcal{F}\left(\phi_2 u_\epsilon^j\right)}(\xi)\psi\left(\frac{\xi}{|\xi|}\right)d\xi\,.$$

The matrix of measures $\mu=(\mu_{ij})_{1\leq i,j\leq p}$ is called the H-measure of the subsequence u_ϵ. It is a hermitian and non-negative matrix.

Let us explain the notations of Theorem 3.1.1 : S_{N-1} is the unit sphere in $\mathbb{R}^N$, $C(S_{N-1})$ is the space of continuous functions on S_{N-1}, $C_0(\mathbb{R}^N)$ that of continuous functions decreasing to 0 at infinity in $\mathbb{R}^N$, and $\overline{z}$ denotes the complex conjugate of the complex number z. Finally, $\mathcal{F}$ is the Fourier transform operator defined in $L^2(\mathbb{R}^N)$ by

$$(\mathcal{F}\phi)(\xi) = \int_{\mathbb{R}^N} \phi(x) e^{-2i\pi(x\cdot\xi)} dx.$$

In Theorem 3.1.1, the role of the test functions ϕ_1 and ϕ_2 is to localize in space, while that of ψ is to localize in the directions of oscillations.

Remark 3.1.2 *Theorem 3.1.1 furnishes a representation formula for the limit of quadratic objects of the sequence u_ϵ. When we take $\psi \equiv 1$, we recover the usual default measure in the physical space, i.e. $\int_{S_{N-1}} \mu_{ij}(\cdot, d\xi)$ is just the limit measure of the bounded sequence $u_\epsilon^i \overline{u}_\epsilon^j$ in $L^1(\mathbb{R}^N)$. Therefore, the H-measure gives a more precise representation of the compactness default, taking into account oscillation directions.*

The main property of the H-measure μ (apart from being a hermitian non-negative matrix) is its localization principle which is a generalization of the compensated compactness theory of Murat and Tartar [48], [63]. We shall not use it in the sequel, but for the sake of completeness we recall it below.

Theorem 3.1.3 *Let u_ϵ be a sequence which converges weakly to 0 in $L^2(\mathbb{R}^N)^p$ and defines a H-measure μ. If u_ϵ is such that*

$$\sum_{j=1}^{p} \sum_{k=1}^{N} \frac{\partial}{\partial x_k} \left(A_{jk}(x) u_\epsilon^j \right) \to 0 \quad \textit{in } H^{-1}_{loc}(\Omega) \textit{ strongly}$$

where the coefficients A_{jk} are continuous in the open set Ω of $\mathbb{R}^N$, then the H-measure satisfies

$$\sum_{j=1}^{p} \sum_{k=1}^{N} A_{jk}(x) \xi_k \mu_{jm} = 0 \textit{ in } \Omega \textit{ for every } m.$$

The most simple example of a weakly converging sequence is a periodically oscillating sequence as in the first chapter. More precisely, we assume that

$$u_\epsilon(x) = u\left(x, \frac{x}{\epsilon}\right),$$

with $u(x,y)$ a function defined on $\mathbb{R}^N \times Y$ which is Y-periodic in the last variable y and satisfies $\int_Y u(x,y)dy = 0$. For simplicity, we assume that $u(x,y)$ is continuous in x with values in $L^\infty(Y)$. The H-measure of such a sequence can be computed explicitly.

Lemma 3.1.4 *Writing $u(x,y)$ as a Fourier series in y, i.e.*

$$u^i(x,y) = \sum_{m\in\mathbb{Z}^N} u^i_m(x) e^{2i\pi m\cdot y}, \tag{3.1}$$

the H-measure of the entire sequence $u_\epsilon(x)$ is

$$\mu_{ij} = \sum_{m\in\mathbb{Z}^N,\ m\neq 0} u^i_m(x)\overline{u}^j_m(x)\delta_{m/|m|}(\xi),$$

where $\delta_{m/|m|}$ is the Dirac mass at $\frac{m}{|m|}$.

Remark that in (3.1) the coefficient $u^i_0(x)$ is necessarily 0 since u_ϵ must converges weakly to 0.

3.2 Periodic case.

In view of Lemma 3.1.4, we can simplify the definition of the H-measure of a periodically oscillating function $u_\epsilon(x) = u(x/\epsilon)$ with $u \in L^2_\#(Y)^p$. We shall no more assume that $u(y)$ has zero average in Y, since we can always subtract its average and apply the previous Lemma 3.1.4. Since we are only interested in real-valued functions, we shall also consider only the real part of the H-measure. After all these minor modifications, by a convenient abuse of language, we shall still talk about the H-measure of $u(y)$ and drop its dependence with respect to x.

Definition 3.2.1 *Let $u(y)$ be a function in $L^2_\#(Y)^p$. Its H-measure μ is the matrix-valued measure defined on S_{N-1} by*

$$\mu_{ij} = \mathcal{R}\rceil \sum_{m\in\mathbb{Z}^N,\ m\neq 0} u^i_m\overline{u}^j_m\delta_{m/|m|}(\xi),$$

where $\mathcal{R}\rceil$ is the real part of a complex number and u^i_m are the Fourier coefficients of the i-th component of $u(y)$, i.e.

$$u^i(y) = \sum_{m\in\mathbb{Z}^N} u^i_m e^{2i\pi m\cdot y}.$$

It is a real symmetric non-negative measure since, for any vector $\lambda \in \mathbb{R}^p$, it satisfies

$$\sum_{i,j=1}^{p} \mu_{ij}\lambda_i\overline{\lambda}_j = \sum_{m\in\mathbb{Z}^N,\ m\neq 0} |u_m\cdot\lambda|^2\,\delta_{m/|m|}(\xi).$$

Remark 3.2.2 *Since we assume that the function $u(y)$ is real-valued, it is easily seen that $\mu_{ij}(-e) = \mu_{ij}(e)$, i.e. the H-measure μ is even on S_{N-1}.*

A special case of particular interest for the sequel is obtained when $u(y)$ is a vector of characteristic functions $(\chi^i(y))_{1\leq i\leq p}$ that satisfy

$$\begin{array}{l} \chi^i(y) = 0 \text{ or } 1, \\ \sum_{i=1}^p \chi^i(y) = 1, \\ \chi^i(y)\chi^j(y) = 0 \text{ for } i \neq j. \end{array} \tag{3.2}$$

In such a case the H-measure satisfies special properties which are restrictions on its possible range.

Lemma 3.2.3 *Let μ be the H-measure of the family of characteristic functions $(\chi^i(y))_{1\leq i\leq p}$ satisfying (3.2). Then, μ is such that*

$$\begin{array}{l} \sum_{i=1}^p \mu_{ij} = 0 \textit{ for } 1 \leq j \leq p, \\ \int_{S_{N-1}} \mu_{ij}(de) = -\theta^i\theta^j \textit{ for } i \neq j, \\ \int_{S_{N-1}} \mu_{ii}(de) = \theta^i(1-\theta^i), \end{array} \tag{3.3}$$

where $\theta^i = \int_Y \chi^i(y)dy$ (we have $\sum_{i=1}^p \theta^i = 1$).

The conditions (3.3) are necessary conditions for a real symmetric non-negative even measure μ to be the H-measure of a family of characteristic functions. However, it is believed that there exist further restrictions on such H-measures, at least when $p > 2$. In the case $p = 2$, Lemma 3.2.3 implies that the knowledge of the two by two matrix μ reduces to that of one of its components, say μ_{11} since $\mu_{12} = \mu_{21} = -\mu_{22} = -\mu_{11}$. It turns out that for a single characteristic function, the set of all possible H-measures is known (see [36], [65]).

Lemma 3.2.4 *Let μ be the H-measure of a single characteristic function $\chi(y)$, i.e. taking only the values 0 or 1, such that $\theta = \int_Y \chi(y)dy$. By varying χ, the set of all such H-measures μ is precisely the set of all probability measures $\mathcal{P}(S_{N-1})$ multiplied by the weighting factor $\theta(1-\theta)$.*

Remark 3.2.5 *In the sequel, we denote by $\mathcal{P}(S_{N-1})$ the space of all probability measures on the unit sphere S_{N-1}. Recall that a probability measure ν is a non-negative measure with unit mass, i.e.*

$$\nu(e) \geq 0 \quad \forall e \in S_{N-1}, \quad \textit{and} \int_{S_{N-1}} d\nu(e) = 1. \tag{3.4}$$

Since the set of all H-measures of family of characteristic functions is unknown, we need one way of building explicitly such H-measures. This is the goal of the following "mixing rule" for H-measures which may be found in [36], [65].

Lemma 3.2.6 *Let $(\chi_1^i(y))_{1\leq i\leq p}$ and $(\chi_2^i(y))_{1\leq i\leq p}$ be two families of characteristic functions with volume fractions $(\theta_1^i)_{1\leq i\leq p}$, $(\theta_2^i)_{1\leq i\leq p}$, and H-measures $(\mu_{ij}^1)_{1\leq i,j\leq p}$, $(\mu_{ij}^2)_{1\leq i,j\leq p}$. Let $\psi(y)$ be another characteristic function with average ρ and H-measure ν. By mixing these two families according to the partition ψ on separated scales, we obtain a new family of characteristic functions, namely*

$$\chi_\epsilon^i(y) = \psi(y)\chi_1^i\left(\frac{y}{\epsilon}\right) + (1-\psi(y))\chi_2^i\left(\frac{y}{\epsilon}\right).$$

As the scale ϵ goes to 0, the volume fractions of this new family are

$$\theta^i = \rho\theta_1^i + (1-\rho)\theta_2^i \text{ for } 1\leq i\leq p$$

and its H-measure is

$$\mu_{ij} = \rho\mu_{ij}^1 + (1-\rho)\mu_{ij}^2 + (\theta_1^i - \theta_2^i)(\theta_1^j - \theta_2^j)\nu.$$

The notion of H-measure for a family of characteristic functions is very useful in several fields of material sciences including optimal design (see e.g. [3]), small contrast composite materials (see below in chapter 4 or e.g. [5]), coherent phase transitions (see chapter 5).

Chapter 4

Composite materials.

This chapter is devoted to a brief introduction to the theory of composite materials in the context of homogenization. For more details, the reader is referred to [17], [33] for a mechanical point of view, and to [25], [35], [45] for a mathematical point of view.

We begin by introducing a particular family of composite materials, known as finite-rank sequential laminates, that constitute a class of optimal composites having effective properties explicitly given by an algebraic formula. Then, we recall the well-known Hashin-Shtrikman variational principle that permits to obtain bounds on the elastic energy of a composite material. It turns out that such bounds are also optimal, i.e. thery are realizable, or attained, by finite-rank sequential laminates.

