FINITE SCALE HOMOGENIZATION

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Abstract

Homogenization theory is concerned with the task of extracting effective material parameters for composite media in the limit where the applied wavelength is large compared to the microstructure. Usually, this is analyzed in the extreme limit where the wavelength is infinite, but in this paper we present the framework of a method which deals with wavelengths that are comparable to the microstructure, that is, finite scale homogenization. We also give example of a few typical cases where this theory may be applied.

1 INTRODUCTION

Most materials can be considered to have some kind of microstructure, for instance concrete with reinforcement metallic rods in a regular pattern, laminated wood, or biological tissue. When the applied wavelength is much larger than the microstructure, it is common to replace the complicated microscopic geometry with a fictitious, homogeneous material for calculational purposes. This greatly reduces the computational effort of the scattering problem.

Two problems immediately present themselves: how do we compute the fictitious material (it is well known it is not the mean value of the material parameters), and how large does the wavelength have to be for the homogenized problem to make sense? Usually, the answer to the first question is to compute a generic problem in a unit cell, but then the solution is formally only valid in the limit where the wavelength is infinitely large.

In a recent publication [1], the authors showed that it is possible to compute homogenized material coefficients even in the case where the wavelength is not infinitely large. Generalizations of this result have been derived by the author [2], which make it possible to calculate a range of validity for homogenized parameters. The method can be used to make a rigorous study of chiral media based on chiral inclusions, as well as negative refractive index materials.

Mathematically, the problem is to study the limit of solutions to certain partial differential equations when a parameter (the microscopic scale) becomes very small. In the infinite wavelength case, this is a well researched area particularly with applications to solid mechanics, although the results do not seem to be commonplace in the radio science community. For recent reviews, we refer the reader to the introductory text [3], the treatises [4, 5], and references therein. Although most of the homogenization literature deal with the classical case of infinite wavelengths, there has recently emerged some important contributions on finite scale homogenization in the mathematics community [6, 7, 8].

2 BASIC IDEA

The approach taken in this paper is based on a simple idea. The formal solution to Maxwell's equations can be written

$$\begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{pmatrix} = \underbrace{\begin{pmatrix} \mathrm{i}\omega\boldsymbol{\epsilon}_{\mathrm{c}}(\boldsymbol{r},\omega) & -\nabla\times \\ \nabla\times & \mathrm{i}\omega\boldsymbol{\mu}_{\mathrm{c}}(\boldsymbol{r},\omega) \end{pmatrix}^{-1}}_{\mathcal{A}} \begin{pmatrix} \boldsymbol{J} \\ \boldsymbol{0} \end{pmatrix} \tag{1}$$

where $\boldsymbol{\epsilon}_{\mathrm{c}}(\boldsymbol{r},\omega)$ is the complex permittivity, and $\boldsymbol{\mu}_{\mathrm{c}}(\boldsymbol{r},\omega)$ is the complex permeability, both of them generally being matrices, that is, we are studying fully anisotropic media. The operator $\mathcal{A}$ is compact if we consider vector fields $\boldsymbol{J}$, $\boldsymbol{E}$, and $\boldsymbol{H}$ with bounded energy (that is, square integrable), and require that these fields satisfy appropriate divergence conditions. A compact operator can be analyzed by its singular value decomposition, where the action of the operator on a field f can be written

$$\mathcal{A}f = \sum_{n=1}^{\infty} \sigma_n (f, u_n) v_n, \quad \text{where} \quad \mathcal{A}u_n = \sigma_n v_n \text{ and } \mathcal{A}^{\dagger} v_n = \sigma_n u_n \tag{2}$$

We use the notation (f, u_n) to indicate the inner product in the associated function space (that is, an integral of the product of the vector fields x and u_n), and $\mathcal{A}^{\dagger}$ denotes the adjoint operator of $\mathcal{A}$. The real, positive numbers σ_n are the singular values of the operator, and $(u_n)_{n=1}^{\infty}$ and $(v_n)_{n=1}^{\infty}$ are orthonormal function sequences. All these quantities can be computed from a well defined eigenvalue problem.

The idea behind finite scale homogenization is based on the physical experience that as the scale becomes small, we can only observe the average of the electromagnetic field, not the small fluctuations on the microscopic scale. This corresponds to a loss of degrees of freedom, where we ideally would only be bothered with six degrees of freedom, the polarization of the mean values of the electric and the magnetic field, respectively. In terms of the singular value decomposition, this corresponds to having the infinite sum in (2) collapse to a finite sum.

