Higher Order Macro Coefficients in Periodic Homogenization

Carlos Conca
Departamento de Ingeniería Matemática, Facultad de Ciencias Físicas y Matemáticas,
Universidad de Chile and Centro de Modelamiento Matemático, UMR 2071 CNRS-UChile,
Casilla 170/3 - Correo 3, Santiago, Chile.

Jorge San Martín
Departamento de Ingeniería Matemática, Facultad de Ciencias Físicas y Matemáticas,
Universidad de Chile and Centro de Modelamiento Matemático, UMR 2071 CNRS-UChile,
Casilla 170/3 - Correo 3, Santiago, Chile.

Loredana Smaranda
Department of Mathematics, Faculty of Mathematics and Computer Science, University of
Pitești, 110040 Pitești, Str. Târgu din Vale Nr.1, Argeș, Romania.

Muthusamy Vanninathan
TIFR-CAM, Post Bag 6503, GKV Post, Bangalore - 560065, India.
E-mail: cconca@dim.uchile.cl, jorge@dim.uchile.cl, smaranda@dim.uchile.cl,
vanni@math.tifrbng.res.in

Abstract. A first set of macro coefficients known as the homogenized coefficients appear in
the homogenization of PDE on periodic structures. If energy is increased or scale is decreased,
these coefficients do not provide adequate approximation. Using Bloch decomposition, it is first
realized that the above coefficients correspond to the lowest energy and the largest scale. This
naturally paves the way to introduce other sets of macro coefficients corresponding to higher
energies and lower scales which yield better approximation. The next task is to compare their
properties with those of the homogenized coefficients. This article reviews these developments
along with some new results yet to be published.

1. Introduction
In this paper, we revisit the classical problem of homogenization of fine periodic structures
([1], [2], [3]) and report on some fundamental developments that have taken place recently.
In Homogenization Theory, a basic model problem regards such periodic structures as heat
conductors with fine heterogeneities in which heat conductivities vary rapidly. The main feature
in this problem is that the temperature field exhibits oscillations making realistic computations
very difficult. In general, Homogenization Theory [4] is a study of oscillations of physical fields
and one seeks tools and methods to describe these oscillations. Approximation to the physical
fields and heat conductivities at a macro scale is deduced as a consequence. This process
involves averaging of oscillations, **homogenized matrix** and **homogenized equation**. In periodic media, the oscillations of physical fields are somewhat restricted; they are created by periodic distribution of microstructures in the media. Yet, they are rich enough to exhibit a variety of phenomena which require sophisticated theory for their understanding. They provide a fertile ground to study the dependence of physical fields on the coefficients of the equation, and on the microstructure, in particular. Another importance of periodic media is that arbitrary heterogeneous structures can be locally approximated by periodic ones since the homogenization process itself is local in this case.

In the periodic setting, there are many methods of homogenization [5]. Our contribution [6] is a spectral approach based on Bloch Waves. One of the advantages of our method is that it enables us to go beyond the homogenized matrix and introduce other macro coefficients in a systematic manner. We call them **higher order macro coefficients**. While the usual homogenized coefficients correspond to the approximation at the lowest energy and the largest scale, the higher order macro coefficients correspond to higher energy or smaller scales, as we shall see. Naturally, these higher order macro coefficients are useful in the study of finer aspects of oscillations.

Let us now give the plan of this write-up. In Section 2, after formally introducing periodic homogenization problem, we give the conventional definition of the homogenized matrix as well as our principal example of two-phase conducting composite. We realize immediately that it is not clear how to generalize this definition to introduce its higher order version. Our main tool to overcome this difficulty is Bloch waves which are introduced in Section 3. Section 4 establishes the connection between Bloch waves and homogenization and this paves the way to define higher order macro coefficients. Main results of this paper are included in Section 5; they compare the properties of homogenized coefficients and their higher order version. In particular, we will define higher order analogues of two prominent homogenized coefficients in the case of two-phase conductors, namely the Arithmetic Mean and the Harmonic Mean. Section 6 ends the article with conclusions and perspectives.

## 2. Periodic Structures and Homogenization

Starting with the basic reference cell $Y = [0, 2\pi]^N \subset \mathbb{R}^N$, one can tile the entire space $\mathbb{R}^N$ by integer translations of the cell $Y$. This defines the periodic structure in unit scale in which the independent variable is denoted by $y$. We can increase the complexity of the structure by considering the rescaled periodic tiling with period $2\pi \varepsilon$ where $\varepsilon > 0$ is a small parameter. The corresponding independent variable is denoted by $x$ and we note the scaling relation $y = \varepsilon x$. We would like to view these structures as heat conductors. To this end, we introduce conductivity matrix $a(y) = (a_{kl}(y))$ of order $N \times N$ enjoying the following properties:

- $a(y)$ is $Y$-periodic: $a(y + 2\pi p) = a(y)$ $\forall p \in \mathbb{Z}^N$,
- $a(y)$ is symmetric,
- For some $\alpha > 0$, $a(y) \eta \cdot \eta \geq \alpha |\eta|^2$ $\forall \eta \in \mathbb{R}^N$ (uniform positive definiteness),
- For some $M$, $|a_{kl}(y)| \leq M$ (uniform boundedness).