Throughout this chapter, we consider elastic composite materials obtained by mixing two isotropic phases. Their Hooke's law A and B are defined by

$$\begin{aligned} A &= 2\mu_A I_4 + \left(\kappa_A - \frac{2\mu_A}{N}\right) I_2 \otimes I_2, \\ B &= 2\mu_B I_4 + \left(\kappa_B - \frac{2\mu_B}{N}\right) I_2 \otimes I_2, \end{aligned} \tag{4.1}$$

where μ_A, μ_B are the shear moduli and κ_A, κ_B are the bulk moduli. The two phases are assumed to be well-ordered, i.e.

$$0 < \mu_A \leq \mu_B, \quad 0 < \kappa_A \leq \kappa_B. \tag{4.2}$$

It is convenient to introduce a Lamé coefficient, proportional to the Poisson's ratio, defined by

$$\lambda_A = \kappa_A - \frac{2\mu_A}{N}, \quad \lambda_B = \kappa_B - \frac{2\mu_B}{N}. \tag{4.3}$$

4.1 Lamination formula.

As already said, the G_θ-closure is unknown, but its subset of so-called "finite rank sequential laminates" is both, easy to compute, and rich enough for many applications. There exists a nice explicit formula for sequential laminates which is due to Francfort and Murat [25] (inspired by some earlier work of Tartar [64]). This formula is purely algebraic, which is in sharp contrast with the periodic formula for which a p.d.e. has to be solved in the unit cell.

It starts with an explicit computation of the homogenized Hooke's law of a special periodic composite obtained by a single lamination of A and B. Recall from the first chapter that A^* is given by

$$A^*\xi\cdot\xi = \min_{w\in H^1_\#(Y)^N}\int_Y A(y)\,(\xi+e(w))\cdot(\xi+e(w))\,dy. \qquad (4.4)$$

where $A(y)=\chi(y)A+(1-\chi(y))B$, and $\chi(y)$ is the characteristic function of phase A. In the case where $\chi(y)$ corresponds to a layer of A and B, the computation of (4.4) amounts to a simple algebraic calculation since the deformation and stress tensors turn out to be constant in each phase. The result is (see Theorem 4.1 in [25] for details, or [35], [45])

Lemma 4.1.1 *Let A^* be a single lamination of material A and B, in proportion θ and $(1-\theta)$ respectively, in the unit direction e. Then*

$$(1-\theta)\,(A^*-A)^{-1} \;=\; (B-A)^{-1}+\theta f_A(e), \qquad (4.5)$$

where $f_A(e)$ is a positive non-definite fourth-order tensor defined, ξ being a symmetric matrix, by

$$f_A(e)\xi = \frac{1}{\mu_A}\left(\xi e\odot e-(\xi e\cdot e)e\otimes e\right)+\frac{1}{2\mu_A+\lambda_A}(\xi e\cdot e)e\otimes e. \qquad (4.6)$$

or, equivalently, by the quadratic form

$$f_A(e)\xi\cdot\xi = \frac{1}{\mu_A}\left(|\xi e|^2-(\xi e\cdot e)^2\right)+\frac{1}{2\mu_A+\lambda_A}(\xi e\cdot e)^2. \qquad (4.7)$$

Formula (4.5) is written in a strange manner (why not a formula giving directly A^* ?), but it allows to reiterate the lamination process.

The composite A^* is said to be a single lamination in the direction e of the two phases A and B in proportions θ and $(1-\theta)$. By varying the proportion θ and the direction e, we obtain a whole family of composite materials. But this family can still be enlarged by laminating again these simple laminates. Repeating this lamination process in any directions and any proportions yields a subset L_θ of G_θ, made of these laminated materials.

Definition 4.1.2 *The subset $L_\theta \subset G_\theta$ of all laminated materials obtained from the phases A and B in proportions θ and $1-\theta$ is the smallest subset of G_θ which contains all simple laminates, as defined by (4.5), and is stable under lamination.*

A smaller subset of L_θ can be defined by considering only the so-called sequential laminates. Such laminates are obtained by an iterative process where, at each stage, the previous laminate is laminated again with a single pure phase (always the same one). This allows to derive an explicit formula for such homogenized Hooke's law A^* by using the special form of (4.5). A sequential laminate is characterized by a collection of unit vectors $(e_i)_{1\le i\le p}$ and by proportions $(\theta_i)_{1\le i\le p}$ in $[0,1]$. At the first stage, a simple laminate A_1^* is obtained by laminating A and B in proportions θ_1, $1-\theta_1$ and in the direction e_1. This simple laminate A_1^* can again be laminated with phase B, in direction e_2 and in proportions $(1-\theta_2)$, θ_2 respectively, to obtain a new laminate denoted by A_2^*. By induction, we obtain A_p^* by lamination of B and A_{p-1}^*, in direction e_p and in proportions θ_p, $(1-\theta_p)$ respectively. By application of formula (4.5), the homogenized tensor A_p^* is defined by

$$(1-\theta_p)\left(A_p^* - A\right)^{-1} = \left(A_{p-1}^* - A\right)^{-1} + \theta_p f_A(e_p).$$

By iterating this formula, the term $(A_{p-1}^* - A)^{-1}$ can be replaced by a similar expression involving $(A_{p-2}^* - A)^{-1}$, and so on up to $(A_0^* - A)^{-1}$ with $A_0^* \equiv B$. This yields a formula of the same type than (4.5)

$$\left(\prod_{i=1}^{p}(1-\theta_i)\right)\left(A_p^* - A\right)^{-1} = (B-A)^{-1} + \sum_{i=1}^{p}\left(\theta_i \prod_{j=1}^{i-1}(1-\theta_j)\right) f_A(e_i). \tag{4.8}$$

Remark that we always laminate an intermediate laminate with the same phase A. In other words, phase B is coated by several layers of A. One can say that A plays the role of a matrix phase and B that of a core phase. Globally, A_p^* can be seen as a mixture of A and B in different layers having a large separation of scales.

Definition 4.1.3 *The composite material A_p^*, defined by formula (4.8), is called a rank-p sequential laminate with matrix phase A and core phase B. It is characterized by the lamination directions $(e_i)_{1\le i\le p}$ and the proportions $(\theta_i)_{1\le i\le p}$ at each stage of the process.*

In Definition 4.1.3 the word "sequential" means that this type of laminates is iteratively constructed by successive laminations always with the same pure phase. In formula (4.8) the overall volume fraction of phase A is

$$\theta = 1 - \prod_{i=1}^{p}(1-\theta_i).$$

If this overall volume fraction θ is fixed, by varying the proportions $(\theta_i)_{1\le i\le p}$ we obtain a parametrized family of rank-p sequential laminates.

Lemma 4.1.4 *Let $(e_i)_{1\le i\le p}$ be a collection of unit vectors. Let θ be a volume fraction in $[0,1]$. For any collection of non-negative real numbers $(m_i)_{1\le i\le p}$ satisfying*

$$\sum_{i=1}^{p} m_i = 1 \text{ and } m_i \ge 0,\ 1\le i\le p,$$

there exists a rank-p sequential laminate A_p^*, with matrix A and core B, in proportions θ and $(1-\theta)$ respectively, with lamination directions $(e_i)_{1\le i\le p}$ such that

$$(1-\theta)\left(A_p^* - A\right)^{-1} = (B-A)^{-1} + \theta\sum_{i=1}^{p} m_i f_A(e_i), \tag{4.9}$$

where $f_A(e_i)$ is given by (4.7). The numbers $(m_i)_{1\le i\le p}$ are called the lamination parameters.

By interchanging the roles of A and B, a symmetric result is obtained. There exists another homogenized Hooke's law B_p^*, a rank-p sequential laminate with core A and matrix B in proportions θ and $(1-\theta)$, defined by

$$\theta\left(B_p^* - B\right)^{-1} = (A-B)^{-1} + (1-\theta)\sum_{i=1}^{p} m_i f_B(e_i), \tag{4.10}$$

where $f_B(e_i)$ is given by (4.7) with B replacing A.

Remark 4.1.5 *In the elasticity setting, laminated composites have been known for a long time (see e.g. [28], [29], [45]), but the class of sequential laminates with their explicit formula (as delivered by Lemmae 4.1.4) has been introduced by Francfort and Murat [25] following the lead of Tartar [64].*

There is another way of writing the above lamination formulae which uses the inverse tensors A^{-1} and B^{-1} (the so-called compliance tensors) instead of A and B. Formulae (4.9) and (4.10) are convenient when working with strain tensors, while the new formulae below are of interest when using stress tensors. The Hooke's law A^* defined by (4.5) as a single lamination of material A and B, in proportion θ and $(1-\theta)$ respectively, in the direction of the unit vector e, is equivalently defined by

$$(1-\theta)\left(A^{*-1}-A^{-1}\right)^{-1}=\left(B^{-1}-A^{-1}\right)^{-1}+\theta f_A^c(e) \tag{4.11}$$

where $f_A^c(e)$ is a symmetric positive non-definite fourth-order tensor defined, for any symmetric matrix ξ, by the quadratic form

$$f_A^c(e)\xi\cdot\xi = A\xi\cdot\xi-\frac{1}{\mu_A}|A\xi e|^2+\frac{\mu_A+\lambda_A}{\mu_A(2\mu_A+\lambda_A)}((A\xi)e\cdot e)^2. \tag{4.12}$$

Since (4.11) is equivalent to (4.5), we deduce that formula (4.9), defining the rank-p sequential laminate A_p^*, is equivalent to

$$(1-\theta)\left(A_p^{*-1}-A^{-1}\right)^{-1}=\left(B^{-1}-A^{-1}\right)^{-1}+\theta\sum_{i=1}^{p}m_i f_A^c(e_i). \tag{4.13}$$

By interchanging the roles of A and B, formula (4.10), defining the rank-p sequential laminate B_p^*, is equivalent to

$$\theta\left(B_p^{*-1}-B^{-1}\right)^{-1} = \left(A^{-1}-B^{-1}\right)^{-1}+(1-\theta)\sum_{i=1}^{p}m_i f_B^c(e_i), \tag{4.14}$$

where $f_B^c(e_i)$ is given by (4.12) with B replacing A.

