Abstract: We find effective (homogenized) parameters for Maxwell’s equations when the microscopic scale becomes small, but not infinitesimal, compared to the wavelength. The analysis is based on a singular value decomposition of the differential operator in Maxwell’s equations.

1 INTRODUCTION

When the microscopic scale of a material is much smaller than the typical wavelength, it becomes inefficient or even impossible to take into account all interactions between the electromagnetic field and the media. A common approach is to introduce an effective, or homogenized, material, which does not vary on the microscopic scale. It is well known that in order to preserve for instance energy between the exact problem and the homogenized problem, the homogenized material cannot be the mean value of the microscopic variations, but has to be modified. Methods for this have been known for a long time, particularly since the 70s, see for instance Bensoussan et al. [1], Jikov et al. [4], Milton [7] for a thorough review of the mathematical techniques involved.

The typical mathematical example is a scalar elliptic equation,

\[ \nabla \cdot (A(x/\varepsilon)\nabla u^\varepsilon) = f, \]

where \( A(x) \) is a periodic function of its argument, and \( \varepsilon \) is a small parameter which indicates the scale of the microstructure. In the limit \( \varepsilon \to 0 \), corresponding to the unit cell becoming infinitesimally small compared to macroscopic scale, the solution \( u^\varepsilon \to u_0 \), where \( u_0 \) is the solution to the equation

\[ \nabla \cdot (A^h \nabla u_0) = f. \]

The homogenized matrix \( A^h \) is constant and can be calculated by solving a local problem in the unit cell. In this paper, we present a method to compute homogenized parameters when the unit cell is not infinitesimal.

2 NOTATION

In six-vector notation, we gather the field vectors according to

\[ e = \begin{pmatrix} E \\ H \end{pmatrix}, \quad d = \begin{pmatrix} D \\ B \end{pmatrix} = \begin{pmatrix} \varepsilon & 0 \\ 0 & \mu \end{pmatrix} \cdot \begin{pmatrix} E \\ H \end{pmatrix} = \begin{pmatrix} J \\ 0 \end{pmatrix} = \begin{pmatrix} \sigma & 0 \\ 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} E \\ H \end{pmatrix} = \sigma \cdot e \]

(1)

where \( M(x) \) is a real, symmetric, positive definite matrix, and \( \sigma(x) \) is a real, symmetric, positive semi-definite matrix. Maxwell’s equations are then written

\[ \nabla \times J \cdot e + \partial_t M \cdot e + \sigma \cdot e = 0 \]

(2)

where

\[ \nabla \times J \cdot e = \begin{pmatrix} 0 & -\nabla \times I \\ \nabla \times I & 0 \end{pmatrix} \cdot \begin{pmatrix} E \\ H \end{pmatrix} = \begin{pmatrix} -\nabla \times H \\ \nabla \times E \end{pmatrix} \]

(3)

3 FLOQUET-BLOCH REPRESENTATION

We assume the material parameters \( M(x) \) and \( \sigma(x) \) to be periodic functions of \( x \), that is, \( M(x+a_{1,2,3}) = M(x) \) where \( a_{1,2,3} \) are the basis vectors of the spatial lattice, possibly non-orthogonal. The spatial unit cell \( U \) has volume \( |U| = a_1 \cdot (a_2 \times a_3) \), and we define the basis vectors \( b_{1,2,3} \) for the reciprocal lattice according to \( a_i \cdot b_j = 2\pi \delta_{ij} \), see for instance Kittel [5]. The reciprocal unit cell \( U' \) then has volume \( |U'| = b_1 \cdot (b_2 \times b_3) = (2\pi)^3/|U| \).
Any $L^2$-function, in particular the electromagnetic field, can be represented with its Fourier transform,

$$e(x, t) = \int_{\mathbb{R}^3} e^{ik \cdot x} \hat{e}(k, t) \, dv_k = \int_{\mathbb{R}^3} e^{ik \cdot x} \hat{e}(k, t) \, dv_k + \int_{\mathbb{R}^3 \setminus U'} e^{ik \cdot x} \hat{e}(k, t) \, dv_k$$  \hspace{1cm} (4)

