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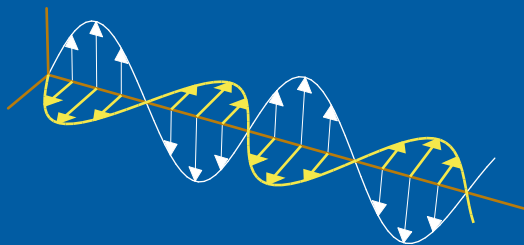
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Homogenization of dispersive material parameters for Maxwell's equations using a singular value decomposition

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Abstract

We find effective, or homogenized, material parameters for Maxwell's equations when the microscopic scale becomes small compared to the scale induced by the frequencies of the imposed currents. After defining a singular value decomposition of the non-selfadjoint partial differential operator, we expand the electromagnetic field in the modes corresponding to the singular values, and show that only the smallest singular values make a significant contribution to the total field when the scale is small. The homogenized material parameters can be represented with the mean values of the singular vectors through a simple formula, which is valid for wavelengths not necessarily infinitely large compared to the unit cell.

1 Introduction

Some problems are hard to solve. The natural reaction is to try and find an easier problem. This is indeed the purpose of this paper: we are interested in the behavior of a strongly heterogeneous microscopic structure (a composite material), when we subject it to electromagnetic fields generated by currents which only have large-scale variations. We expect the microscopic details of the solution to be less important, and want to see what happens on a scale comparable with the imposed currents. In order to do this, we must find a way of replacing the microscopic structure with macroscopic, homogeneous, properties, a process known as homogenization.

Homogenization is not a new topic. It has been dealt with excessively in the literature, see for instance [3] for a general introduction, [2] and [12] for broad overviews, and [6] for a mathematically rigorous presentation. The recent books [11, 15] give a good review of the latest result in this broad field. In principle, the methods presented in these references require that the microscopic scale becomes infinitely small compared to the wavelength applied.

The purpose of the present paper is to provide homogenization results for the case where the microscopic scale is small, but not infinitesimal compared to the wavelength used. In the paper [13], the authors presented a method based on spectral expansions for Maxwell's equations, *i.e.*, utilizing eigenvectors of the curl operators combined with the microscopic description of the material. The homogenized material could be represented using mean values of only a few eigenvectors. This method relies on the material being lossless, since then Maxwell's equations can be associated with a self-adjoint partial differential operator for which there exists suitable spectral theorems.

Unfortunately, most materials cannot be considered lossless. There is almost always a small conductivity or dispersive effects, which makes the corresponding operator in Maxwell's equations non-selfadjoint. The literature on non-selfadjoint operators seems to be very limited, with [4] being the big exception. The most promising tool for analyzing non-selfadjoint operators, is the singular value decomposition, which can be defined for arbitrary compact operators. In this paper, we show how to define proper function spaces so that Maxwell's operator has a compact inverse, thus avoiding problems with the residual spectrum investigated in [10]. We

then show that only a few of the modes corresponding to different singular values make a sizable contribution to the electromagnetic field in the limit where the unit cell becomes very small, which leads to a quite simple homogenization formula in Theorem 6.11.

This paper is organized as follows. In Section 2 we present the notation and basic assumptions used in the paper. Section 3 gives the Floquet-Bloch representation of an L^2 -function, which is advantageous to study periodic media. The singular value decomposition and the function spaces needed to define it are presented in Section 4, and the decomposition is used to represent the solution to Maxwell's equations in Section 5. The homogenized material parameters are deduced in Section 6, and the results are discussed in Section 7. Finally, in Appendix A, we give a complete calculation of the singular values and the associated vectors for the case of a homogeneous, isotropic medium, which is used as a test case for the present algorithm.