Definition 4.1.6 *We denote by L_θ^- the set of all sequential laminates A_p^*, with matrix A and core B, in proportions θ and $(1-\theta)$ respectively, defined by formula (4.9) (or equivalently (4.13)), obtained by varying the number p of laminations and the laminations directions $(e_i)_{1\le i\le p}$, as well as the lamination parameters $(m_i)_{1\le i\le p}$.*
We denote by L_θ^+ the set of all sequential laminates B_p^*, with core A and matrix B, in proportions θ and $(1-\theta)$ respectively, defined by formula (4.10) (or equivalently (4.14)), obtained by varying the number p of laminations and the laminations directions $(e_i)_{1\le i\le p}$, as well as the lamination parameters $(m_i)_{1\le i\le p}$.

It is interesting for the sequel to know these sets $L_\theta^\pm$. This is the purpose of the next result which is due to Avellaneda [10].

Lemma 4.1.7 *The set L^-_θ is the bounded closed subset of all symmetric fourth-order tensors $A^* \in \mathcal{M}^4_N$ such that there exists a probability measure ν on the unit sphere S_{N-1} satisfying*

$$(1-\theta)\left(A^*-A\right)^{-1} \ = \ (B-A)^{-1} + \theta \int_{S_{N-1}} f_A(e) d\nu(e), \qquad (4.15)$$

where $f_A(e)$ is given by (4.7). Furthermore, any tensor A^* in L^-_θ is the Hooke's law of a finite rank sequential laminate defined by (4.9) with rank $p \leq (N+3)(N+2)(N+1)N/24$.

Similarly, L^+_θ is the bounded closed subset of all symmetric fourth-order tensors $B^* \in \mathcal{M}^4_N$ such that there exists a probability measure ν on the unit sphere S_{N-1} satisfying

$$\theta\left(B^*-B\right)^{-1} \ = \ (A-B)^{-1} + (1-\theta) \int_{S_{N-1}} f_B(e) d\nu(e), \qquad (4.16)$$

where $f_B(e)$ is given by (4.7) with B replacing A. Furthermore, any tensor B^* in L^+_θ is the Hooke's law of a finite rank sequential laminate defined by (4.10) with rank $p \leq (N+3)(N+2)(N+1)N/24$.

Remark 4.1.8 *The space $\mathcal{P}(S_{N-1})$ of all probability measures on the unit sphere S_{N-1} has been defined in Remark 3.2.5. Remark that, up to a multiplicative factor $\theta(1-\theta)$, the measure ν in the formulae of Lemma 4.1.7 is just the H-measure of the characteristic function of one phase of the sequential laminate A^*.*

Proof. Clearly, any sequential laminate A^*_p, defined by (4.9), satisfies (4.15) with a discrete probability measure ν, namely

$$\nu(e) = \sum_{i=1}^{p} m_i \delta(e - e_i),$$

where δ is the Dirac mass at the origin. Conversely, let us show that any tensor A^* defined by (4.15), with a probability measure ν, is indeed a finite rank sequential laminate. Remark that $f_A(e)$ is a homogeneous polynomial of degree four on the unit sphere. Therefore, there exists a linear map L_A, acting in the space $\mathcal{M}^4_N$, such that

$$\int_{S_{N-1}} f_A(e) d\nu(e) = L_A\left(\int_{S_{N-1}} e \otimes e \otimes e \otimes e \, d\nu(e)\right). \qquad (4.17)$$

When ν runs into $\mathcal{P}(S_{N-1})$, the fourth order tensor $\int_{S_{N-1}} e\otimes e\otimes e\otimes e\, d\nu(e)$ describes a convex subset of the set of fully symmetric fourth order tensor A satisfying

$$A_{ijkl} = A_{kjil} = A_{klij} = A_{jikl},$$

with unit trace $\sum_{i,j=1}^{N} A_{ijij} = 1$, having dimension $n = (N+3)(N+2)(N+1)N/24 - 1$. By Lemma 4.1.9 below, the extremal points of this subset are precisely of the type $e \otimes e \otimes e \otimes e$. Thus, applying Caratheodory's theorem which states that any point of a convex set in a space of finite dimension n can be represented as a convex combination of at most $n+1$ extremal points of this convex set, we can replace any probability measure ν by a discrete one in (4.15). Consequently, A^* is the effective tensor of a rank-$(n+1)$ sequential laminate defined by (4.9). This yields the desired characterization of L_θ^-. A symmetric argument works for L_θ^+. Furthermore, since the set $\mathcal{P}(S_{N-1})$ is sequentially compact for the vague convergence of measures, it implies that L_θ^- and L_θ^+ are closed in $\mathcal{M}_N^4$. $\square$

Lemma 4.1.9 *Let $\mathcal{C}$ denote the convex hull, in the space of fourth order tensors $\mathcal{M}_N^4$, of $e \otimes e \otimes e \otimes e$ when e runs into S_{N-1}. The extremal points of $\mathcal{C}$ are exactly the points $e \otimes e \otimes e \otimes e$.*

Proof. This convex hull $\mathcal{C}$ is defined by

$$\mathcal{C} = \left\{ \int_{S_{N-1}} e \otimes e \otimes e \otimes e \, d\nu(e) \in \mathbb{R}^{N^2} \text{ with } \nu \in \mathcal{P}(S_{N-1}) \right\},$$

wher $\mathcal{P}(S_{N-1})$ is the space of all probability measures defined in Remark 3.2.5. Let us prove that the extremal points of $\mathcal{C}$ correspond to a measure ν being a Dirac mass, i.e. are exactly of the type $e \otimes e \otimes e \otimes e$. Let M be such an extremal point defined by

$$M = \int_{S_{N-1}} e \otimes e \otimes e \otimes e \, d\nu(e).$$

Recall that an extremal point is such that it can not be decomposed as a convex combination of two other points in the same convex set. If we can prove that, for any linear form L, the function $e \to L(e \otimes e \otimes e \otimes e)$ is constant on the support of the measure ν, then one can replace ν by a Dirac mass supported at any e in the support of ν without changing the value of the matrix M, which proves that $M = e \otimes e \otimes e \otimes e$ as desired.

Let L be a linear form on the spce of fourth-order tensors. We assume that $L(e \otimes e \otimes e \otimes e)$ is not constant on the support of ν. Upon defining the essential minimum L^- and maximum L^+ of $L(e \otimes e \otimes e \otimes e)$ by

$$L^- = \sup \left\{ \alpha \in \mathbb{R} \mid \nu\{e \in S_{N-1} \mid L(e \otimes e \otimes e \otimes e) \leq \alpha\} = 0 \right\},$$

and

$$L^+ = \inf \{\beta \in \mathbb{R} \mid \nu\{e \in S_{N-1} \mid L(e \otimes e \otimes e \otimes e) \geq \beta\} = 0\},$$

our assumption implies $L^- < L^+$. Therefore, there exists L^0 such that $L^- < L^0 < L^+$. Introducing

$$S^- = \{e \in S_{N-1} | L(e \otimes e \otimes e \otimes e) \leq L^0\}$$

and

$$S^+ = \{e \in S_{N-1} | L(e \otimes e \otimes e \otimes e) > L^0\},$$

by construction we have $\theta^- = \nu(S^-) > 0$ and $\theta^+ = \nu(S^+) > 0$ with $\theta^- + \theta^+ = 1$. The measure ν can be decomposed as a convex combination of probability measures

$$\nu = \theta^+ \frac{\nu_{|S^+}}{\theta^+} + \theta^- \frac{\nu_{|S^-}}{\theta^-},$$

where $\nu_{|S^\pm}$ is the restriction to $S^\pm$ of ν. Similarly, the tensor M can be decomposed as a convex combination of two points in $\mathcal{C}$

$$M = \theta^+ M^+ + \theta^- M^-,$$

with

$$M^\pm = \int_{S_{N-1}} e \otimes e \otimes e \otimes e \frac{d\nu_{|S^\pm}}{\theta^\pm},$$

which contradicts the extremal character of M. Thus, for any linear form, $L(e \otimes e \otimes e \otimes e)$ is constant on the support of ν, which can therefore be replaced by a Dirac mass. This proves that the extremal points of $\mathcal{C}$ are of the type $e \otimes e \otimes e \otimes e$. □

Lemma 4.1.7 gives a convenient parametrization of the sets of sequential laminates $L_\theta^\pm$ in terms of probability or H-measures. Nevertheless, it leaves open two important questions. First, is there a simple algebraic characterization of $L_\theta^\pm$? Second, what is the minimal number of laminations necessary to attain any tensor in these sets $L_\theta^\pm$? By a matter of theory, we know from Lemma 4.1.7 that any tensor in $L_\theta^\pm$ corresponds to a rank-p sequential laminate with $p \leq (N+3)(N+2)(N+1)N/24$. However, this number is not optimal and is rather a crude upper bound (it gives $p = 5$ in 2-D and $p = 15$ in 3-D). These questions have been addressed in [11] for the two-dimensional case, $N = 2$, and in [26] for the three-dimensional case, $N = 3$. Their results are summarized in the following

Lemma 4.1.10 *Any tensor in $L^{\pm}_{\theta}$ corresponds to a rank-p sequential laminate with $p=3$ if $N=2$ and $p=6$ if $N=3$. Furthermore, if $N=2$ or 3, any tensor A^* in L^{-}_{θ} is characterized by*

$$(1-\theta)\left(A^*-A\right)^{-1} \;=\; (B-A)^{-1}+\theta L_A(M), \tag{4.18}$$

with L_A a linear map on the space of fourth-order tensors defined by

$$\begin{aligned} L_A(M)_{ijkl} \;&= \left(\frac{1}{2\mu_A+\lambda_A}-\frac{1}{\mu_A}\right) M_{ijkl} \\ &+\frac{1}{4\mu_A}\sum_{m=1}^{N}\left(M_{imml}\delta_{jk}+M_{imkm}\delta_{jl}+M_{mjml}\delta_{ik}+M_{mjkm}\delta_{il}\right), \end{aligned} \tag{4.19}$$

where M is any fourth order tensor, being fully symmetric, i.e.

$$M_{ijkl}=M_{kjil}=M_{klij}=M_{jikl}, \tag{4.20}$$

with unit trace

$$\sum_{i,j=1}^{N} M_{ijij}=1, \tag{4.21}$$

which is positive in the sense of quadratic forms, i.e. for any symmetric matrix ξ

$$\sum_{i,j,k,l=1}^{N} M_{ijkl}\xi_{ij}\xi_{kl}\geq 0. \tag{4.22}$$

A symmetric result holds for L^{+}_{θ}.