The corresponding $\varepsilon$-scaled conductivity matrix is denoted by $a^\varepsilon(x) = a(\frac{x}{\varepsilon})$. Steady state heat conduction in such media is governed by the following elliptic operators in divergence form:

$$Au \equiv -\frac{\partial}{\partial y_k} \left(a_{kl}(y) \frac{\partial u}{\partial y_l}\right),$$

$$A^\varepsilon u^\varepsilon \equiv -\frac{\partial}{\partial x_k} \left(a_{kl}(\frac{x}{\varepsilon}) \frac{\partial u^\varepsilon}{\partial x_l}\right).$$
These operators represent periodic structures in the same way as Laplace operator did for homogeneous media.

**Example** (Two - Phase conductor). Let $\alpha_0 > 0, \alpha_1 > 0$ represent the conductivities and let $0 < \gamma < 1$. We define the conductivity matrix by $a_{kl}(y) = a(y)\delta_{kl}$ with $a(y) = \alpha_1\chi_T(y) + \alpha_0\chi_{Y\setminus T}(y)$. Here $T \subset Y$ is a measurable subset and $\gamma = \frac{|T|}{|Y|}$. In other words, we have two phases $(\alpha_0, \alpha_1)$ in volume proportions $(1 - \gamma, \gamma)$ respectively in our heat conductor. We call the arrangement of the subset $T$ inside $Y$, alternatively, the characteristic function $\chi_T$, as the microstructure of the two-phase medium.

One of the fundamental questions of Homogenization Theory can now be phrased as follows: Consider oscillating temperature fields $\{u^\varepsilon\}$ with weak limit (average) $u$ as $\varepsilon \to 0$. Their oscillations are restricted by

$$\int_{\mathbb{R}^N} |u^\varepsilon|^2 + \int_{\mathbb{R}^N} |\nabla u^\varepsilon|^2 \leq c,$$

$$A^\varepsilon u^\varepsilon = f \text{ in } \mathbb{R}^N.$$  

Here the constant $c > 0$ and the heat source density $f$ are independent of $\varepsilon$. Under the above conditions, one wishes to describe the oscillations in $u^\varepsilon$ as $\varepsilon \to 0$; in particular, one is interested in the equation satisfied by $u$. The real issue involved is to compute the weak limit (average) of the heat fluxes

$$a_{kl}(\varepsilon) \frac{\partial u^\varepsilon}{\partial x_k}(x), \quad k = 1, 2, \ldots, N.$$

Taking averages of nonlinear functionals of oscillating quantities being not easy, one can easily appreciate the difficulties involved in this homogenization problem which requires the average of the above quadratic functional. These were first overcome and the equation satisfied by $u$ was found in [7].

The pioneering approach in [4] solves this problem in two steps. In the first, one shows that the limit of Fourier materials is a material of same type. More precisely, one shows that the (weak) limit of the heat flux is of the form $q_{kl} \frac{\partial u}{\partial x_k}$ for some constant matrix $q = (q_{kl})$, called the homogenized matrix. This is a general phenomenon going well beyond periodic microstructures. In particular, this step shows the existence of a composite medium which is really a mixture of several individual phases with given volume proportions and with arbitrary micro-geometry of mixing. The underlying mathematical theory is the so-called compensated compactness. For a nice account of this, see [4].

In the second step, one computes the matrix $q$ by placing the periodic medium in the temperature field $\eta \cdot y$ and computing the average of the resulting heat flux [4]. This amounts to solving the following cell test problem:

$$Aw = 0 \text{ in } \mathbb{R}^N, \quad w(y) - \eta \cdot y \text{ is } Y\text{-periodic}.$$  

Then the homogenized matrix $q$ is given by

$$q\eta = \langle a(y)\nabla w(y) \rangle \quad \forall \eta \in \mathbb{R}^N,$$

where the angle brackets represent average over the periodic cell $Y$. Alternatively, setting $\chi^{(1)}(y) = w(y) - \eta \cdot y$, we see that the cell test function $\chi^{(1)}$ satisfies

$$A\chi^{(1)} = \eta \frac{\partial a_{kl}}{\partial y_k}(y), \quad \chi^{(1)} \text{ is } Y\text{-periodic}.$$
Further, the homogenized matrix $q$ can be expressed in terms of $\chi^{(1)}$ as follows:

$$q\eta = \langle a(y) \nabla(\chi^{(1)} + \eta \cdot y) \rangle \quad \forall \eta \in \mathbb{R}^N.$$ 

Apart from the explicit dependence on the microstructure via $a(y)$, the homogenized matrix $q$ depends on the microstructure implicitly through the cell test function $\chi^{(1)}$. In the sequel, it will be convenient to express $\chi^{(1)}$ as a linear superposition of $\chi_l$, $l = 1, 2, \ldots, N$ : $\chi^{(1)} = \eta_l \chi_l$,

where $\chi_l$ is solution of

$$A\chi_l = \frac{\partial a_{kl}}{\partial y_k}(y), \quad \chi_l \text{ is } Y\text{-periodic.}$$

Finally, combining the two previous steps, we conclude that the weak limit $u$ satisfies the homogenized equation:

$$Qu \equiv -\frac{\partial}{\partial x_k} \left( q_{kl} \frac{\partial u}{\partial x_l} \right) = f \text{ in } \mathbb{R}^N.$$ 

3. Bloch Waves

In this section, we briefly sketch the Bloch waves associated with the periodic structure and the operator $A$ on it. Some of the original references in the subject are [8], [9], [10]. For further details, the interested reader is referred to our papers on Bloch waves and their applications cited in the list of References.