2 Notation

For notational convenience, we use scaled fields in this paper, *i.e.*, the SI-unit fields \mathbf{E}_{SI} , \mathbf{H}_{SI} , \mathbf{D}_{SI} , and \mathbf{B}_{SI} are related to the fields \mathbf{E} , \mathbf{H} , \mathbf{D} , and \mathbf{B} used in this paper by

$$\mathbf{E}_{\text{SI}}(\mathbf{x}, t_{\text{SI}}) = \epsilon_0^{-1/2} \mathbf{E}(\mathbf{x}, t) \quad \mathbf{H}_{\text{SI}}(\mathbf{x}, t_{\text{SI}}) = \mu_0^{-1/2} \mathbf{H}(\mathbf{x}, t) \quad (2.1)$$

$$\mathbf{D}_{\text{SI}}(\mathbf{x}, t_{\text{SI}}) = \epsilon_0^{1/2} \mathbf{D}(\mathbf{x}, t) \quad \mathbf{B}_{\text{SI}}(\mathbf{x}, t_{\text{SI}}) = \mu_0^{1/2} \mathbf{B}(\mathbf{x}, t) \quad (2.2)$$

where the permittivity and permeability of vacuum are denoted by ϵ_0 and μ_0 , respectively. The time is scaled according to $t = c_0 t_{\text{SI}}$, where $c_0 = 1/\sqrt{\epsilon_0 \mu_0}$ is the speed of light in vacuum. With this scaling, all the electromagnetic fields have the same physical dimension $\sqrt{\text{power}/\text{volume}}$, *i.e.*, $(\text{J s}^{-1} \text{m}^{-3})^{1/2}$, and the space and time variables \mathbf{x} and t both have the physical dimension length (m). The corresponding relations for the current density \mathbf{J}_{SI} and the charge density ρ_{SI} are

$$\mathbf{J}_{\text{SI}}(\mathbf{x}, t_{\text{SI}}) = \mu_0^{-1/2} \mathbf{J}(\mathbf{x}, t), \quad \rho_{\text{SI}}(\mathbf{x}, t_{\text{SI}}) = \epsilon_0^{1/2} \rho(\mathbf{x}, t) \quad (2.3)$$

In these units, Maxwell's equations are

$$\begin{cases} \nabla \times \mathbf{E} + \partial_t \mathbf{B} = \mathbf{0} \\ \nabla \times \mathbf{H} - \partial_t \mathbf{D} = \mathbf{J} \end{cases} \quad (2.4)$$

which are supplemented by the continuity equation

$$\nabla \cdot \mathbf{J} + \partial_t \rho = 0 \quad (2.5)$$

2.1 Six-vector notation

We now introduce a six-vector notation, which considerably shortens the notation. We group the fields according to

$$\mathbf{e} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} \mathbf{D} \\ \mathbf{B} \end{pmatrix}, \quad \mathbf{j} = \begin{pmatrix} \mathbf{J} \\ \mathbf{0} \end{pmatrix}, \quad \varrho = \begin{pmatrix} \rho \\ 0 \end{pmatrix} \quad (2.6)$$

Collections of vectors like \mathbf{e} , \mathbf{d} , and \mathbf{j} are called six-vectors in the following, and collections of scalars like ϱ are called two-scalars. On occasions, we also make reference to different parts of these vectors and scalars if they are associated with the electric or magnetic fields. This is indicated by indices e or h. For instance, we may describe a two-scalar as $\varrho = [\varrho_e, \varrho_h]^T$, where ϱ_e and ϱ_h are traditional scalars.

Note that even though there are physical reasons to say that there are no magnetic charges, it may still be advantageous to include the possibility in the model. Indeed, sometimes it is *necessary* since we might be solving not the full problem but only a subproblem. In this case, sources which may appear non-physical at first sight can be used to provide a coupling between different parts of the problem. Examples are for instance the Born approximation and various scattering problems, where we need to be able to treat arbitrary current densities \mathbf{j} and charge densities ϱ .

Define differential operators according to

$$\nabla \times \mathbf{J} \cdot \mathbf{e} = \begin{pmatrix} \mathbf{0} & -\nabla \times \mathbf{I} \\ \nabla \times \mathbf{I} & \mathbf{0} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \begin{pmatrix} -\nabla \times \mathbf{H} \\ \nabla \times \mathbf{E} \end{pmatrix}, \quad \nabla \cdot \mathbf{d} = \begin{pmatrix} \nabla \cdot \mathbf{D} \\ \nabla \cdot \mathbf{B} \end{pmatrix} \quad (2.7)$$

where \mathbf{I} is the identity matrix in three dimensions. The material is described by the constitutive relations

$$\mathbf{d}(\mathbf{x}, t) = \mathbf{M}(\mathbf{x}) \cdot \mathbf{e}(\mathbf{x}, t) + \int_{-\infty}^t (\boldsymbol{\sigma}(\mathbf{x}) + \boldsymbol{\chi}(\mathbf{x}, t - t')) \cdot \mathbf{e}(\mathbf{x}, t') dt' \quad (2.8)$$