4.2 Hashin-Shtrikman variational principle.

This section is devoted to the Hashin-Shtrikman variational principle which allows to derive optimal bounds on the effective or homogenized energy of a composite material. Denoting by A^* the homogenized Hooke's law and by ξ a symmetric matrix in $\mathbb{R}^{N^2}$, the homogenized elastic energy evaluated at the strain tensor ξ is the quantity $A^*\xi\cdot\xi$. The method, introduced by Hashin and Shtrikman in [33], has been further developed by many individuals, e.g., [7], [10], [32], [37], [46], [47], [68], [69].

Of course, any homogenized Hooke's law $A^*\in G_\theta$ satisfies the trivial harmonic and arithmetic mean bounds, i.e.,

$$\left(\theta A^{-1}+(1-\theta)B^{-1}\right)^{-1} \;\leq\; A^* \;\leq\; \left(\theta A+(1-\theta)B\right).$$

For certain choices of the strain ξ there are composites A^* such that their effective energy $A^*\xi\cdot\xi$ saturates either one of these upper and lower bounds. But there are also other choices of ξ for which none of these bounds is attained by a composite $A^* \in G_\theta$. In this sense, the harmonic and arithmetic mean bounds are not optimal. As was shown by Avellaneda [10], the Hashin-Shtrikman variational principle allows to improve considerably the harmonic and arithmetic mean bounds by bounding any homogenized Hooke's law between two effective tensors of sequential laminates.

Theorem 4.2.1 *Let A^* be any effective Hooke's law in G_θ. There exist two sequential laminates $A^+ \in L_\theta^+$ (i.e. with core A and matrix B) and $A^- \in L_\theta^-$ (i.e. with matrix A and core B), such that*

$$A^- \leq A^* \leq A^+,$$

in the sense of quadratic forms (of course, the sequential laminates A^+, A^- vary with A^*).

Remark 4.2.2 *As a byproduct of Theorem 4.2.1, we shall prove that, even if A^* does not share the same H-measure than $A^\pm$, the fourth-order moments of their H-measures are the same.*

Proof of Theorem 4.2.1. The proof relies on the Hashin-Shtrikman variational principle. Since G_θ is the closure of the set of periodic composites, and since the sets $L_\theta^\pm$ are closed (cf. Lemma 4.1.7), we may restrict ourselves to a periodic composite A^*. Such an effective tensor A^* is defined through a characteristic function $\chi(y)$ in the unit cell Y, which satisfies $\int_Y \chi(y)dy = \theta$. By periodic homogenization, A^* is given by the formula

$$A^*\xi\cdot\xi = \min_{\phi\in H^1_\#(Y)^N} \int_Y (\chi A + (1-\chi)B)\,(\xi + e(\phi))\cdot(\xi+e(\phi))dy, \quad (4.23)$$

where ξ is any symmetric matrix in $\mathbb{R}^{N^2}$. We first establish a lower bound to this effective energy (4.23). By adding and subtracting a reference energy $A(\xi + e(\phi))\cdot(\xi + e(\phi))$, we obtain

$$A^*\xi\cdot\xi = \min_{\phi\in H^1_\#(Y)^N} \left[\int_Y (1-\chi)(B-A)(\xi+e(\phi))\cdot(\xi+e(\phi))dy \right.$$
$$\left. + \int_Y A(\xi+e(\phi))\cdot(\xi+e(\phi))dy\right]. \quad (4.24)$$

Using the positivity of $B - A$ and convex duality, the first integral in the right hand side of (4.24) is rewritten

$$\sup_{\eta(y)\in L^2_\#(Y;\mathbf{R}^{N^2})} \int_Y (1-\chi)\left(2\eta\cdot(\xi+e(\phi)) - (B-A)^{-1}\eta\cdot\eta\right) dy. \quad (4.25)$$

One can get a lower bound in (4.25) by specializing to constant matrices η. Since $\int_Y \chi(y)dy = \theta$, this yields the following lower bound for (4.25)

$$2(1-\theta)\eta\cdot\xi - (1-\theta)(B-A)^{-1}\eta\cdot\eta + \int_Y 2(1-\chi)\eta\cdot e(\phi)dy.$$

On the other hand, since by periodicity $\int_Y e(\phi)dy = 0$, we have

$$\int_Y A(\xi+e(\phi))\cdot(\xi+e(\phi))dy = A\xi\cdot\xi + \int_Y Ae(\phi)\cdot e(\phi)dy.$$

Therefore, (4.24) leads to

$$A^*\xi\cdot\xi \geq A\xi\cdot\xi + 2(1-\theta)\xi\cdot\eta - (1-\theta)(B-A)^{-1}\eta\cdot\eta - g(\chi,\eta) \quad (4.26)$$

where $g(\chi,\eta)$ is a non-local term defined, through a cell problem, by

$$g(\chi,\eta) = -\min_{\phi(y)\in H^1_\#(Y)^N} \int_Y \left[Ae(\phi)\cdot e(\phi) + 2(1-\chi)\eta\cdot e(\phi)\right] dy. \quad (4.27)$$

The infimum over ϕ in (4.27) is easily computed by Fourier analysis since it involves only bi-linear terms depending on y. By periodicity, the characteristic function is written as a Fourier series

$$\chi(y) = \sum_{k\in\mathbf{Z}^N} \hat{\chi}(k)e^{2i\pi k\cdot y},$$

as well as the test function $\phi(y)$

$$\phi(y) = \sum_{k\in\mathbf{Z}^N} \hat{\phi}(k)e^{2i\pi k\cdot y}.$$

Since χ and ϕ are real-valued, the relationship

$$\overline{\hat{\chi}(k)} = \hat{\chi}(-k), \text{ and } \overline{\hat{\phi}(k)} = \hat{\phi}(-k) \quad (4.28)$$

holds true. The strain tensor of ϕ is given by

$$e(\phi)(y) = \sum_{k\in\mathbf{Z}^N} 2i\pi e^{2i\pi k\cdot y}\hat{\phi}(k)\odot k.$$

Plancherel formula yields

$$
\begin{aligned}
& -\int_Y \left(Ae(\phi)\cdot e(\phi) - 2\chi\eta\cdot e(\phi)\right) dy \\
&= -\sum_{k\in\mathbb{Z}^N} \left[4\pi^2 A(\hat{\phi}(k)\odot k)\cdot(\hat{\phi}(k)\odot k) - 4i\pi\eta\cdot(\hat{\phi}(k)\odot k)\right] \qquad (4.29)\\
&= -\sum_{k\in\mathbb{Z}^N} \left[4\pi^2\left(2\mu_A|k|^2|\hat{\phi}(k)|^2 + \lambda_A(\hat{\phi}(k)\cdot k)^2\right) + 4\pi\mathcal{I}m\left(\overline{\hat{\chi}(k)}(\eta k)\cdot\hat{\phi}(k)\right)\right].
\end{aligned}
$$

The minimization over $\phi(y)$ in $H^1_\#(Y)^N$ is equivalent to the minimizations over all vectors $\hat{\phi}(k)$ in $\mathbb{C}^N$, for each frequency k (and the minimization can be performed on each component independently). Remark that the frequency $k=0$ contributes for nothing in the sum (4.29). For all other frequencies the minimum is attained by

$$
\hat{\phi}(k) = -\frac{i\hat{\chi}(k)}{4\pi\mu_A|k|^2}\left(\eta k - \frac{\lambda_A}{2\mu_A+\lambda_A}\frac{\eta k\cdot k}{|k|^2}k\right),
$$

and the minimum value is

$$
|\hat{\chi}(k)|^2 f_A(\frac{k}{|k|})\eta\cdot\eta, \tag{4.30}
$$

where $f_A(e)\eta\cdot\eta$ is defined by

$$
f_A(e)\eta\cdot\eta = \frac{1}{\mu_A}\left(|\eta e|^2 - (\eta e\cdot e)^2\right) + \frac{1}{2\mu_A+\lambda_A}(\eta e\cdot e)^2. \tag{4.31}
$$

Therefore

$$
g(\chi,\eta) = \sum_{k\in\mathbb{Z}^N,\ k\neq 0} |\hat{\chi}(k)|^2 f_A(\frac{k}{|k|})\eta\cdot\eta. \tag{4.32}
$$

On the other hand, Plancherel formula gives

$$
\sum_{k\in\mathbb{Z}^N,\ k\neq 0} |\hat{\chi}(k)|^2 = \int_Y |\chi(y)-\theta|^2\, dy = \theta(1-\theta).
$$

Thus, introducing the H-measure $\theta(1-\theta)\nu$ of the characteristic function χ (where ν is a probability measure on the unit sphere S_{N-1}), the non-local term (4.32) can be rewritten

$$
g(\chi,\eta) = \theta(1-\theta)\int_{S_{N-1}} f_A(e)\eta\cdot\eta\, d\nu(e),
$$

where ν is defined by

$$\theta(1-\theta)\int_{S_{N-1}} f(e)\,d\nu(e) = \sum_{k\in\mathbb{Z}^N,\ k\neq 0} |\hat{\chi}(k)|^2 f(\frac{k}{|k|}) \tag{4.33}$$

for any continuous function $f : S_{N-1} \to \mathbb{R}$. The notion of H-measure (due to Gerard [27] and Tartar [65]) has been discussed in chapter 3.

Recall that, by its definition (4.31), $f_A(e)\eta\cdot\eta$ is an homogeneous polynomial of degree four as a function of e. Therefore, the value of the non-local term $g(\chi,\eta)$ depends only on the fourth-order moments of the H-measure ν. By Caratheodory's theorem and Lemma 4.1.9, any probability measure can be replaced by a convex combination of Dirac masses as far as their fourth-order moments are concerned. In other words, there exist an integer $p \geq 1$, unit vectors $(e_i)_{1\leq i\leq p}$, positive parameters $(m_i)_{1\leq i\leq p}$ such that $m_i \geq 0$ and $\sum_{i=1}^p m_i = 1$

$$\int_{S_{N-1}} e\otimes e\otimes e\otimes e\,d\nu(e) = \sum_{i=1}^p m_i e_i\otimes e_i\otimes e_i\otimes e_i.$$

Thus, we have

$$g(\chi,\eta) = \theta(1-\theta)\left(\sum_{i=1}^p m_i f_A(e_i)\right)\eta\cdot\eta,$$

where the vectors e_i and parameters m_i do not depend on η. Consequently, the right hand side of (4.26) is a simple Legendre transform of a quadratic function which yields

$$A^*\xi\cdot\xi \geq A\xi\cdot\xi + (1-\theta)\left((B-A)^{-1} + \theta\sum_{i=1}^p m_i f_A(e_i)\right)^{-1}\xi\cdot\xi. \tag{4.34}$$

Comparing (4.34) with the lamination formula (4.9) immediately implies that there exists a sequential laminate A^-, with matrix A and core B, such that

$$A^*\xi\cdot\xi \geq A^-\xi\cdot\xi.$$

Since A^- is independent of ξ (it depends only on the H-measure of the characteristic function χ), it gives the desired inequality $A^* \geq A^-$.