Just as plane waves/Fourier waves $\{e^{iy\eta}; \eta \in \mathbb{R}^N\}$ form an orthonormal basis (in a generalized sense) in homogeneous media, Bloch waves form an orthonormal basis of eigenvectors of $A$ in periodic media. To introduce them as a generalization of plane waves, let us recall the property characterizing the plane waves; namely they are common eigenvectors for all general non-periodic microstructures admitting an invariance group.

To rephrase $($\eta,Y$)$ periodicity condition, there are advantages: it points to a way of treating general non-periodic microstructures admitting an invariance group.

Finally, combining the two previous steps, we conclude that the weak limit $u$ satisfies the homogenized equation:

$$Qu \equiv -\frac{\partial}{\partial x_k} \left( q_{kl} \frac{\partial u}{\partial x_l} \right) = f \text{ in } \mathbb{R}^N.$$ 

Since $($\eta,Y$)$ periodicity condition is invariant if we replace $\eta$ by $\eta + q, q \in \mathbb{Z}^N$, it is enough to restrict $\eta$ in the dual cell $Y' = [ -\frac{1}{2}, \frac{1}{2} ]^N$. Undoubtedly, the novelty of the above system is the periodicity condition. One can offer one more explanation for it, based on the Theory of Group Representations. In fact, the microstructure being periodic, has invariance group $\mathbb{Z}^N$ which is abelian. According to the general theory [11], all its irreducible unitary representations are one-dimensional and given by its characters. Though this may be a more abstract way of rephrasing $($\eta,Y$)$ periodicity condition, there are advantages: it points to a way of treating general non-periodic microstructures admitting an invariance group.

By means of the change of variables $\psi(y, \eta) = e^{iy\eta} \phi(y, \eta)$, the above problem is transformed to the following one:

$$A(\eta)\phi = \lambda(\eta)\phi \text{ in } \mathbb{R}^N,$$

where we see the appearance of the translated operator:

$$A(\eta) \equiv -\left( \frac{\partial}{\partial y_k} + i\eta_k \right) \left\{ a_{kl}(y) \left( \frac{\partial}{\partial y_l} + i\eta_l \right) \right\}.$$
Spectral theory of compact self-adjoint operators applies here. It shows that the operator $A(\eta)$ can be diagonalized in an orthonormal basis $\{\phi_m(y,\eta); m \in \mathbb{N}\}$ with the corresponding eigenvalues $\{\lambda_m(\eta); m \in \mathbb{N}\}$.

Finally to get the spectral decomposition of $A$ in $\mathbb{R}^N$, it is enough to put the previous elements together by varying $\eta$ continuously in the dual cell $Y' = [-\frac{1}{2}, \frac{1}{2}]^N$. This process gives rise to what is known as Bloch decomposition of functions, analogous to the classical Fourier decomposition. Roughly speaking, any square integrable function $f(y)$ defined on $\mathbb{R}^N$ can be expressed as a superposition of basis functions $\{\phi_m(y,\eta) e^{i m \cdot \eta}; \eta \in Y', m \in \mathbb{N}\}$, each of which is an eigenvector for $A$. The coefficients appearing in this superposition are called Bloch coefficients which are analogous to Fourier coefficients. Finally, the above decomposition is unitary, i.e., it preserves the respective norms. For details, see for instance [6].

### 4. Bloch waves, Homogenization and Macro Coefficients

Though not evident, somewhat surprising connections exist between homogenization and Bloch waves and our idea is to exploit them further and introduce macro coefficients at various orders. Roughly speaking, Bloch eigenvalue problem introduced in the last section contains a wealth of information about the periodic structure; in particular, its infinitesimal versions at $\eta = 0$ yield information on homogenization. To make this statement more meaningful, we need to make a few observations.

Consider the parametrized eigenvalue problem for the translated operator $A(\eta)$ written down in the last section. Even though $A(\eta)$ depends quadratically on $\eta$, it does not imply any regularity beyond Lipschitz property of its eigenvalues $\{\lambda_m(\eta); m \in \mathbb{N}\}$ with respect to $\eta$. This is because eigenvalues may coalesce as $\eta$ varies and become degenerate. However miracle occurs at $\eta = 0$. Indeed, when $\eta = 0$, the first eigenvalue $\lambda_1(0) = 0$ of $A(0) = A$ is simple with eigenvectors being constants. Under such circumstances, regular perturbation theory of Kato-Rellich ([12], [13]) can be applied to show that for a suitable choice of first eigenvector $\phi_1(y,\eta)$, the map $\eta \mapsto (\lambda_1(\eta), \phi_1(y,\eta))$ is analytic near $\eta = 0$. Further, starting from “initial condition” $(\lambda_1(0), \phi_1(y,0))$, one can compute all Taylor coefficients by differentiating the eigen-equation successively and evaluating at $\eta = 0$. In this way, one shows that (see [6]):

- All odd order derivatives of $\lambda_1(\eta)$ at $\eta = 0$ vanish; thus we have
  \[ \lambda_1(\eta) = \frac{1}{2!} \lambda_1^{(2)}(0) \eta^2 + \frac{1}{4!} \lambda_1^{(4)}(0) \eta^4 + \frac{1}{6!} \lambda_1^{(6)}(0) \eta^6 + \cdots \]

- Taylor coefficient $\frac{1}{2!} \lambda_1^{(2)}(0)$ coincides with the homogenized matrix $q$ (see [14]).