The optical response of the medium is then modeled by the real, symmetric, positive definite matrix $\mathbf{M}(\mathbf{x})$, the conduction currents are modeled by the real, symmetric, positive semi-definite conductivity matrix $\boldsymbol{\sigma}(\mathbf{x})$, and the remaining dispersive effects (such as resonances or relaxation processes) are modeled by the susceptibility kernel $\boldsymbol{\chi}(\mathbf{x}, t)$. The Laplace transform and its inverse are defined as [1, Ch. 15]

$$f(s) = \int_0^{\infty} e^{-st} f(t) dt, \quad f(t) = \frac{1}{2\pi i} \int_{s \in \gamma} e^{st} f(s) ds \quad (2.9)$$

where $\gamma = (\eta - i\infty, \eta + i\infty)$ is an integration path chosen so that the singularities of $f(s)$ are for $\text{Re } s < \eta$. With the Laplace transform we have the usual relations $\partial_t \rightarrow s$, $\int_{-\infty}^t \rightarrow 1/s$, and convolutions become products, which is used to write

$$\mathbf{d}(\mathbf{x}, s) = (\mathbf{M}(\mathbf{x}) + \boldsymbol{\sigma}(\mathbf{x})/s + \boldsymbol{\chi}(\mathbf{x}, s)) \cdot \mathbf{e}(\mathbf{x}, s) = \mathbf{M}_c(\mathbf{x}, s) \cdot \mathbf{e}(\mathbf{x}, s) \quad (2.10)$$

In order to guarantee a passive medium, *i.e.*, one that does not generate energy, we require [5, p. 15]

$$\text{Re}(s\mathbf{M}_c(\mathbf{x}, s)) \geq 0 \quad \forall \mathbf{x} \in \mathbb{R}^3, \text{Re } s \geq 0 \quad (2.11)$$

In the following, we often write $\mathbf{M}_c(s)$ or \mathbf{M}_c with the \mathbf{x} - and s -dependence implicitly understood. Maxwell's equations and the continuity equation are then compactly written in the Laplace domain as

$$(\nabla \times \mathbf{J} + s\mathbf{M}_c) \cdot \mathbf{e} + \mathbf{j} = \mathbf{0}, \quad \nabla \cdot \mathbf{j} + s\varrho = 0 \quad (2.12)$$

2.2 Periodic media

We further assume the medium is periodic. The unit cell is denoted with U , and the periodic material satisfies $\mathbf{M}_c(\mathbf{x} + \mathbf{x}_n, s) = \mathbf{M}_c(\mathbf{x}, s)$, $\mathbf{n} \in \mathbb{Z}^3$, where $\mathbf{x}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$ and \mathbf{a}_i , $i = 1, 2, 3$, are the basis vectors for the lattice. The reciprocal unit cell is denoted with U' , and a vector in the reciprocal lattice is $\mathbf{k}_n = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3$, where $\mathbf{b}_1 = \frac{2\pi}{|U|} \mathbf{a}_2 \times \mathbf{a}_3$, $\mathbf{b}_2 = \frac{2\pi}{|U|} \mathbf{a}_3 \times \mathbf{a}_1$, $\mathbf{b}_3 = \frac{2\pi}{|U|} \mathbf{a}_1 \times \mathbf{a}_2$, and $|U| = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$. This implies $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}$, where δ_{ij} is the Kronecker delta. For more on the description of periodic media, see the introductory chapters in most books on solid state physics, for instance [8]. We denote the typical length of the unit cell by a , *i.e.*, the physical vectors $\mathbf{a}_{1,2,3}$ and $\mathbf{b}_{1,2,3}$ can be expressed in dimensionless vectors $\hat{\mathbf{a}}_{1,2,3}$ and $\hat{\mathbf{b}}_{1,2,3}$ through the scaling $\mathbf{a}_{1,2,3} = a \hat{\mathbf{a}}_{1,2,3}$ and $\mathbf{b}_{1,2,3} = a^{-1} \hat{\mathbf{b}}_{1,2,3}$, where the dimensionless vectors $\hat{\mathbf{a}}_{1,2,3}$ have a typical length of 1.