The other inequality $A^* \leq A^+$ is derived similarly by establishing an upper bound on the effective energy. We subtract to (4.23), the other *reference material* B

$$A^*\xi\cdot\xi = \min_{\phi\in H^1_\#(Y)^N}\Big[-\int_Y \chi(B-A)(\xi+e(\phi))\cdot(\xi+e(\phi))dy$$

$$+\int_Y B(\xi + e(\phi)) \cdot (\xi + e(\phi))dy \Big] . \tag{4.35}$$

Using the positivity of $B - A$ and convex duality, the first integral in the right hand side of (4.35) is rewritten

$$-\sup_{\eta(y)\in L^2_\#(Y;\mathbb{R}^{N^2})} \int_Y \chi \left(2\eta \cdot (\xi + e(\phi)) - (B-A)^{-1}\eta \cdot \eta\right) dy. \tag{4.36}$$

One can get an upper bound in (4.36) by specializing the maximization in η to constant matrices in Y

$$-\theta \left(2\xi \cdot \eta - (B-A)^{-1}\eta \cdot \eta\right) - 2\int_Y \chi e(\phi) \cdot \eta dy.$$

On the other hand, by periodicity we have

$$\int_Y B(\xi + e(\phi)) \cdot (\xi + e(\phi))dy = B\xi \cdot \xi + \int_Y Be(\phi) \cdot e(\phi)dy.$$

Therefore (4.35) yields, for any $\eta \in \mathbb{R}^{N^2}$,

$$A^*\xi \cdot \xi \le B\xi \cdot \xi + \theta \left(-2\xi \cdot \eta + (B-A)^{-1}\eta \cdot \eta\right) - h(\chi, \eta), \tag{4.37}$$

where $h(\chi, \eta)$ is another non-local term defined by

$$h(\chi, \eta) = -\min_{\phi(y)\in H^1_\#(Y)^N} \int_Y \left(Be(\phi) \cdot e(\phi) - 2\chi e(\phi) \cdot \eta\right) dy. \tag{4.38}$$

As for the lower bound, a simple computation by Fourier analysis shows that

$$h(\chi, \eta) = \sum_{k\in\mathbb{Z}^N,\ k\neq 0} |\hat{\chi}(k)|^2 f_B(\frac{k}{|k|})\eta \cdot \eta, \tag{4.39}$$

which, using the same H-measure ν of χ, can be rewritten

$$h(\chi, \eta) = \theta(1-\theta) \int_{S_{N-1}} f_B(e)\eta \cdot \eta \, d\nu(e).$$

Replacing the measure ν by the same convex combination of Dirac masses, we obtain

$$h(\chi, \eta) = \theta(1-\theta) \left(\sum_{i=1}^p m_i f_B(e_i)\right) \eta \cdot \eta.$$

Consequently, the right hand side of (4.37) is the Legendre transform of a quadratic function, and this yields

$$A^*\xi\cdot\xi \le B\xi\cdot\xi - \theta\left((B-A)^{-1} - (1-\theta)\sum_{i=1}^{p} m_i f_B(e_i)\right)^{-1}\xi\cdot\xi. \quad (4.40)$$

Comparing (4.40) with the lamination formula (4.10) immediately implies that there exists a sequential laminate A^+, with core A and matrix B, such that $A^* \le A^+$. □

As an immediate application of Theorem 4.2.1, we obtain optimal bounds on the effective energy of a composite material. We recall the definition of an optimal bound.

Definition 4.2.3 *Let ξ be a symmetric matrix in $\mathbb{R}^{N^2}$. A real-valued function $f^+(\theta,A,B,\xi)$ (respectively $f^-(\theta,A,B,\xi)$) is called an upper bound (respectively a lower bound) if, for any homogenized tensor $A^* \in G_\theta$,*

$$A^*\xi\cdot\xi \le f^+(\theta,A,B,\xi) \quad \big(\textit{respectively } \ge f^-(\theta,A,B,\xi)\big)\,.$$

The upper bound f^+ (respectively lower bound f^-) is said to be optimal if, for any $\xi \in \mathbb{R}^{N^2}$, there exists $A^*_\xi \in G_\theta$ (which may depend on ξ) such that

$$A^*_\xi\xi\cdot\xi = f^+(\theta,A,B,\xi) \quad (\textit{respectively } = f^-(\theta,A,B,\xi)).$$

There is no special reason for restricting our attention to a single effective energy, i.e. to a unique strain tensor ξ, and Definition 4.2.3 extends easily to sum of energies

$$\sum_{i=1}^{p} A^*\xi_i\cdot\xi_i = A^* : \left(\sum_{i=1}^{p}\xi_i\otimes\xi_i\right),$$

where $(\xi_i)_{1\le i\le p}$ is a collection of strain tensors. The sum $\sum_{i=1}^{p}\xi_i\otimes\xi_i$ is a symmetric fourth-order tensor, and any symmetric fourth-order tensor M can always be diagonalized as

$$M = \sum_{i=1}^{N(N+1)/2}\tilde{\xi}_i\otimes\tilde{\xi}_i,$$

where each $\tilde{\xi}_i \in \mathbb{R}^{N^2}$, and $N(N+1)/2$ is the dimension of the space $\mathbb{R}^{N^2}$. Therefore, there is no loss of generality in assuming that the number of energies is exactly $p = N(N+1)/2$. Such energy bounds are also called trace bounds [46] since they can be written

$$\sum_{i=1}^{p} A^*\xi_i \cdot \xi_i = \mathrm{tr}\,(A^*M) = A^* : M \quad \text{with} \quad M = \sum_{i=1}^{p} \xi_i \otimes \xi_i .$$

Proposition 4.2.4 *Let $\xi_1, ..., \xi_p$ be symmetric matrices in $\mathbb{R}^{N^2}$. Any homogenized tensor $A^* \in G_\theta$ satisfies*

$$\sum_{i=1}^{p} A^*\xi_i \cdot \xi_i \geq \sum_{i=1}^{p} A\xi_i \cdot \xi_i + (1-\theta) \max_{(\eta_i)_{1\leq i\leq p}\in\mathbb{R}^{N^2}} \tag{4.41}$$

$$\left[\sum_{i=1}^{p} \left(2\xi_i \cdot \eta_i - (B-A)^{-1}\eta_i \cdot \eta_i \right) - \theta g(\eta_1, ..., \eta_p) \right],$$

where the non-local term g is given by

$$g(\eta_1, ..., \eta_p) = \max_{e\in S_{N-1}} \sum_{i=1}^{p} f_A(e)\eta_i \cdot \eta_i, \tag{4.42}$$

and

$$\sum_{i=1}^{p} A^*\xi_i \cdot \xi_i \leq \sum_{i=1}^{p} B\xi_i \cdot \xi_i + \theta \min_{(\eta_i)_{1\leq i\leq p}\in\mathbb{R}^{N^2}} \tag{4.43}$$

$$\left[\sum_{i=1}^{p} \left(2\xi_i \cdot \eta_i + (B-A)^{-1}\eta_i \cdot \eta_i \right) - (1-\theta) h(\eta_1, ..., \eta_p) \right],$$

where the non-local term h is given by

$$h(\eta_1, ..., \eta_p) = \min_{e\in S_{N-1}} \sum_{i=1}^{p} f_B(e)\eta_i \cdot \eta_i, \tag{4.44}$$

and $f_{A,B}(e)$ is defined by

$$f_{A,B}(e)\eta \cdot \eta = \frac{1}{\mu_{A,B}} \left(|\eta e|^2 - (\eta e \cdot e)^2 \right) + \frac{1}{2\mu_{A,B} + \lambda_{A,B}} (\eta e \cdot e)^2. \tag{4.45}$$

Furthermore, these upper and lower bounds are optimal in the sense of Definition 4.2.3 and optimality is always achieved by a finite-rank sequential laminate, of rank 3 in 2-D and rank 6 in 3-D.

Remark 4.2.5 *The functions g and h are called non-local terms since they are the only terms in the Hashin-Shtrikman bounds that contain informations on the microstructure of the homogenized Hooke's law A^*. Clearly, g is convex, and the lower bound (4.41) is therefore given as the result of a finite-dimensional concave maximization. On the other hand, one can check that*

$$h(\eta_1, ..., \eta_p) \leq \sum_{i=1}^{p} B^{-1}\eta_i \cdot \eta_i,$$

and since $(B-A)^{-1} - (1-\theta)B^{-1} \geq 0$, the upper bound (4.43) is given as the result of a finite-dimensional convex minimization.

In principle, the bounds (4.41) and (4.43) can be computed explicitly since they reduce to a finite-dimensional optimization. In practice, this is almost impossible because, even for isotropic phases, there are no simple formula for the non-local terms g and h. Indeed, the optimization with respect to $e \in S_{N-1}$ in (4.42) and (4.44) is untractable (the optimal e's are usually not eigenvectors of any matrix η_i).

Remark that the positive non-definite fourth-order tensors $f_A(e), f_B(e)$ defined by (4.45) are exactly the same than those appearing in the lamination formula (see (4.7)). This is at the root of the optimality of these bounds. Theorem 4.2.1 and Proposition 4.2.4 can easily be generalized to the case of non-isotropic Hooke's law A and B.

Deriving the Hashin-Shtrikman bounds given by Proposition 4.2.4 is a classical matter : it goes back to the original work of Hashin and Shtrikman [33] (modern expositions may be found in [7], [46], or in [28], [29] where the translation method is used rather than the Hashin-Shtrikman variational principle).