As the spatial unit cell $U$ goes to zero, the reciprocal cell $U'$ fills $\mathbb{R}^3$, which means the last integral must vanish in this limit and the field is given by Fourier components with $k \in U'$. Another way to represent the field is with a Floquet-Bloch representation, first given by Floquet [3] in a one-dimensional setting and later rediscovered by Bloch [2].

$$e(x, t) = \int_{U'} e^{ik \cdot x} \hat{e}(x, k, t) \, dv_k$$ \hspace{1cm} (5)

where the Bloch amplitude $\hat{e}(x, k, s)$ is a $U$-periodic function of $x$. Since the Bloch amplitude is periodic, any variation with $x$ corresponds to fluctuations in the electromagnetic field on a scale smaller than the unit cell. We define the mean value as

$$\langle \hat{e} \rangle = \frac{1}{|U|} \int_{U'} \hat{e}(x, k) \, dv_x$$ \hspace{1cm} (6)

It can be shown that $\langle \hat{e}(k, t) \rangle = \hat{e}(k, t)$, where $\hat{e}(k, t)$ is the Fourier amplitude of the electromagnetic field. Thus, when the unit cell $U \rightarrow 0$, the electromagnetic field is determined by the mean value of the Bloch amplitude.

The homogenized material parameters are defined according to

$$\langle d \rangle = \langle M \cdot \hat{e} \rangle = M^h \cdot \langle \hat{e} \rangle \quad \text{and} \quad \langle j \rangle = \langle \sigma \cdot \hat{e} \rangle = \sigma^h \cdot \langle \hat{e} \rangle$$ \hspace{1cm} (7)

Using the Floquet-Bloch representation and the fact that the material parameters $M(x)$ and $\sigma(x)$ are $U$-periodic, Maxwell’s equations can be formulated in terms of the Bloch amplitude as

$$(\nabla + ik) \times J + \delta M \cdot \hat{e} + \sigma \cdot \hat{e} = 0$$ \hspace{1cm} (8)

where the shifted curl operator is a consequence of $\nabla \times J \cdot (e^{ik \cdot x} \hat{e}) = e^{ik \cdot x} (\nabla + ik) \times J \cdot \hat{e}$. Using a Laplace transformation in time, which replaces the time derivative with the Laplace parameter $s$, we see that this is essentially an eigenvalue problem:

$$M^{-1} \cdot [(\nabla + ik) \times J + \sigma] \cdot \hat{e} = -s \hat{e}$$ \hspace{1cm} (9)

Sjöberg et al. [8] make a detailed analysis of this problem in the case when $\sigma = 0$. Since the operator can then be associated with a self-adjoint compact operator, there is a solid spectral theory available which makes it possible to derive an expression for $M^h$, based on the eigenvectors associated with the smallest eigenvalues. This makes intuitive sense, since small eigenvalues correspond to small frequencies $s$.

In the present case, the operator $M^{-1} \cdot [(\nabla + ik) \times J + \sigma]$ is not self-adjoint, or even normal. This means there is practically no spectral theory at all available, but we can do the next best thing, that is, a singular value decomposition.

4 SINGULAR VALUE DECOMPOSITION

The decomposition in this section is a consequence of the corresponding decomposition of the resolvent operator $[M^{-1} \cdot ((\nabla + ik) \times J + \sigma) + z]^{-1}$, which can be shown to be a compact operator, see Kress [6, p. 277] for details. The singular value decomposition of our operator is defined as

$$\begin{cases}
M^{-1} \cdot ((\nabla + ik) \times J + \sigma) \cdot u_n + z u_n = \lambda_n v_n \\
M^{-1} \cdot ((\nabla + ik) \times J + \sigma) \cdot v_n + z^* v_n = \lambda_n u_n
\end{cases}$$ \hspace{1cm} (10)

where the function sequences $\{u_n\}$ and $\{v_n\}$ are each complete and orthonormal in the weighted scalar product $(u_1, M \cdot u_2) = \int_U u_1(x) \cdot M(x) \cdot u_2(x) \, dv_x$. The complex number $z$ is chosen so that there is no singular value $\lambda_n$ equal to zero.