Denote by $C_{\#}^{\infty}(U; \mathbb{C}^{6,2})$ the space of infinitely differentiable periodic functions on U with values in $\mathbb{C}^{6,2}$. We work primarily with the space

$$L_{\#}^2(U; \mathbb{C}^6) = \text{the completion of } C_{\#}^{\infty}(U; \mathbb{C}^6) \text{ in the } L^2 \text{ norm} \quad (2.13)$$

Due to the periodic boundary conditions, this space contains functions which are constants. The scalar product in $L_{\#}^2(U; \mathbb{C}^6)$ is

$$(\mathbf{u}, \mathbf{v}) = \frac{1}{|U|} \int_U \mathbf{u} \cdot \mathbf{v}^* dv_{\mathbf{x}} \quad (2.14)$$

and we often use the mean value operator

$$\langle \mathbf{u} \rangle = \frac{1}{|U|} \int_U \mathbf{u} dv_{\mathbf{x}} \quad (2.15)$$

3 Floquet-Bloch representation

In [13], the authors derived a Floquet-Bloch decomposition of Maxwell's equations in periodic media, *i.e.*, the electromagnetic field can be represented as

$$\mathbf{e}(\mathbf{x}, s) = \int_{U'} e^{i\mathbf{k} \cdot \mathbf{x}} \tilde{\mathbf{e}}(\mathbf{x}, \mathbf{k}, s) dv_{\mathbf{k}} \quad (3.1)$$

where the Bloch amplitude $\tilde{\mathbf{u}}(\mathbf{x}, \mathbf{k})$ of an L^2 -function $\mathbf{u}(\mathbf{x})$ is [13]

$$\tilde{\mathbf{u}}(\mathbf{x}, \mathbf{k}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} \hat{\mathbf{u}}(\mathbf{k} + \mathbf{k}_n) e^{i\mathbf{k}_n \cdot \mathbf{x}} = \frac{|U|}{(2\pi)^3} \sum_{\mathbf{n} \in \mathbb{Z}^3} \mathbf{u}(\mathbf{x} + \mathbf{x}_n) e^{-i\mathbf{k} \cdot (\mathbf{x} + \mathbf{x}_n)} \quad (3.2)$$

with $\hat{\mathbf{u}}(\mathbf{k})$ being the Fourier transform of $\mathbf{u}(\mathbf{x})$. The Bloch amplitude $\tilde{\mathbf{e}}$ is a U -periodic function of \mathbf{x} . Maxwell's equations for the Bloch amplitude are then

$$((\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c) \cdot \tilde{\mathbf{e}} + \tilde{\mathbf{j}} = \mathbf{0}, \quad \mathbf{x} \in U, \mathbf{k} \in U' \quad (3.3)$$

and the continuity equation is $(\nabla + i\mathbf{k}) \cdot \tilde{\mathbf{j}} + s\tilde{\rho} = 0$. The advantage with this formulation is that the differential equations only have to be solved in a unit cell U , although the price is paid through the fact that we must solve it for every \mathbf{k} in the reciprocal unit cell U' .

4 Singular value decomposition

The following theorem is from [9, p. 277].

Theorem 4.1 (Singular value decomposition). *Let (μ_n) denote the sequence of the nonzero singular values of the compact linear operator A (with $A \neq 0$) repeated according to their multiplicity, i.e., according to the dimension of the nullspaces $N(\mu_n^2 I - A^* A)$. Then there exist orthonormal sequences (ϕ_n) in X and (g_n) in Y such that*

$$A\phi_n = \mu_n g_n, \quad A^* g_n = \mu_n \phi_n \quad (4.1)$$

for all $n \in \mathbb{N}$. For each $\phi \in X$ we have the singular value decomposition

$$\phi = \sum_{n=1}^{\infty} (\phi, \phi_n) \phi_n + Q\phi \quad (4.2)$$

with the orthogonal projection operator $Q : X \rightarrow N(A)$ and

$$A\phi = \sum_{n=1}^{\infty} \mu_n (\phi, \phi_n) g_n \quad (4.3)$$

Each system (μ_n, ϕ_n, g_n) , $n \in \mathbb{N}$, with these properties is called a singular system of A . When there are only finitely many singular values, the series (4.2) and (4.3) degenerate into finite sums. (Note that for an injective operator A the orthonormal system $\{\phi_n : n \in \mathbb{N}\}$ provided by the singular system is complete in X .)