- First order derivatives of the first eigenvector coincide with the cell test functions introduced in Section 2:
  \[ \frac{\partial \phi_1}{\partial \eta}(y,0) = i \chi_l(y), \quad l = 1, 2, \ldots, N. \]

Above results lead to the following nice spectral interpretation of homogenization process: since Bloch waves diagonalize $A$ with eigenvalues $\{\lambda_m(\eta); m \in \mathbb{N}, \eta \in Y'\}$, we have a nice decomposition of the operator $A$ on the periodic structure in terms of discrete energy levels $m \in \mathbb{N}$ and continuous (quasi) momentum $\eta \in Y'$. Homogenization approximation corresponds to the lowest energy level $m = 1$ and the lowest momentum $\eta = 0$ or equivalently the largest length scale.

Above interpretation shows two directions to proceed further.

**Direction 1.** (High Energy Homogenization). One can rise the energy level and fix it at an arbitrary value $m \in \mathbb{N}$ and seek homogenization approximation at that level. This leads entirely
to a new set of structural conditions on the periodic structure under which one can perform homogenization [15]. They are as follows:

(a) $\eta = 0$ is the minimizer of $\lambda_m(\eta)$ as $\eta$ varies over the dual cell and it is unique:

$$\lambda_m(0) = \min \{ \lambda_m(\eta) : \eta \in Y' \}.$$ 

(b) $\lambda_m(0)$ is a simple eigenvalue of the operator $A(0) = A$.

(c) The Hessian matrix $\lambda_m^{(2)}(0)$ is positive definite.

When $m = 1$, all the above conditions (a) - (c) are automatically satisfied. When $m > 1$, they need not be satisfied and we need to postulate them. If they are not satisfied, new physical phenomena appear ([16], [17]). For instance, if the condition (c) above is not satisfied, we have loss of convexity of $\lambda_m(\eta)$ at $\eta = 0$. This leads to a leakage of energy from the $m^{th}$ mode to other modes and as a consequence, the homogenized limit will not be a scalar equation, but it is a system coupling all these modes. However, if the above conditions are satisfied, one can prove a homogenization theorem involving only the $m^{th}$ mode and show that the homogenized matrix at the energy level $m \in \mathbb{N}$ is given by $\frac{1}{n!} \lambda_m^{(2)}(0)$. The main difficulty at high energy levels is that the factorization principle is not valid; that is, the eigenvector $\phi_m(y, 0)$ need not conserve a constant sign. This principle states roughly that if the eigenvector keeps a constant sign, it can be factorized out, giving place to a simpler problem to homogenize. High energy homogenization problems do not fall in this class. To overcome this difficulty, we exploit Bloch decomposition along with the above structural conditions and the notion of two-scale convergence [18] to carry out homogenization process. See [15] for details. It is an open problem to translate the above conditions (a) - (c) concretely in terms of microstructures in the physical space.

**Direction 2.** (Homogenization with smaller scales) We start with the remark that one approximates $\lambda_1(\eta)$ by $\frac{1}{2} \lambda_1^{(2)}(0) \eta^2$ in the homogenization process. Now, one maintains the energy level at $m = 1$ and decreases the length scale to have a closer look at the effects of microstructure, that is, one increases slightly the value of $|\eta|$ to the extent that $\frac{1}{2} \lambda_1^{(2)}(0) \eta^2$ is no more a good approximation for $\lambda_1(\eta)$ and we need the next term of the Taylor expansion to have a good approximation:

$$\lambda_1(\eta) \approx \frac{1}{2} \lambda_1^{(2)}(0) \eta^2 + \frac{1}{4!} \lambda_1^{(4)}(0) \eta^4.$$ 

In such situations, one observes that the homogenized matrix $q$ alone is not good enough to provide a good approximation to the inhomogeneous medium at the energy level $m = 1$ and the chosen length scale. We need the $4^{th}$ order tensor $d = \frac{1}{4!} \lambda_1^{(4)}(0)$ also. Indeed, let us consider the periodic medium with fine microstructure described by $A^\varepsilon$ introduced in Section 2. The first Bloch eigenvalue on this structure satisfies the scaling relation: $\lambda_1^\varepsilon(\xi) = \varepsilon^{-2} \lambda_1(\varepsilon \xi)$. Expanding this around $\xi = 0$, we get

$$\lambda_1^\varepsilon(\xi) = \frac{1}{2!} \lambda_1^{(2)}(0) \xi^2 + \frac{1}{4!} \varepsilon^2 \lambda_1^{(4)}(0) \xi^4 + \frac{1}{6!} \varepsilon^4 \lambda_1^{(6)}(0) \xi^6 + \cdots.$$ 

Consider now the problem of acoustic wave propagation in such a medium with well-prepared initial conditions at energy level $m = 1$:

$$v_\varepsilon^{\xi} + A^\varepsilon v_\varepsilon = 0 \text{ in } \mathbb{R}^N \times \mathbb{R},$$

$$v_\varepsilon^{\xi}(x, 0) = \phi_1 \left( \frac{x}{\varepsilon}, 0 \right) v_0(x),$$
\[ v^l(x, 0) = \phi_1 \left( \frac{x}{\varepsilon}, 0 \right) v_1(x). \]