Since $\{u_n\}$ is a complete system, we can expand the Bloch amplitude using these functions, that is, $\hat{e} = \sum_n (\hat{e}, M \cdot u_n) u_n$. The homogenized matrices in (7) can then be defined according to $\langle M \cdot u_n \rangle = M^h \cdot \langle u_n \rangle$ etc.
5 AVERAGING THE EQUATIONS

Multiplying (10) with $M$ and taking the mean value implies

$$\begin{cases}
  i\mathbf{k} \times \mathbf{J} \cdot (\mathbf{u}_n) + \langle \mathbf{\sigma} \cdot \mathbf{u}_n \rangle + z \langle \mathbf{M} \cdot \mathbf{u}_n \rangle = \lambda_n \langle \mathbf{M} \cdot \mathbf{v}_n \rangle \\
  -i\mathbf{k} \times \mathbf{J} \cdot \langle \mathbf{v}_n \rangle + \langle \mathbf{\sigma} \cdot \mathbf{v}_n \rangle + z^* \langle \mathbf{M} \cdot \mathbf{v}_n \rangle = \lambda_n \langle \mathbf{M} \cdot \mathbf{u}_n \rangle
\end{cases}$$  \hspace{1cm} (11)

and by introducing the homogenized matrices according to (7) we obtain

$$\begin{cases}
  (i\mathbf{k} \times \mathbf{J} + \mathbf{\sigma}^h + z\mathbf{M}^h) \cdot (\mathbf{u}_n) = \lambda_n \mathbf{M}^h \cdot \langle \mathbf{v}_n \rangle \\
  (-i\mathbf{k} \times \mathbf{J} + \mathbf{\sigma}^h + z^*\mathbf{M}^h) \cdot \langle \mathbf{v}_n \rangle = \lambda_n \mathbf{M}^h \cdot (\mathbf{u}_n)
\end{cases}$$  \hspace{1cm} (12)

Now, this is identified as a singular value decomposition of a finite dimensional matrix $i\mathbf{k} \times \mathbf{J} + \mathbf{\sigma}^h + z\mathbf{M}^h$. This is usually written $A = VDU^H$, where $V$ and $U$ are unitary matrices and $D$ is a diagonal matrix with the singular values on the diagonal.

Introduce the real and imaginary part of $z$ according to $z = z' + iz''$. After a lengthy analysis, based on identifying $i\mathbf{k} \times \mathbf{J} + iz^*\mathbf{M}^h$ as the anti-hermitian part and $\mathbf{\sigma}^h + z\mathbf{M}^h$ as the hermitian part of the finite-dimensional matrix, we obtain the following expression for the homogenized matrices:

$$\mathbf{M}^h = \frac{1}{2} \sum_{m \in I} \langle \mathbf{M} \cdot \mathbf{u}_m \rangle \langle \mathbf{u}_m^* \cdot \mathbf{M} \rangle + \langle \mathbf{M} \cdot \mathbf{v}_m \rangle \langle \mathbf{v}_m^* \cdot \mathbf{M} \rangle$$  \hspace{1cm} (13)

$$\mathbf{\sigma}^h = \frac{1}{2} \sum_{m \in I} \lambda_m \langle \mathbf{M} \cdot \mathbf{v}_m \rangle \langle \mathbf{u}_m^* \cdot \mathbf{M} \rangle + \langle \mathbf{M} \cdot \mathbf{u}_m \rangle \langle \mathbf{v}_m^* \cdot \mathbf{M} \rangle - z'\mathbf{M}^h$$  \hspace{1cm} (14)

where $I$ is an index set comprising only the modes corresponding to the six smallest singular values $\lambda_n$. Note that the expressions in the numerator are dyadic products, that is, matrices.

6 DISCUSSION

The importance of the homogenized materials in (13) and (14) is that they are defined for a wave vector $\mathbf{k} \neq 0$. This means the unit cell $U$ does not have to be infinitesimal compared to the applied wavelength. In the case of $\mathbf{\sigma} = 0$, these formulas have been compared to the classical homogenization formulas by Sjöberg et al. [9], in order to deduce the validity range of classical homogenization. A similar comparison in the present case has to await the development of suitable numerical algorithms, which are not presently available.

REFERENCES