This section is devoted to the adaptation of this theorem to the differential operator $(\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c$. The strategy is to first formulate function spaces X and Y such that the inverse operator $((\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c)^{-1} : X \rightarrow Y$, called the resolvent, is compact. Then the above theorem can be used to establish a singular value decomposition of the resolvent, which can be inverted to apply to the original differential operator. The result is Theorem 4.4.

4.1 Compactness of the resolvent

As is explained in more depth in [13], the space $L_{\#}^2(U; \mathbb{C}^6)$ is a bit too big for our purposes. Therefore, we introduce the smaller spaces

$$X = \{\mathbf{v} \in L_{\#}^2(U; \mathbb{C}^6) : \exists z', z'' \in \mathbb{C}, (\nabla + i\mathbf{k}) \cdot \mathbf{v} = [z' \tilde{\varrho}_e, z'' \tilde{\varrho}_h]^T\} \quad (4.4)$$

$$Y = \{\mathbf{u} \in L_{\#}^2(U; \mathbb{C}^6) : \exists z', z'' \in \mathbb{C}, (\nabla + i\mathbf{k}) \cdot [\mathbf{M}_c \cdot \mathbf{u}] = [z' \tilde{\varrho}_e, z'' \tilde{\varrho}_h]^T\} \quad (4.5)$$

which contain all functions in $L_{\#}^2(U; \mathbb{C}^6)$ with divergences proportional to the electric charge distribution $\tilde{\varrho}_e$ and the magnetic charge distribution $\tilde{\varrho}_h$.

Theorem 4.2. *The spaces X and Y are closed subspaces in $L_{\#}^2(U; \mathbb{C}^6)$, i.e., they are Hilbert spaces with the standard L^2 scalar product.*

Proof. (See also [13] for a proof when $z' = z''$.) Since the spaces are related through $Y = M_c^{-1}X$, we only need to prove the theorem for X .

Any function $\mathbf{v} \in L_{\#}^2(U; \mathbb{C}^6)$ can be decomposed according to

$$\mathbf{v} = \mathbf{v}_0 + \mathbf{v}_1, \quad \mathbf{v}_0 \in \ker((\nabla + i\mathbf{k}) \cdot), \quad \mathbf{v}_1 = \ker((\nabla + i\mathbf{k}) \cdot)^\perp \quad (4.6)$$

All functions \mathbf{v}_0 in the kernel of the divergence operator obviously belong to X (with $z' = z'' = 0$). The kernel is a closed subspace of $L_{\#}^2(U; \mathbb{C}^6)$, and is defined by

$$\mathbf{v}_0 \in \ker((\nabla + i\mathbf{k}) \cdot) \Leftrightarrow (\mathbf{v}_0, (\nabla + i\mathbf{k})\phi) = 0 \quad \forall \phi \in H_{\#}^1(U; \mathbb{C}^2) \quad (4.7)$$

From this it is clear that any function in the orthogonal complement to the kernel, $\mathbf{v}_1 \in \ker((\nabla + i\mathbf{k}) \cdot)^\perp$, can be written as a gradient, $\mathbf{v}_1 = (\nabla + i\mathbf{k})\phi_1$. The equations

$$(\nabla + i\mathbf{k}) \cdot (\nabla + i\mathbf{k})\phi_e = \tilde{\varrho}_e, \quad (\nabla + i\mathbf{k}) \cdot (\nabla + i\mathbf{k})\phi_h = \tilde{\varrho}_h \quad (4.8)$$

are uniquely solvable for the scalar functions ϕ_e and ϕ_h when $\mathbf{k} \neq \mathbf{0}$. When $\mathbf{k} = \mathbf{0}$, we need to require $\langle \phi_e \rangle = \langle \phi_h \rangle = 0$ in order to find a unique solution (in this case all constant functions are included in the kernel, *i.e.*, $\mathbb{C}^6 \subset \ker(\nabla \cdot)$). All functions $(\nabla + i\mathbf{k})\phi$ in X must then be linear combinations of the functions $[(\nabla + i\mathbf{k})\phi_e, \mathbf{0}]^T = \mathbf{v}_e$ and $[\mathbf{0}, (\nabla + i\mathbf{k})\phi_h]^T = \mathbf{v}_h$.