Proof of Proposition 4.2.4. We focus on the lower bound (the case of the upper bound is completely symmetric). Applying Theorem 4.2.1 yields

$$\sum_{i=1}^{p} A^*\xi_i \cdot \xi_i \geq \min_{A^- \in L_\theta^-} \sum_{i=1}^{p} A^-\xi_i \cdot \xi_i. \tag{4.46}$$

The closed character of L_θ^- immediately implies that (4.46) is an optimal lower bound. It remains to evaluate the right hand side of (4.46) with the help of characterization (4.15) of L_θ^- which associates to each tensor A^- a probability measure ν. Applying the Legendre transform to $A^- - A$ leads to

$$\sum_{i=1}^{p} A^-\xi_i \cdot \xi_i = \sum_{i=1}^{p} A\xi_i \cdot \xi_i + (1-\theta) \max_{(\eta_i)_{1\leq i\leq p} \in \mathbf{R}^{N^2}}$$

$$\left[\sum_{i=1}^{p}\left(2\xi_i\cdot\eta_i-(B-A)^{-1}\eta_i\cdot\eta_i\right)-\theta g_\nu(\eta_1,...,\eta_p)\right],$$

where g_ν is defined by

$$g_\nu(\eta_1,...,\eta_p)=\sum_{i=1}^{p}\left(\int_{S_{N-1}} f_A(e)d\nu(e)\right)\eta_i\cdot\eta_i. \tag{4.47}$$

To obtain a lower bound, we have to maximize g_ν over all H-measures ν. This is easily realized by taking a Dirac mass concentrated on the unit vectors where $\sum_{i=1}^{p} f_A(e)\eta_i\cdot\eta_i$ is maximal, i.e. $\max_\nu g_\nu = g$. This yields the lower bound (4.41). □

Remark 4.2.6 *The proof of Proposition 4.2.4 delivers also necessary and sufficient conditions for a periodic microstructure to be optimal in the Hashin-Shtrikman bounds. Actually, the lower bound is obtained by making two inequalities. The first one is made in (4.25) by restricting the tensors η_i to be constant. Therefore, the microscopic strain of an optimal tensor must be constant in phase B. The second inequality is made in (4.47) when maximizing with respect to the H-measure ν of the microstructure χ. By definition (4.33) of ν, this yields restrictions on the Fourier coefficients of χ.*

As an application of these trace bounds, we can recover the famous original Hashin-Shtrikman bounds [33] on the bulk and shear moduli of an isotropic two-phase composite material (which have been shown to be attainable by finite rank sequential laminate in [25]).

Theorem 4.2.7 *Let A^* be an isotropic homogenized tensor in G_θ, i.e.*

$$A^* \;=\; 2\mu_* I_4+\left(\kappa_*-\frac{2\mu_*}{N}\right)I_2\otimes I_2.$$

Its bulk and shear moduli κ_* and μ_* satisfy

$$\frac{1-\theta}{\kappa_*-\kappa_A}\le\frac{1}{\kappa_B-\kappa_A}+\frac{\theta}{2\mu_A+\lambda_A} \tag{4.48}$$

$$\frac{\theta}{\kappa_B-\kappa_*}\le\frac{1}{\kappa_B-\kappa_A}+\frac{1-\theta}{2\mu_B+\lambda_B} \tag{4.49}$$

and

$$\frac{1-\theta}{2(\mu_*-\mu_A)}\le\frac{1}{2(\mu_B-\mu_A)}+\frac{\theta(N-1)(\kappa_A+2\mu_A)}{(N^2+N-2)\mu_A(2\mu_A+\lambda_A)} \tag{4.50}$$

$$\frac{\theta}{2(\mu_B - \mu_*)} \leq \frac{1}{2(\mu_B - \mu_A)} + \frac{(1-\theta)(N-1)(\kappa_B + 2\mu_B)}{(N^2 + N - 2)\mu_B(2\mu_B + \lambda_B)} \tag{4.51}$$

Furthermore, the lower bounds (4.48) and (4.50), as well as the upper bounds (4.49) and (4.51), are simultaneously attained by an isotropic rank-p sequential laminate with $p = N(N+1)/2$.

Remark 4.2.8 *The bounds (4.48), (4.50), (4.49) and (4.51) do not characterize all possible isotropic homogenized tensor A^* in G_θ. In other words, there exist isotropic elasticity tensors with moduli satisfying these bounds which are not composite materials obtained by mixing phases A and B in proportions θ, $(1-\theta)$. Better bounds (i.e. which define a smaller region of the (κ_*, μ_*) plane) can be obtained.*

Proof. The lower bound (4.41) can be rewritten

$$\phi_1(\xi_1, ..., \xi_p) \ \geq \ \phi_2(\xi_1, ..., \xi_p), \tag{4.52}$$

where

$$\phi_1(\xi_1, ..., \xi_p) = \frac{1}{1-\theta} \sum_{i=1}^{p} (A^* - A)\xi_i \cdot \xi_i,$$

and

$$\phi_2(\xi_1, ..., \xi_p) = \max_{\eta_i \in \mathbb{R}^{N^2}} \left[\sum_{i=1}^{p} \left(2\xi_i \cdot \eta_i - (B-A)^{-1}\eta_i \cdot \eta_i \right) - \theta g(\eta_1, ..., \eta_p) \right].$$

Since ϕ_1 and ϕ_2 are convex functions, by application of the Legendre or Fenchel transform, the family of inequality (4.52) is equivalent to

$$\phi_1^*(\eta_1, ..., \eta_p) \ \leq \ \phi_2^*(\eta_1, ..., \eta_p), \tag{4.53}$$

with

$$\phi_k^*(\eta_1, ..., \eta_p) = \max_{\xi_i \in \mathbb{R}^{N^2}} \left[\sum_{i=1}^{p} 2\xi_i \cdot \eta_i - \phi_k(\xi_1, ..., \xi_p) \right].$$

Since for a convex function ϕ one has $\phi^{**} = \phi$, we deduce from (4.53) that

$$\sum_{i=1}^{p} (B-A)^{-1}\eta_i \cdot \eta_i + \theta g(\eta_1, ..., \eta_p) \geq (1-\theta) \sum_{i=1}^{p} (A^* - A)^{-1}\eta_i \cdot \eta_i, \tag{4.54}$$

for any choice of the matrices $(\eta_i)_{1 \leq i \leq p} \in \mathbb{R}^{N^2}$. Similarly, the family of upper bound (4.43) is equivalent to

$$\sum_{i=1}^{p} (B-A)^{-1}\eta_i \cdot \eta_i - (1-\theta) h(\eta_1, ..., \eta_p) \geq \theta \sum_{i=1}^{p} (B - A^*)^{-1}\eta_i \cdot \eta_i. \tag{4.55}$$

Taking $\eta_1 = \cdots = \eta_p = I_2$ (the identity matrix) yields the desired bounds for κ_* since $f_A(k)I_2 \cdot I_2$, as well as $f_B(k)I_2 \cdot I_2$, are independent of k, i.e.

$$f_A(k)I_2 \cdot I_2 = \frac{1}{2\mu_A + \lambda_A}.$$

On the other hand, we now choose $(\eta_i)_{1\le i\le p} \in \mathbb{R}^{N^2}$ with $p = N(N+1)/2$ such that

$$\sum_{i=1}^{N(N+1)/2} \eta_i \otimes \eta_i = I_4 - \frac{1}{N} I_2 \otimes I_2 = P_s,$$

where the positive fourth-order tensor P_s is the orthogonal projection operator on trace-free matrices (i.e. pure shear tensors). One can check that

$$\sum_{i=1}^{N(N+1)/2} (B-A)^{-1}\eta_i \cdot \eta_i = \operatorname{tr}\left((B-A)^{-1}P_s\right) = \frac{1}{2(\mu_B - \mu_A)},$$

and

$$\sum_{i=1}^{N(N+1)/2} f_A(k)\eta_i \cdot \eta_i = \operatorname{tr}\left(f_A(k)P_s\right) = \frac{(N-1)(\kappa_A + 2\mu_A)}{(N^2+N-2)\mu_A(2\mu_A+\lambda_A)},$$

which is independent of k. This leads to the desired bounds on μ_*. These bounds on κ_* and μ_* are necessarily optimal and attained by finite rank sequential laminates, since the families of bounds (4.54) and (4.55) are equivalent to the other families (4.41) and (4.43) which are optimal by virtue of Proposition 4.2.4.

A more direct way of checking the optimality of these bounds in dimension $N = 2$ or 3 is, following [25], to exhibit a particular isotropic and optimal sequential laminate given by one of the two formulae (4.9) and (4.10) (symmetric by interchanging the roles of A and B). When $N = 2$, we choose a rank-3 sequential laminate with lamination parameters $m_1 = m_2 = m_3 = 1/3$ and lamination directions

$$e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, e_2 = \begin{pmatrix} \cos\frac{\pi}{3} \\ \sin\frac{\pi}{3} \end{pmatrix}, e_3 = \begin{pmatrix} \cos\frac{2\pi}{3} \\ \sin\frac{2\pi}{3} \end{pmatrix}.$$

A simple but tedious computation shows that it is isotropic and saturates the two lower bounds (4.48) and (4.50) for formula (4.9) (with a matrix of A and a core of B), or the two upper bounds (4.49) and (4.51) for the symmetric formula (4.10) (with a matrix of B and a core of A).

When $N = 3$, we choose a rank-6 sequential laminate with lamination parameters $m_1 = m_2 = m_3 = m_4 = m_5 = m_6 = 1/6$ and lamination directions corresponding to the six northern hemisphere vertices of the regular icosahedron

$$e_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, e_2 = \begin{pmatrix} \sin 2\beta \\ 0 \\ \cos 2\beta \end{pmatrix}, e_3 = \begin{pmatrix} \sin 2\beta \cos 2\alpha \\ \sin 2\beta \sin 2\alpha \\ \cos 2\beta \end{pmatrix},$$

$$e_4 = \begin{pmatrix} \sin 2\beta \cos 4\alpha \\ \sin 2\beta \sin 4\alpha \\ \cos 2\beta \end{pmatrix}, e_5 = \begin{pmatrix} \sin 2\beta \cos 6\alpha \\ \sin 2\beta \sin 6\alpha \\ \cos 2\beta \end{pmatrix}, e_6 = \begin{pmatrix} \sin 2\beta \cos 8\alpha \\ \sin 2\beta \sin 8\alpha \\ \cos 2\beta \end{pmatrix},$$

with $\alpha = \frac{\pi}{5}$ and $\cos 2\beta = \sqrt{5}/5$. A tedious computations shows that it is isotropic and saturates the two lower bounds (4.48) and (4.50) for formula (4.9) (with a matrix of A and a core of B), or the two upper bounds (4.49) and (4.51) for the symmetric formula (4.10) (with a matrix of B and a core of A). □

Remark 4.2.9 *In all the previous bounds, optimality has been proved by exhibiting sequential laminates which saturate these bounds. Laminates are not the only possible optimal microstructures but they are the more general ones. The optimal bounds (4.48) and (4.49) on the bulk modulus are known since Hashin to be achieved by a concentric sphere assemblage of the two phases (see e.g. [17]). However, for the other optimal bounds (4.50) and (4.51) on the shear modulus, the only available optimal microstructure is the sequential laminated one. In the case of a single energy bound, there are also other optimal microstructures, at least in some restricted regimes of these bounds. Grabovsky [30] has shown that Tartar's confocal ellipsoid construction [64] is optimal under some conditions. Vigdergauz distribution of periodic inclusions [66] is also conditionally optimal in an energy bound (see [31]).*

4.3 Small amplitude G-closure

On the contrary of the conductivity case, the G-closure of two isotropic elastic phases in prescribed proportions is unknown. In other words, there is no explicit algebraic characterization of the set G_θ defined as the set of all constant effective Hooke's law obtained by homogenization of phases A and B in volume fractions $\theta, 1-\theta$. The main reason for this lack of knowledge of the G-closure is that the Hashin-Shtrikman energy bounds given by Proposition 4.2.4, or Avellaneda's Theorem 4.2.1, are unsufficient to characterize all homogenized tensors.