Since the size of the microstructure and the wave length of propagating waves are of same order, there is a resonant interaction between them. Thus, homogenization process and Bloch waves play a role in this propagation problem. For waves satisfying \( |\xi| = o(\varepsilon^{-\frac{1}{2}}) \), we see that \( \varepsilon^2|\xi|^4 = o(1) \) which shows that all terms in the expansion except the first one can be neglected and so the usual homogenized medium provides a good description of propagation of such waves. For shorter waves satisfying \( |\xi| = o(\varepsilon^{-\frac{3}{2}}) \), we have \( \varepsilon^4|\xi|^6 = o(1) \) and \( \varepsilon^2|\xi|^4 = o(\varepsilon^{-\frac{3}{2}}) \) and so we cannot neglect the first term as well as the second one for reasonable approximation. Thus both \((q, d)\) are relevant for the approximate description of propagation of such short waves. To see the consequence, let us focus on the one-dimensional case, for simplicity. According to the above discussion, we have the approximation

\[ A^\varepsilon \approx -q d^2 dx^2 + \varepsilon^2 d^4 dx^4. \]

The presence of 4th order derivatives signifies that the short waves under consideration undergo dispersion, a feature not captured by the homogenized operator. This dispersion effect is due to the decrease of scales.

Taking together the two directions described above, we have a general picture of periodic structures: Derivatives of various orders of eigenvalues \( \lambda_m(\eta) \) at \( \eta = 0 \) (if they exist) provide macro coefficients associated with the periodic structure at various orders of scales. Similarly, derivatives of various orders of eigenvectors \( \phi_m(y, \eta) \) at \( \eta = 0 \) (if they exist) yield different cell test functions containing hierarchy of information about the microstructure. Viewing through Bloch decomposition, we see that at each energy level \( m \in \mathbb{N} \), there is a sequence of intermediate scales indexed by \( l \in \mathbb{N} \) ranging from the macroscopic level (at which the usual homogenization is done) up to the scale corresponding to microstructure. Taking \( m = 1 \) for instance, for each such scale \( l \in \mathbb{N} \), there is a new macro coefficient given by the \( (2l)^{th} \) order derivative of \( \lambda_1(\eta) \) at \( \eta = 0 \) which incorporates the microstructure information through the cell test functions defined by derivatives of \( \phi_1(y, \eta) \) at \( \eta = 0 \) up to order \( l \). The new tensors which emerge out of the above picture, namely \( q_m = \frac{1}{2l} \lambda_m^{(2l)}(0) \), \( d = \frac{1}{2l} \lambda_1^{(4)}(0) \) etc. are called higher order macro coefficients.

In the sequel, we pursue the Direction 2 and report on the results obtained. When \( m = 1 \), because of analyticity, all derivatives of \( \lambda_1(\eta) \) and \( \phi_1(y, \eta) \) exist at \( \eta = 0 \). Thus the existence question regarding macro coefficients is settled and we focus on their properties.

**Example:** Before proceeding to the next section, let us consider the example of homogeneous medium defined by the conductivity matrix \( a_{kl}(y) \equiv \delta_{kl} \). In this case, the Bloch waves are naturally indexed by \( m \in \mathbb{Z}^N \), they are independent of \( \eta \) and given by \( \phi_m(y, \eta) = e^{imv.y} \). The associated eigenvalues are quadratic and given by \( \lambda_m(\eta) = |m + \eta|^2 \) \( \forall m \in \mathbb{Z}^N \). Further, the cell test functions \( \chi^{(1)} \), \( \chi^{(2)} \) are all constants and consequently, the homogenized matrix and their higher order versions are trivially found to be

\[ q = I, \quad q_m = I, \quad d = 0. \]

**5. Properties of Macro Coefficients**

This is the main part of this article, which recalls some properties of the homogenized matrix \( q \) and gives parallel developments about the tensor \( d \). For a detailed study of \( q \), see [19], [20] or [21]. Our presentation will highlight the differences between \( q \) and \( d \). As is evident from two-phase conductors, these quantities depend on conductivities of individual phases and more importantly on the microstructure (e.g.: their volume proportions and other statistical measures). Motivated by applications in Optimal Design Problems, the goal of the theory is to bring out
the dependence on the microstructure in its entirety at various intermediate scales mentioned in the previous section. Our results are mainly in the form of bounds on these macro quantities valid independent of microstructure or at best depending on volume proportions of phases.

5.1. Spatial Representation
For \((q,d)\), we already have a representation in the (energy-momentum) space:

\[
q = \frac{1}{2!} \lambda_1^{(2)}(0), \quad d = \frac{1}{4!} \lambda_1^{(4)}(0).
\]

In order to bring out their dependence on the microstructure, it is essential that we seek spatial representation for them. In the case of \(q\), we saw such a representation, namely a spatial average in Section 2. Let us recall it here:

\[
q_\eta = \left\langle a(y) \nabla (\chi^{(1)} + \eta \cdot y) \right\rangle
\]

which can be used to deduce an expression for the quadratic form associated with \(q\):

\[
q_\eta^2 = q_\eta \cdot \eta = \left\langle a(y) \nabla (\chi^{(1)} + \eta \cdot y) \cdot \nabla (\chi^{(1)} + \eta \cdot y) \right\rangle \quad \forall \ \eta \in \mathbb{R}^N,
\]

from which bounds below follow at once

\[
\min \{|a(y)|; y \in Y\} \leq q \leq \max \{|a(y)|; y \in Y\}.
\]