To conclude, this means

$$X = \ker((\nabla + i\mathbf{k}) \cdot) \oplus \overline{\{\mathbf{v}_e\}} \oplus \overline{\{\mathbf{v}_h\}} \quad (4.9)$$

where $\overline{\{\mathbf{v}\}}$ denotes the linear hull of the function \mathbf{v} . Thus, X is the direct sum of closed, linear subspaces of $L_{\#}^2(U; \mathbb{C}^6)$ and is therefore a Hilbert space with the standard L^2 scalar product. \square

Lemma 4.1. *The vacuum resolvent operator*

$$R_0(s) = [(\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{I}]^{-1} : X \rightarrow X \quad (4.10)$$

*is compact for all s in the resolvent set, *i.e.*, when $R_0(s)$ is bounded, it is also compact. Furthermore, there exists a number $s' = i\omega$, $\omega \in \mathbb{R}$, such that $iR_0(i\omega)$ is a compact, self-adjoint operator.*

Proof. The resolvent operator is associated with the solution of a differential equation

$$[(\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{I}] \cdot \mathbf{v} = \mathbf{w} \quad \Leftrightarrow \quad \mathbf{v} = R_0(s) \cdot \mathbf{w} \quad (4.11)$$

Choosing $s = 1$ for simplicity and taking the Fourier transform of this equation, we have

$$[i(\mathbf{k}_n + \mathbf{k}) \times \mathbf{J} + \mathbf{I}] \cdot \hat{\mathbf{v}}_{\mathbf{n}} = \hat{\mathbf{w}}_{\mathbf{n}} \quad (4.12)$$

Introduce the decomposition $\hat{\mathbf{v}}_{\mathbf{n}\perp} + \hat{\mathbf{v}}_{\mathbf{n}\parallel}$, where the index \perp indicates components orthogonal to $\mathbf{k}_n + \mathbf{k}$. We then have

$$[i(\mathbf{k}_n + \mathbf{k}) \times \mathbf{J} + \mathbf{I}] \cdot \hat{\mathbf{v}}_{\mathbf{n}\perp} = \hat{\mathbf{w}}_{\mathbf{n}\perp}, \quad \mathbf{v}_{\mathbf{n}\parallel} = \mathbf{w}_{\mathbf{n}\parallel} \quad (4.13)$$

which demonstrates that the resolvent is equivalent to the identity operator for the \perp components. These components correspond precisely to the space $\overline{\{v_e\}} \oplus \overline{\{v_h\}}$ from the previous proof. Since this is a finite-dimensional space, the resolvent is compact on this space.

For the \perp components, we square the equation and obtain

$$(|\mathbf{k}_n + \mathbf{k}|^2 + 1)|\hat{v}_{n\perp}|^2 = |\hat{w}_{n\perp}|^2 \quad (4.14)$$

Using the notation $\mathbf{w}_\perp = \sum_{\mathbf{n} \in \mathbb{Z}^3} e^{i\mathbf{k}_n \cdot \mathbf{x}} \hat{w}_{n\perp}$, we have

$$\|\mathbf{R}_0(1) \cdot \mathbf{w}_\perp\|_{L^2}^2 = \|\mathbf{v}_\perp\|_{L^2}^2 = \sum_{\mathbf{n} \in \mathbb{Z}^3} \frac{|\hat{w}_{n\perp}|^2}{|\mathbf{k}_n + \mathbf{k}|^2 + 1} \quad (4.15)$$

Define the operator S_N , which restricts the number of Fourier coefficients, as

$$[S_N \mathbf{v}](\mathbf{x}) = \sum_{|\mathbf{n}| \leq N} \hat{v}_n e^{i\mathbf{k}_n \cdot \mathbf{x}} \quad (4.16)$$