The goal of this section is therefore to characterize the G-closure in the low contrast, or small amplitude, limit. Indeed, if we assume that the two phases A and B have very close moduli, then the full G-closure is known in 2 and 3 dimensions up to second order terms in the contrast $B - A$. More precisely, we assume that there exist a small positive parameter γ and a positive isotropic fourth order tensor D such that

$$B = A + \gamma D. \tag{4.56}$$

The next lemma gives a formula for a periodic composite A^* in terms of its H-measure (see chapter 3), up to second order in γ.

Lemma 4.3.1 *Let A^* be any periodic homogenized tensor associated to a characteristic function χ. Introducing the H-measure ν of χ, defined as a probability measure on S_{N-1} by*

$$\theta(1-\theta)\int_{S_{N-1}} f(e)\, d\nu(e) = \sum_{k\in\mathbb{Z}^N,\ k\neq 0} |\hat{\chi}(k)|^2 f(\frac{k}{|k|})$$

for any continuous function f on S_{N-1}, we have

$$A^* = \theta A + (1-\theta)B - \gamma^2\theta(1-\theta)D\left(\int_{S_{N-1}} f_A(e) d\nu(e)\right) D + \mathcal{O}(\gamma^3),$$

where, for any $\eta \in \mathbb{R}^{N^2}$,

$$f_A(e)\eta\cdot\eta = \frac{1}{\mu_A}\left(|\eta e|^2 - (\eta e\cdot e)^2\right) + \frac{1}{2\mu_A+\lambda_A}(\eta e\cdot e)^2,$$

and the remainder is uniform with respect to A^* in the sense that, there exists a positive constant C, independent of γ and χ, such that

$$\left\|\mathcal{O}(\gamma^3)\right\| \le C\gamma^3.$$

Upon recalling Lemma 4.1.10 (on the characterization of fourth-order moments of probability measures, due to [26]), we immediately obtain the following

Theorem 4.3.2 *Assume that the space dimension is $N = 2$ or 3. Then, any tensor A^* in G_θ is of the form*

$$A^* = \theta A + (1-\theta)B - \gamma^2\theta(1-\theta)DL_A(M)D + \mathcal{O}(\gamma^3)$$

where M is any fully symmetric fourth order tensor, i.e.

$$M_{ijkl} = M_{kjil} = M_{klij} = M_{jikl},$$

with unit trace $\sum_{i,j=1}^N M_{ijij} = 1$, and non-negative in the sense of quadratic forms, i.e. for any symmetric matrix ξ

$$\sum_{i,j,k,l=1}^{N} M_{ijkl}\xi_{ij}\xi_{kl} \geq 0,$$

and L_A is the following linear map on the space of fourth-order tensors

$$\begin{aligned} L_A(M)_{ijkl} &= \left(\frac{1}{2\mu_A+\lambda_A} - \frac{1}{\mu_A}\right) M_{ijkl} \\ &+\frac{1}{4\mu_A}\sum_{m=1}^{N}\left(M_{imml}\delta_{jk} + M_{imkm}\delta_{jl} + M_{mjml}\delta_{ik} + M_{mjkm}\delta_{il}\right). \end{aligned}$$

Proof of Lemma 4.3.1. Recall from chapter 1 that a periodic composite A^* is defined through the solution of a cell problem. Namely, for any tensor $\xi \in \mathbb{R}^{N^2}$,

$$A^*\xi\cdot\xi = \int_Y A(y)\left(\xi + e(w)\right)\cdot\xi dy,$$

where $A(y) = \chi(y)A + (1-\chi(y))B$ and w is the unique solution in $H^1_\#(Y)^N$ (up to a rigid body displacement) of

$$\begin{cases} -\mathrm{div_y}\ \left(A(y)\left(\xi + e(w(y))\right)\right) = 0 & \text{in } Y \\ y \to w(y) & Y\text{-periodic.} \end{cases}$$

Remark that $A(y) = A + \gamma(1-\chi(y))D$, and therefore the solution w depends analytically on the small contrast parameter γ. We shall not use this fact, but rather expand w as

$$w(y) = \gamma v(y) + \gamma^2 r(y),$$

where v is the unique solution in $H^1_\#(Y)^N$ (up to a rigid body displacement) of

$$\begin{cases} -\mathrm{div_y}\ \left(Ae(v) + (1-\chi(y))D\xi\right) = 0 & \text{in } Y \\ y \to v(y) & Y\text{-periodic.} \end{cases}$$

By subtraction, it is easily checked that r is the solution of

$$\begin{cases} -\mathrm{div_y}\ \left(A(y)e(r) + (1-\chi(y))De(v)\right) = 0 & \text{in } Y \\ y \to r(y) & Y\text{-periodic.} \end{cases}$$

Remark that v is independent of γ, but not r. Nevertheless, since $A(y) \geq A$, r satisfies the following a priori estimate

$$\|e(r)\|_{L^2(\Omega;\mathbb{R}^{N^2})} \leq C|\xi|,$$

where C is a positive constant that does not depend on γ nor χ. Plugging the ansatz for w in the definition of A^* and integrating by parts leads to

$$A^*\xi\cdot\xi = A\xi\cdot\xi+\gamma(1-\theta)D\xi\cdot\xi-\gamma^2\int_Y Ae(v)\cdot e(v)dy+\gamma^3\int_Y De(r)\cdot\xi dy. \quad (4.57)$$

Thanks to the a priori estimate on r, the last term in (4.57) is a uniform remainder term of order γ^3. The term of order γ^2 in (4.57) can be computed by Fourier analysis as in the proof of Theorem 4.2.1. Indeed, it is the same computation than that of the non-local term defined by (4.27). More precisely, we have

$$\int_Y Ae(v)\cdot e(v)dy = g(\chi, D\xi) = \sum_{k\in\mathbb{Z}^N,\ k\neq 0} |\hat{\chi}(k)|^2 f_A(\frac{k}{|k|})(D\xi)\cdot(D\xi),$$

where $f_A(\cdot)$ is defined by (4.31). Introducing the H-measure ν and remarking that $\sum_{k\in\mathbb{Z}^N,\ k\neq 0}|\hat{\chi}(k)|^2 = \theta(1-\theta)$ yield the desired result. □

Proof of Theorem 4.3.2. By density of periodic composites in the set G_θ of all possible composites, and by the closed character of the set $\mathcal{C}$ of fourth-order tensors of probability measures, the small amplitude formula of Lemma 4.3.1 is easily extended to any composite tensor $A^* \in G_\theta$ (this can be obtained directly by using the proper notion of H-measure, see [65] for details). In dimensions $N = 2$ or 3, Lemma 4.1.10 furnishes a characterization of this set $\mathcal{C}$ which yields the desired result. □

Chapter 5

Multiple well energies.

This chapter is devoted to the relaxation of so-called multiwell energies in the elasticity setting which are models of coherent phase transitions. The modelling aspects of this problem are discussed at length in e.g. [14], [36] (or see the metallurgical literature [34], [57]). We content ourselves in discussing some mathematical aspects of the geometrically linear version of this problem, enlightening the role played by H-measures.

5.1 Setting of the problem.

We consider a bounded open set $\Omega \in \mathbb{R}^N$ occupied by several phases of a same material. For simplicity, we assume that there are no volume forces but only surface loadings that are represented by non homogeneous boundary conditions. The material chooses its preferred phase at each point by minimizing its elastic energy. In the framework of linearized elasticity, the unknown is the displacement vector u, and we denote by $e(u) = (\nabla u + \nabla^t u)/2$ its strain tensor. Each phase, indexed by $1 \leq i \leq p$, has its Hooke's law A_i, its stress-free strain a_i, and its minimum energy w_i. Its elastic energy is therefore

$$W_i(\xi) = A_i(\xi - a_i) \cdot (\xi - a_i) + w_i.$$

The multiwell energy is the minimum of all phase energies

$$W(\xi) = \min_{1 \leq i \leq p} W_i(\xi). \tag{5.1}$$

For some smooth boundary conditions u_0 we look for minimizers of

$$\inf_{u \in u_0 + H_0^1(\Omega)^N} \int_\Omega W\left(e(u)\right) dx. \tag{5.2}$$

In truth, the interesting object is not really the minimizer u but rather the characteristic functions of the p phases which are defined (possibly non uniquely) by

$$W(e(u)) = \sum_{i=1}^{p} \chi_i(x) W_i(e(u)) .$$

Exploring further this idea, we show that (5.2) is equivalent to an optimal design problem. Indeed, we can rewrite

$$W(\xi) = \min_{(\chi_i)_{1\le i\le p}\in C} \sum_{i=1}^{p} \chi_i W_i(\xi),$$

where the set C is defined by

$$(\chi_i)_{1\le i\le p} \in C \Leftrightarrow \begin{cases} \chi_i = 0 \text{ or } 1 \\ \sum_{i=1}^{p} \chi_i = 1 \end{cases}$$

Thus, for any $u \in H^1(\Omega)^N$,

$$\int_\Omega W(e(u))\, dx = \min_{(\chi_i)_{1\le i\le p}\in L^\infty(\Omega;C)} \int_\Omega \sum_{i=1}^{p} \chi_i(x) W_i(e(u))\, dx.$$

Switching the two minimizations implies that (5.2) is equivalent to

$$\inf_{(\chi_i)_{1\le i\le p}\in L^\infty(\Omega;C)} \min_{u\in u_0+H_0^1(\Omega)^N} \int_\Omega \int_\Omega \sum_{i=1}^{p} \chi_i(x) W_i(e(u))\, dx. \tag{5.3}$$

It turns out that both formulations (5.2) and (5.3) are not well-posed, i.e. they usually do not admit minimizers. The reason is that the integrand W is not quasiconvex (and a fortiori not convex) and thus the energy in (5.2) is not sequentially lower semi-continuous. These problems need therefore to be relaxed. Relaxation for (5.2) is a matter of quasiconvexification (see e.g. [18] for details on this notion), while for (5.3) it is a problem of homogenization (see e.g. [42], [50]). The link between these two approachs of the same problem is extensively studied in [38].