In particular, \(q\) is positive definite. These results are classical and well-known in the literature. What is perhaps not well-known is that an analogous representation exists for the tensor \(d\). In fact, the corresponding 4\textsuperscript{th} order form is given by [22]:

\[
d_\eta^4 = -\left\langle a(y) \nabla (\chi^{(2)} - \frac{1}{2} (\chi^{(1)})^2) \cdot \nabla (\chi^{(2)} - \frac{1}{2} (\chi^{(1)})^2) \right\rangle \quad \forall \ \eta \in \mathbb{R}^N.
\]

Here appears a new cell test function \(\chi^{(2)}\) capturing more information on the microstructure, and it is defined as follows: \(\chi^{(2)}\) is \(Y\)-periodic and satisfies

\[
-\text{div}(a(y)\nabla \chi^{(2)}) = (a(y) - q)\eta^2 + a(y)\nabla \chi^{(1)} \cdot \eta + \text{div}(a(y)\eta \chi^{(1)}).
\]

As one may expect, \(\chi^{(2)}\) is related to the second order derivatives of \(\phi_1(y,\eta)\) with respect to \(\eta\) at \(\eta = 0\). An immediate consequence of above representation is the following universal sign for \(d\) independent of microstructure:

\[
d_\eta^4 \leq 0, \quad \forall \eta \in \mathbb{R}^N.
\]

This result is somewhat surprising because one does not expect the tensor \(d\) to have a sign at this generality. Secondly, the sign of \(d\) is opposite to that of \(q\). One may ask whether the next order macro tensor \(\frac{1}{6!} \lambda_1^{(6)}(0)\) keeps a non-negative sign. Unfortunately, this is not so [23].

Another observation on the above representation is the following: while \(q\) depends on the microstructure implicitly through \(\chi^{(1)}\), the dependence of \(d\) is through both \((\chi^{(1)}, \chi^{(2)})\). Further, the representation for \(d\) contains some nonlinear terms signifying interaction between the scales including a self interaction term \((\chi^{(1)})^2\). This is a new feature which is absent in \(q\).
5.2. One Dimensional Results
Let us consider the case of conductors with two-phases \( \{\alpha_0, \alpha_1\} \) in proportions \( \{1 - \gamma, \gamma\} \). In this case, it is well-known that the value of the homogenized coefficient (which is a scalar) remains fixed at the Harmonic Mean of \( \{\alpha_0, \alpha_1\} \) as microstructure varies:

\[
\frac{1}{q} = \frac{1 - \gamma}{\alpha_0} + \frac{\gamma}{\alpha_1}.
\]

In contrast, as we shall see, (the scalar) \( d \) shows rich variation with the microstructure. In such a case, one would like to exploit the negativity of \( d \) in optimization problems involving microstructures. This begs the following questions: how negative \( d \) can be when microstructure varies? To answer this, we must minimize \( d \) over microstructures. Is the minimizing microstructure classical or generalized/relaxed one? What is the minimum value? In the present one dimensional case, we provide complete answers to these questions. In multi-dimensional problems, these questions remain open, in general. Let us state our precise results.

**Theorem** ([25]) Under the above situation, we have

(i) The minimum value of \( d \) is given by

\[
\min d = -\frac{1}{12} |Y|^2 q^3 \gamma^2 (1 - \gamma)^2 \left( \frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2.
\]

(ii) The maximum value of \( d \) is zero.

(iii) The minimizer is unique upto translations and is given by the following classical microstructure: the phases \( \{\alpha_0, \alpha_1\} \) occupy intervals of lengths \( \{(1 - \gamma)|Y|, \gamma|Y|\} \) inside \( Y \).

(iv) The maximizer is also unique and is given by the following generalized/relaxed microstructure: the phases \( \{\alpha_0, \alpha_1\} \) are present everywhere with uniform local proportions \( \{1 - \gamma, \gamma\} \) at every point \( y \).

(v) The values of \( d \) over classical microstructures range over the entire interval \([\min d, \max d]\).

(vi) \( d \) has the monotonicity property: more interfaces between the two phases in the microstructure, the higher the value of \( d \).

Let us make several remarks on the above Theorem. One general lesson learnt from the above Theorem is the following: many complicated microstructures may be associated with a particular value of \( q \); however when \( d \) is considered along with \( q \), a particularly simple microstructure is chosen among them as minimizer for \( d \). This remarkable property is stated in (iii) above in the one dimensional case. The minimum value \( d \) is a curious combination of \( \langle|Y|, \gamma, \alpha_0, \alpha_1\rangle \). Unlike the Harmonic Mean, it is not clear how this is related to the standard statistical quantities associated with the microstructure. In optimization problems involving microstructures, the optimizers are, in general, generalized/relaxed microstructures. It is exceptional here that one finds the minimizer to be a classical microstructure. This is due to the monotonicity property of (vi): At its minimum value, \( d \) has just two interfaces between the two phases \( \{\alpha_0, \alpha_1\} \), whereas \( d \) has a continuum of interfaces at its maximum value. These properties could be exploited in high contrast materials to produce ones with negative index, particularly at scales where \( d \) is significant. Finally, it is surprising to see continuous variation of \( d \) over periodic classical microstructures: \( d \) assumes all intermediate values between its minimum and its maximum. This is very different from the behaviour of \( q \). In one-dimension, its value does not change at all and remains fixed at the Harmonic Mean. In higher dimensions, the eigenvalues of \( q \) over all periodic microstructures are merely dense in the corresponding set over arbitrary microstructures [20].