This means the bounded operator $S_N \mathbf{R}_0(1)$ has finite rank, and is therefore compact. We then have

$$\|(1 - S_N) \mathbf{R}_0(1) \cdot \mathbf{w}_\perp\|_{L^2}^2 = \sum_{|\mathbf{n}| > N} \frac{|\hat{w}_{n\perp}|^2}{|\mathbf{k}_n + \mathbf{k}|^2 + 1} \leq \frac{\|\mathbf{w}_\perp\|^2}{|\mathbf{k}_N + \mathbf{k}|^2 + 1} \rightarrow 0 \quad (4.17)$$

uniformly for all \mathbf{w}_\perp of unit norm, as $N \rightarrow \infty$. This shows that $\mathbf{R}_0(1)$ is the limit of finite rank operators $S_N \mathbf{R}_0(1)$ in the operator norm, and is therefore compact. Since any function $\mathbf{w} \in X$ can be decomposed according to $\mathbf{w} = \mathbf{w}_\perp + \mathbf{w}_\parallel$ and the resolvent is compact on each associated subspace, it is compact on all X .

Thus, the spectrum of $\mathbf{R}_0(1)$ is a discrete subset of \mathbb{C} , which in turn implies that $\mathbf{R}_0(s)$ is compact for all s in the resolvent set due to the resolvent equation $\mathbf{R}_0(s_1) - \mathbf{R}_0(s_2) = (s_1 - s_2) \mathbf{R}_0(s_1) \cdot \mathbf{R}_0(s_2)$, see for instance [14, p. 516]. Furthermore, there exists a number $s' = i\omega$, $\omega \in \mathbb{R}$, such that $i\mathbf{R}_0(i\omega)$ is a compact, self-adjoint operator. \square

Theorem 4.3. *The resolvent operator*

$$\mathbf{R}(s) = ((\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c(s))^{-1} : X \rightarrow Y \quad (4.18)$$

is compact for all s in the resolvent set such that $s\mathbf{M}_c(s)$ is bounded.

Proof. The resolvent $\mathbf{R}(s)$ can be written in terms of the vacuum resolvent $\mathbf{R}_0(s)$,

$$\begin{aligned} \mathbf{R}(s) &= [(\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{I} + s(\mathbf{M}_c(s) - \mathbf{I})]^{-1} = [\mathbf{R}_0(s)^{-1} + s(\mathbf{M}_c(s) - \mathbf{I})]^{-1} \\ &= [\mathbf{I} + \mathbf{R}_0(s) \cdot s(\mathbf{M}_c(s) - \mathbf{I})]^{-1} \cdot \mathbf{R}_0(s) \end{aligned} \quad (4.19)$$

A product of operators AB is compact if A is bounded and B is compact, or *vice versa*. The operator $[\mathbf{I} + \mathbf{R}_0(s) \cdot s(\mathbf{M}_c - \mathbf{I})]^{-1}$ is bounded unless -1 is an eigenvalue of

the compact operator $\mathbf{R}_0(s) \cdot s(\mathbf{M}_c - \mathbf{I})$. Choose $s' = i\omega$, $\omega \in \mathbb{R}$. Since $i\mathbf{R}_0(i\omega)$ is self-adjoint it has only real eigenvalues, and for passive media we have $\text{Re}(i\omega\mathbf{M}_c(i\omega)) \geq 0$. This means the eigenvalues of $\mathbf{R}_0(s') \cdot s'(\mathbf{M}_c - \mathbf{I})$ generally have a non-zero imaginary part, and thus the operator $[\mathbf{I} + \mathbf{R}_0(s') \cdot s'(\mathbf{M}_c(s') - \mathbf{I})]^{-1}$ is bounded. This means $\mathbf{R}(s')$ is compact, and the generalized resolvent equation

$$\mathbf{R}(s_1) - \mathbf{R}(s_2) = \mathbf{R}(s_1) \cdot (s_1\mathbf{M}_c(s_1) - s_2\mathbf{M}_c(s_2)) \cdot \mathbf{R}(s_2) \quad (4.20)$$

then implies that $\mathbf{R}(s)$ is compact for all s in the resolvent set, provided $s\mathbf{M}_c(s)$ is bounded. \square

Remark 1. With $\mathbf{R}(s)$ a compact operator, the resolvent set consists of all \mathbb{C} except for a countable set of points (the point spectrum, eigenvalues).

