Lippmann-Schwinger spectra, composite materials eigenstates and their role in computational homogenization

Cédric Bellis*†[1] and Hervé Moulinec[2]

[1]Laboratoire de Mécanique et d'Acoustique [Marseille] (LMA) – Aix Marseille Université, Ecole Centrale de Marseille, Centre National de la Recherche Scientifique, Aix Marseille Université : UMR7031, Ecole Centrale de Marseille : UMR7031, Centre National de la Recherche Scientifique : UMR7031 – 4 impasse Nikola TeslaCS 4000613453 Marseille Cedex 13, France

[2]Aix-Marseille Université, CNRS, Centrale Marseille, LMA UMR 7031 – Aix Marseille Univ, CNRS, Centrale Marseille, LMA UMR 7031, Marseille, France – 4 impasse Nikola Tesla, 13013 Marseille, France

Abstract

When considering the homogenization of heterogeneous materials, one has to solve for the local fields in a representative volume element subjected to a uniform loading. This defines a cell problem, which can take the form of local equations or of an equivalent volume integral equation. When the composite material considered is made of constituents with linear behaviors, such an integral equation reduces to the so-called Lippmann-Schwinger equation. Establishing such a formulation relies on the introduction of a linear, and in most cases also uniform, comparison medium with its companion Green's function. In the case of periodic composites, this type of formulation has provided the foundation for the fast Fourier transform-based numerical method developed in (1) to compute the effective properties of linear and non-linear composites. This has opened the door to a breadth of successful developments since.

Theoretical results were also obtained using variational principles and volume integral formulations, in particular to establish bounds on the homogenized properties. In addition, the analytic properties of the effective tensor of the composite as a function of the parameters of its constituents have been the subject of a number of studies, initiated with (2, 3, 4) for dielectric composites. In the specific case of two-component materials, it is shown that the effective properties can be represented as an integral of a rational function of the material contrast between phases. This formulation turns out to be a Stieltjes integral representation associated with the spectral measure of the linear integral operator featured in the Lippmann-Schwinger formulation of the homogenization problem. Describing the spectrum of this operator and its associated eigenvectors, also referred to as eigenstates of the composite as in (5), is thus key for understanding the expression of the effective properties as functions of the composite micro-geometry and constituent parameters.

To bridge the gap between the generic computational methods on the one hand and the theoretical homogenization results for two-phase composites on the other hand, the perspective adopted in the present study is that the introduction of the comparison medium amounts

*Speaker

†Corresponding author: bellis@lma.cnrs-mrs.fr

to a preconditioning of the original cell problem. In the context of solving partial differential equations, preconditioning is a well-known method, see e.g. (6). It is then crucial to analyze the spectral properties of the preconditioned operator as the performances of iterative solution schemes, such as the conjugate gradient or fixed-point iterations, depend on them, a study that is carried out for example in (7) for second-order differential operators relevant to the problems considered here. This makes it possible to find an optimal preconditioner, i.e., in the present context, an optimal comparison medium.

In the context of computational homogenization methods and to connect with the known theoretical results, the overall objective of the present study is to shed some light on the implications of the preconditioning strategy by the introduction of the comparison medium and, in the linear case, on the role of the spectral properties of the integral operator of the Lippmann-Schwinger equation in computing the solution to the cell problem and thus the effective properties of a given composite. The results presented hereinafter are intended to be formulated in a framework as general as possible, encompassing in particular the conductivity and elasticity cases.

The homogenization problem is presented first in a variational setting for generic composite materials, potentially governed by a non-quadratic energy density. The introduction of the comparison medium is made through the definition of an energetic inner product. This naturally leads to the identification of the gradient of the energy functional as a preconditioned version of the original cell problem governing the local fields. Iterative solutions methods are then studied, starting with steepest descent, which we connect to fixed-point iterations, revisiting the convergence criteria conventionally adopted. Although a formulation using the unknown potential (or displacement) field is adopted in this study, the link is made with the gradient (or strain) based formulations that are widely used in the applications. This analysis is then particularized to the case of linear composites, so as to obtain the well-known Lippmann-Schwinger integral equation. The featured linear operator, which is bounded and self-adjoint, is then analyzed with bounds on its eigenvalues and a description, in the conductivity setting, of the associated eigenvectors, referred to as eigenstates of the composite. Then, we will focus on the role of the spectral properties of the operator considered, namely how the solution to the cell problem and the effective properties are expressed in terms of the eigenvalues and eigenvectors in the case of multiple phase composites. These developments are then particularized to two-component materials. This analysis conducted in an infinite-dimensional functional setting is then transposed in the context of numerical methods, with a suitable discretization scheme. A matrix formulation of the eigenvalue problem is investigated in connection with the conventional tools of FFT-based homogenization methods. Finally, some numerical results will be presented and discussed for a set of synthetic microstructures. Some numerical spectra will be described together with the associated eigenstates, highlighting in particular the very small portion of the spectrum that actually plays a role in computing the solution to the homogenization problem.

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