From the representation (2) of the compact operator $\mathcal{A}$, it is seen that control of the singular values produces some control of the action of the operator. In our case, we are interested in the case where the microscopic scale becomes small. Studying a nonmagnetic material (that is, $\boldsymbol{\mu}_{\mathrm{c}} = \mu_0 \mathbf{I}$) with periodic microstructure as a model example, we denote the period by a. Choose a fixed frequency with vacuum wavelength λ_0, and let it be restricted by the condition $\lambda_0 > 2a\,\|\boldsymbol{\epsilon}_{\mathrm{c}}/\epsilon_0\|$ (less restrictive but more complicated conditions are possible). As is shown in [2], this implies that $\sigma_n < a$ if $n > 6$, that is, all singular values go to zero as $a \to 0$ except for the first six. This corresponds precisely to the number of degrees of freedom to choose the $2 \times 3 = 6$ vector components of the mean values $\langle \boldsymbol{E} \rangle$ and $\langle \boldsymbol{H} \rangle$, which are the only observable parts of the electric and magnetic fields as the scale becomes small. This reduction of the degrees of freedom for the electromagnetic field is just what is needed to be able to define homogenized material properties, and we refer to [1, 2] for details.

3 FINITE SCALE HOMOGENIZATION AND DISPERSION

The fact that the vacuum wavelength of the incident field is restricted only by a condition of the type $\lambda_0 > Ca$, where C is typically in the range 1–10, indicates that we can use wavelengths that are finite compared to the microscopic scale a, and still be able to define homogenized material parameters. In classical homogenization, it is usually necessary to require that $a/\lambda_0 \to 0$ in order to do that. However, there is of course a price to pay: even though it does not show in the heuristic derivation in the previous section, the resulting homogenized parameters will exhibit spatial dispersion, that is, the constitutive relation between the macroscopic fields $\boldsymbol{D}$ and $\boldsymbol{E}$ depends on the wave vector employed,

$$\boldsymbol{D}(\boldsymbol{k}) = \boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}(\boldsymbol{k})\boldsymbol{E}(\boldsymbol{k}) \tag{3}$$

where $\boldsymbol{E}(\boldsymbol{k})$ is the amplitude of a plane wave with wave vector $\boldsymbol{k}$ and $\boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}(\boldsymbol{k})$ is the homogenized permittivity. The dependence of $\boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}$ on $\boldsymbol{k}$ may be more or less pronounced, depending on the contrast and microscopic geometry.

From a design point of view, it may be desirable to design materials which are as broad band as possible, that is, depend as little as possible on $\boldsymbol{k}$. However, there is one more dispersion source. The microscopic constituents, which are used to fabricate the composite material, may exhibit temporal dispersion, that is, depend on ω. This opens the possibility of compensating one kind of dispersion with the other, producing more broad band solutions. In other applications, it may instead be desirable to enhance the dispersion by combining the sources.

Another point that should be made, is that the dependence on $\boldsymbol{k}$, where $|\boldsymbol{k}| = 2\pi/\lambda_0$, can be used to study the validity range of the extreme homogenization limit, where $a/\lambda_0 \to 0$. By considering the $\boldsymbol{k}$-dependent homogenized coefficient $\boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}(\boldsymbol{k})$ as the "true" value, it makes sense to study the relative error $|\boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}(\boldsymbol{0}) - \boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}(\boldsymbol{k})|/|\boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}(\boldsymbol{k})|$, and use this as a measure to determine the validity range of the classical homogenization result, $\boldsymbol{\epsilon}_{\mathrm{c}}^{\mathrm{h}}(\boldsymbol{0})$. This was done for composite media consisting of two phases in [9], where it was found that, for a few test geometries, the validity range depends strongly on the contrast of the microscopics constituents employed. Typically, for a contrast of the order of 10, the classical homogenized result turned out to be correct within a tolerance of 10% for vacuum wavelengths down to $\lambda_0 \approx 2.5a$.

4 CONCLUSIONS

In this paper we have drawn a rough picture of a framework which allows homogenization results to be extracted even when the microscopic scale is comparable to the wavelength employed. Some possible applications are: 1) The rigorous study of media with chiral effects or negative index of refraction, 2) The design of media based on spatial dispersion from the microstructure combined with temporal dispersion from the constituents, and 3) The study of the validity range of classical homogenization results. The results are new even in the mathematical community, where similar approaches only recently have emerged.

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