Let us say a few words about the proof of the above result. First of all, two simplifications occur in the physical space representation formula for \( d \), given in Subsection 5.1. Dependence of
on the microstructure through the cell test function $\chi^{(2)}$ can be taken into account explicitly and thus $\chi^{(2)}$ can be eliminated. Similarly, the self-interaction term also disappears from the scene yielding a simple representation formula for $d$ ([22]) :

$$d = -q \langle v^2 \rangle,$$

where $v$ is defined more directly in terms of microstructure via

$$-\frac{dv}{dy} = 1 - q \left( \frac{\chi_T(y)}{\alpha_1} + \frac{1 - \chi_T(y)}{\alpha_0} \right)$$

in $\mathbb{R}$, $v$ is $Y$-periodic.

Observe that the minimization problem for $d$ has the structure of Optimal Control Problem with microstructures being controls and the equation for $v$ as the state equation and $d$ as the cost functional. As usual, the main difficulty in minimization problems over microstructures is the non-convexity.

In the problem at hand, we see non-convexity at two places. One is the non-convexity of the constraint set on controls: convex combination of characteristic functions need not be a characteristic function. This can be rectified by replacing the original problem by its relaxed version in which characteristic functions are replaced by local density functions $0 \leq \theta(y) \leq 1$, which are weak limits of characteristic functions. This process called relaxation does not alter the minimum value of the problem. For a general description of relaxation procedures in optimal design problems, the reader may refer to [24], for instance. The second source of non-convexity is in the functional to be minimized and this is more serious. The major technical point of our paper [25] is to show how to overcome this difficulty. Last but not least, one exploits the fact that one-dimensional minimal microstructures cannot display complicated patterns. For instance, any open set in $\mathbb{R}$ is a countable union of open intervals. Various covering theorems show that this is not the case in multi-dimensions.

In the proof of above theorem, we follow the usual procedure for solving Optimal Control Problems. We derive first order optimality conditions which are necessary at minimum. This is formulated in terms of the state and the adjoint state. This reduces greatly the set of possible minimizers. The task of finding the minimizer is reduced to comparing the values of the cost functional on the above set. An informed guess for the minimizer enables us to finish the proof.

5.3. Bounds on Laminates

Let us now consider the multi-dimensional case of a two-phase conductor with phases $\{\alpha_0, \alpha_1\}$ in given proportions $\{1 - \gamma, \gamma\}$. A celebrated theorem describes the variation of the eigenvalues of the homogenized matrix $q$ as the microstructure varies. More precisely, the eigenvalues $\{\mu_j\}$ of $q$ are characterized by the following bounds (assuming $\alpha_0 > \alpha_1$) :

$$\mu-(\gamma) \leq \mu_j \leq \mu+(\gamma),$$

$$\sum_{j=1}^{N} \frac{1}{\mu - \alpha_1} \leq \frac{1}{\mu-(\gamma) - \alpha_1} + \frac{N - 1}{\mu+(\gamma) - \alpha_1},$$

$$\sum_{j=1}^{N} \frac{1}{\alpha_0 - \mu_j} \leq \frac{1}{\alpha_0 - \mu-(\gamma)} + \frac{N - 1}{\alpha_0 - \mu+(\gamma)}.$$

Here, we have used the following notations for the Arithmetic and Harmonic Means:

$$\mu+(\gamma) = (1 - \gamma)\alpha_0 + \gamma\alpha_1,$$
\( \frac{1}{\mu_-(\gamma)} = \frac{1 - \gamma}{\alpha_0} + \frac{\gamma}{\alpha_1}. \)

Above result has a long history of developments. Many authors have made their contributions. K. Lurie and A. Cherkaev are some of the original contributors [26], [27], [28], [29]. The reader can also refer to [4] for proofs based on compensated compactness and H-measures. Obtaining such a characterization for the tensor \( d \) is a far away dream.

In the above description, laminates play a crucial role. Indeed, they are optimal microstructures for \( q \) in the sense that the eigenvalues of \( q \) on laminates provide upper and lower bounds for the eigenvalues of \( q \) on arbitrary microstructures.

In this subsection, our attention turns to multi-dimensional aspects of macro coefficients by studying their variation on laminates. One of the first phenomena which comes to our mind is the direction-dependence of physical properties, i.e., lack of isotropy at the macro scale even when the materials at microstructure level are isotropic. In particular, we are aware of different longitudinal and transverse behaviour in laminates. Further, there is no interaction between longitudinal and transverse modes in these structures. Somewhat surprisingly, this is no more true when we decrease the scale, as seen below.

The first task in our endeavour is to find a replacement which will play the role of eigenvalues. In this context, let us recall that bounds on eigenvalues of a symmetric matrix such as \( q \) are equivalent to the bounds on the associated quadratic form \( q \eta^2 = q_{kl} \eta_k \eta_l \). This motivates us to consider the quartic form \( d \eta^4 \equiv d_{ijkl} \eta_k \eta_j \eta_l \eta_l \) associated to the 4th order tensor \( d \) and study its variation on laminated microstructures. Another reason for considering the quadratic or quartic form is to capture direction-dependent phenomena.