5.2 Relaxation.

We first recall the notion of quasi-convexification for a real-valued functional W defined on strains in $\mathbb{R}^{N^2}$. Assume that W is continuous and satisfy

$$c \le W(\lambda) \le C(1+|\lambda|^2), \quad \lambda \in \mathbb{R}^{N^2}.$$

The quasi-convex envelope of W (or its quasi-convexification) is defined for every λ in $\mathbb{R}^{N^2}$ as

$$QW(\lambda) = \inf_{\phi \in H_0^1(Y)^N} \int_Y W\left(\lambda + e(\phi)(x)\right) dx, \tag{5.4}$$

where $Y = (0,1)^N$ is the unit cube of $\mathbb{R}^N$. The function QW is a locally Lipschitz function as easily seen upon noting that QW is rank-1 convex and satisfies the same growth assumption as W (see e.g. [44]). The main property of the quasi-convexification is its link with relaxation. For any bounded open set Ω of $\mathbb{R}^N$, the lower semi-continuous envelope in $H^1(\Omega)^N$ of

$$I(u) = \int_\Omega W(e(u))dx$$

for the sequential weak topology of $H^1(\Omega)^N$, *i.e.*, the functional

$$RI(u) = \inf_{\substack{u_n \in H^1(\Omega)^N \\ u_n \rightharpoonup u \text{weakly in } H^1(\Omega)^N}} \liminf I(u_n)$$

is given by

$$RI(u) = \int_\Omega QW(e(u))dx. \tag{5.5}$$

According to [13] and [18], in the definition (5.4) of QW it is possible to replace the space $H_0^1(Y)^N$ of test fields by that of periodic fields $H_\#^1(Y)^N$ (at least when W is non negative, continuous and grows at most quadratically). Thus, QW is equivalently defined by

$$QW(\lambda) = \inf_{\phi \in H_\#^1(Y)^N} \int_Y W\left(\lambda + e(\phi)(x)\right) dx, \tag{5.6}$$

where $H_\#^1(Y)^N$ is the Sobolev space of Y-periodic vector-valued functions. A proof of (5.5) may be found in [18], Theorems 1.1 and 2.1 in Chapter 5, and in [1], Statement 3.7.

The computation of the quasiconvex envelope of (5.1) with the help of formula (5.6) amounts to solve a problem of periodic homogenization in practice. Plugging the definition of W in (5.6) and introducing families of characteristic functions $(\chi_i)_{1\leq i\leq p}$ yields

$$QW(\lambda) = \inf_{\phi \in H_\#^1(Y)^N} \min_{(\chi_i)_{1\leq i\leq p} \in L_\#^\infty(Y;C)} \int_Y \sum_{i=1}^p \chi_i(x) W_i\left(\lambda + e(\phi)(x)\right) dx \tag{5.7}$$

Switching the two minimizations in (5.7) leads to

$$QW(\lambda) = \inf_{(\chi_i)_{1\le i\le p}\in L^\infty_\#(Y;C)} W_{(\chi_i)}(\lambda)$$

where $W_{(\chi_i)}$ is an effective or homogenized energy at fixed repartition of the phases, defined by

$$W_{(\chi_i)}(\lambda) = \min_{\phi\in H^1_\#(Y)^N} \int_Y \sum_{i=1}^{p} \chi_i(x) W_i\left(\lambda + e(\phi)(x)\right) dx \tag{5.8}$$

The computation of $W_{(\chi_i)}$ in full generality is yet an open problem, and we focus in the sequel on two important special cases where it is possible.

5.2.1 First example.

To explore further (5.8), we now assume that there are only two phases $A_1 = A$, $A_2 = B$ which are well ordered, i.e. $A < B$ in the sense of quadratic forms. We rewrite the original energy integrand as

$$W(\lambda + e(\phi)) = \min\left(W_A(\lambda + e(\phi)), W_B(\lambda + e(\phi))\right)$$

with

$$\begin{array}{l} W_A(\lambda + e(\phi)) = A(\lambda + e(\phi) - a)\cdot(\lambda + e(\phi) - a) + w_A, \\ W_B(\lambda + e(\phi)) = B(\lambda + e(\phi) - b)\cdot(\lambda + e(\phi) - b) + w_B. \end{array}$$

To simplify the integrand in (5.8), we introduce another constant strain ξ and we write

$$\begin{array}{l} \chi W_A(\lambda + e(\phi)) + (1-\chi) W_B(\lambda + e(\phi)) = \\ (\chi A + (1-\chi)B)(\xi + e(\phi))\cdot(\xi + e(\phi)) \\ +2\left(\xi + e(\phi)\right)\cdot\left(\chi A(\lambda - \xi - a) + (1-\chi)B(\lambda - \xi - b)\right) \\ +\chi\left(w_A + A(\lambda - \xi - a)\cdot(\lambda - \xi - a)\right) \\ +(1-\chi)\left(w_B + B(\lambda - \xi - b)\cdot(\lambda - \xi - b)\right). \end{array} \tag{5.9}$$

Taking ξ given by

$$\xi = (B-A)^{-1}\left(B(\lambda - b) - A(\lambda - a)\right)$$

implies that $A(\lambda - \xi - a) = B(\lambda - \xi - b)$, so the second term of (5.9) is a null lagrangian. Denoting by θ the average of χ in Y, we thus have

$$\begin{array}{rcl} W_{(\chi_i)}(\lambda) & = & 2\xi\cdot A(\lambda - \xi - a) + \theta\left(w_A + A(\lambda - \xi - a)\cdot(\lambda - \xi - a)\right) \\ & + & (1-\theta)\left(w_B + B(\lambda - \xi - b)\cdot(\lambda - \xi - b)\right) \\ & + & \displaystyle\min_{\phi\in H^1_\#(Y)^N} \int_Y (\chi A + (1-\chi)B)(\xi + e(\phi))\cdot(\xi + e(\phi)) dx \end{array} \tag{5.10}$$

The last term in (5.10) is, by definition of homogenization, equal to

$$A^*\xi \cdot \xi$$

where A^* is the homogenized Hooke's law corresponding to the periodic mixture of A and B corresponding to χ. Rewriting (5.10) as

$$W_{(\chi_i)}(\lambda) = m(\theta, \lambda) + A^*\xi \cdot \xi,$$

the quasiconvex envelope is thus

$$QW(\lambda) = \min_{0 \le \theta \le 1} \min_{A^* \in G_\theta} m(\theta, \lambda) + A^*\xi(\lambda) \cdot \xi(\lambda).$$

Although the G-closure set G_θ is still unknown, in a previous chapter we have computed the Hashin-Shtrikman lower bound which gives the value of

$$g(\theta, \xi) = \min_{A^* \in G_\theta} A^*\xi \cdot \xi.$$

Recall from Proposition 4.2.4 that the bound $g(\theta, \xi)$ is computed through a so-called non-local term which depends on the H-measure of the optimal tensor A^*. Therefore, the only relevant informations of the optimal microstructure in the relaxed formulation is its proportion θ and its H-measure. Explicit computations of $g(\theta, \xi)$ have been done in e.g. [7], [8], [4], [28], [29]. Finding in which case the optimal microstructures are actually optimal also for the original, non-relaxed, problem is discussed in [6], [9].

5.3 Second example.

We now assume that all phases have the same Hooke's law $A_i = A$, i.e. the original energy integrand is

$$W(\xi) = \min_{1 \le i \le p} \left(A(\xi - a_i) \cdot (\xi - a_i) + w_i \right).$$

This case was considered e.g. in [24], [36], [43], [55], [59]. Formula (5.8) simplifies as

$$\begin{aligned} W_{(\chi_i)}(\lambda) = & \min_{\phi \in H^1_\#(Y)^N} \int_Y \left(Ae(\phi) \cdot e(\phi) - 2Ae(\phi) \cdot \sum_{i=1}^p \chi_i a_i \right) dx \\ & + \sum_{i=1}^p \theta_i \left(w_i + A(\lambda - a_i) \cdot (\lambda - a_i) \right), \end{aligned} \tag{5.11}$$

where θ_i is the average of χ_i. The computation of (5.11) has already been performed in Lemma 4.3.1 for two wells $p = 2$. The computation is similar for more wells and the result is given in terms of the H-measure $\mu = (\mu_{ij})_{1\leq i,j\leq p}$ of the family of characteristic functions $(\chi_i)_{1\leq i\leq p}$. The result is

$$\begin{aligned} g(\theta,\mu) = & \min_{\phi\in H^1_{\#}(Y)^N} \int_Y \left(Ae(\phi)\cdot e(\phi) + 2Ae(\phi)\cdot \sum_{i=1}^p \chi_i a_i \right) dx \\ = & -\sum_{i,j=1}^p \int_{S_{N-1}} P_e(A^{1/2}a_i)\cdot A^{1/2}a_j\, m_{ij}(de) \end{aligned} \tag{5.12}$$

where P_e is a projection operator (depending on the unit vector e) defined on $\mathbb{R}^{N^2}$ as the orthogonal projection on the set $V(e)$ of rank-one matrices of the type

$$V(e) = \left\{ e\otimes v + v\otimes e,\ v\in \mathbb{R}^N \right\}.$$

The precise value of $g(\theta,\mu)$ is not important. However, (5.12) shows that $g(\theta,\mu)$ does not depend on a precise knowledge of the microstructure (χ_i), but just of its H-measure μ and its average θ. Thus, the quasiconvex envelope of W is

$$QW(\lambda = \min_{(\theta,\mu)} g(\theta,\mu) + \sum_{i=1}^p \theta_i \left(w_i + A(\lambda - a_i)\cdot(\lambda - a_i) \right),$$

where the minimization takes place over all $\theta = (\theta_1, ..., \theta_p)$ satisfying the constraints

$$\theta_i \geq 0, \text{ and } \sum_{i=1}^p \theta_i = 1,$$

and all H-measures $\mu = (\mu_{ij})_{1\leq i,j\leq p}$ of families of characteristic functions with averages θ (cf. section 3.2). Acording to Lemmas 3.2.3 and 3.2.4 the set of all such H-measures in known only in the case of two wells $p = 2$ (for $p > 2$ there are only necessary conditions on μ). Thus an explicit formula can be obtained only in the case $p = 2$ (see [36], [55]) and merely partial results are available if $p > 2$ (see [24], [36], [59]).

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