**Periodic laminates**, by definition, correspond to the following choice of the conductivity matrix: \( a_{kl}(y) = a(y) \delta_{kl} \) with \( a(y) = a(y_1) \) which is \( 2\pi \)-periodic function of a single variable. Further, since we are considering two-phase media, we have

\[
a(y_1) = \alpha_0 \chi_{T} - \alpha_1 \chi_{T}(y_1), \quad \text{with} \quad \gamma = \frac{|T|}{|Y|}.
\]

It is implicitly assumed that \( T \) as a subset of the basic reference cell \( Y \) has one-dimensional structure: \( T = T_1 \times [0, 2\pi]^{N-1} \) where \( T_1 \) is an arbitrary measurable subset of \([0, 2\pi]\). Examples include vertical strips and their unions. Note that there are two types of directions in this microstructure: parallel (longitudinal) and perpendicular (transverse) directions to lamination. Accordingly, we split the (momentum) variable \( \eta = (\eta_1, \tilde{\eta}) \) with \( \eta_1 \in \mathbb{R}, \tilde{\eta} = (\eta_2, \eta_3, \ldots, \eta_N) \in \mathbb{R}^{N-1} \).

As before, the aim is to study the variation of \((q, d)\) as the laminated microstructure \( T \) varies inside the basic cell \( Y \), assuming that the volume proportion \( \gamma = \frac{|T|}{|Y|} \) remains fixed. Here are our results:

**Theorem** Under the above situation, we have

(i) the value \( q \eta^2 = q_{kl} \eta_k \eta_l \) remains fixed at

\[
q \eta^2 = \mu_-(\gamma) \eta_1^2 + \mu_+(\gamma) \tilde{\eta}^2 \quad \forall \eta \in \mathbb{R}^N,
\]

as microstructure varies.

(ii) The minimum value of \( d \eta^4 = d_{klmn} \eta_k \eta_l \eta_m \eta_n \) is given by

\[
\min d \eta^4 = -\frac{1}{12} |Y|^2 \gamma^2 (1 - \gamma^2 (\mu_-(\gamma)))^{-1} \left( \left( \mu_-(\gamma) \right) \eta_1^2 \left( \frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) + |\tilde{\eta}|^2 (\alpha_1 - \alpha_0) \right)^2.
\]
(iii) The maximum value of $d\eta^4$ is zero.

(iv) As microstructure varies among classical laminates, $d\eta^4$ fills up the entire interval $[\min d\eta^4, \max d\eta^4]$.

(v) Minimizer for $d\eta^4$ exists and is unique up to translations. It is the classical laminate consisting of a single vertical strip inside $Y$.

(vi) Maximizer for $d\eta^4$ exists and is unique. It is however a relaxed laminated microstructure defined by the local density $a(y_1) \equiv \gamma \forall y_1 \in [0, 2\pi]$.

A few remarks about the previous Theorem are in order. It is a natural generalization of our one-dimensional result in Section 5.2; indeed, if $\tilde{\eta} = 0$, the above result is reduced to the result in one dimension. Thus all our remarks on one-dimensional results of Subsection 5.2 hold good. So we comment only on additional features here. The statement (i) of the above Theorem is rephrasing the well-known fact, namely the conductivities in the transverse and the longitudinal directions are given by the Harmonic and the Arithmetic Means respectively. Further, there is no interaction between the two modes. Because of the presence of the cross term in statement (ii), there is interaction between the longitudinal and the transverse modes in the case of higher order macro coefficient $d$. This is a new phenomenon occurring because of the decrease of scale. The origin of this macro phenomenon lies in the presence of interaction terms $(\chi^{(1)})^4, \chi^{(2)}(\chi^{(1)})^2$ etc. in the spatial representation formula for $d$. (Section 5.1).

Finally, taking successively one after the other $\tilde{\eta} = 0$ or $\eta_1 = 0$ in the statement (ii), and comparing it with the statement (i), we realize that the quantities

$$-\frac{1}{12}|Y|^2\gamma^2(1-\gamma)^2(\mu_- (\gamma))^3 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)^2,$$

$$-\frac{1}{12}|Y|^2\gamma^2(1-\gamma)^2(\mu_- (\gamma))^{-1} (\alpha_1 - \alpha_0)^2,$$

represent the next order corrections to the Harmonic and the Arithmetic Means respectively as the scale is decreased. The details of the proof of the above results will appear elsewhere.

### 6. Conclusions and Perspectives

Probing the matter and the space-time at high energies and fine scales through experiments, observations and theoretical studies of models is part of modern day trend. One can hope to carry out similar activities to understand the behaviour of heterogeneous structures at fine scales and at high energies. This article has treated periodically heterogeneous structures with the above point of view. In this context, we have introduced higher order macro coefficients and studied their properties. Several new phenomena that appear with the decrease of scale or with the increase of energy are pointed out. Analogous treatment of arbitrary heterogeneous structures is a huge program for the future. Even among the restricted class of periodic structures with two-phases but with arbitrary micro-geometry, the analysis of behaviour of higher order macro coefficients is a challenging task and efforts are being taken to face up to it.

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