Remark 2. The null space of the resolvent is empty by definition for all s in the resolvent set: the resolvent is associated with the solution of a differential equation,

$$[(\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c(s)] \cdot \mathbf{v} = \mathbf{w} \quad \Leftrightarrow \quad \mathbf{v} = \mathbf{R}(s) \cdot \mathbf{w} \quad (4.21)$$

If there is a \mathbf{w} such that $\mathbf{R}(s) \cdot \mathbf{w} = \mathbf{0}$, it is clear that this requires $\mathbf{w} = \mathbf{0}$.

4.2 Singular value decomposition for the differential operator

Since the resolvent operator $\mathbf{R}(s)$ is compact with empty null space for all s in the resolvent set, we have the following adaptation of the singular value decomposition:

$$\mathbf{R}(s) \cdot \mathbf{v}_n = \mu_n \mathbf{u}_n, \quad \mathbf{R}(s)^* \cdot \mathbf{u}_n = \mu_n \mathbf{v}_n \quad (4.22)$$

and we have the following generalized Fourier series expansions

$$\mathbf{v} = \sum_n (\mathbf{v}, \mathbf{v}_n) \mathbf{v}_n, \quad \mathbf{u} = \sum_n (\mathbf{u}, \mathbf{u}_n) \mathbf{u}_n \quad (4.23)$$

for all $\mathbf{v} \in X$ and $\mathbf{u} \in Y$. The singular values $\{\mu_n\}$ are all nonzero since the nullspace is empty, which means the orthogonal functions $\{\mathbf{u}_n\}$ and $\{\mathbf{v}_n\}$ can be equivalently defined in terms of the inverse operator,

$$\mathbf{R}(s)^{-1} \cdot \mathbf{u}_n = \mu_n^{-1} \mathbf{v}_n, \quad (\mathbf{R}(s)^*)^{-1} \cdot \mathbf{v}_n = \mu_n^{-1} \mathbf{u}_n \quad (4.24)$$

Since $(\mathbf{R}(s)^*)^{-1} = (\mathbf{R}(s)^{-1})^*$, see [7, Thm. III-5.30, p. 169], we have now proved the following theorem, where we write $\sigma_n = \mu_n^{-1}$.

Theorem 4.4. *There exist a sequence of real, positive numbers $\{\sigma_n\}$ and orthonormal sequences $\{\mathbf{u}_n\}$ in Y and $\{\mathbf{v}_n\}$ in X such that*

$$\begin{cases} ((\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c) \cdot \mathbf{u}_n = \sigma_n \mathbf{v}_n \\ (-\nabla + i\mathbf{k}) \times \mathbf{J} + s^* \mathbf{M}_c^H \cdot \mathbf{v}_n = \sigma_n \mathbf{u}_n \end{cases} \quad (4.25)$$

For each $\mathbf{u} \in Y$ and $\mathbf{v} \in X$ we have the expansions

$$\mathbf{u} = \sum_n (\mathbf{u}, \mathbf{u}_n) \mathbf{u}_n, \quad \text{and} \quad \mathbf{v} = \sum_n (\mathbf{v}, \mathbf{v}_n) \mathbf{v}_n \quad (4.26)$$

and

$$((\nabla + \mathbf{i}\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c) \cdot \mathbf{u} = \sum_n \sigma_n (\mathbf{u}, \mathbf{u}_n) \mathbf{v}_n \quad (4.27)$$

The numbers $\{\sigma_n\}$ are the singular values for the differential operator $(\nabla + \mathbf{i}\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c$.

Remark 3. For some s , it may happen that there is an n such that $\sigma_n = 0$. In this case, \mathbf{u}_n corresponds to an eigenvector of the operator bundle $(\nabla + \mathbf{i}\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c(s)$, and we call such an s a characteristic frequency [4, p. 265]. Observe that the resolvent $\mathbf{R}(s)$ is not bounded for such an s .

5 The solution of Maxwell's equations

Expanding the electromagnetic field in the modes $\{\mathbf{u}_n\}$ implies

$$\tilde{\mathbf{e}} = \sum_n (\tilde{\mathbf{e}}, \mathbf{u}_n) \mathbf{u}_n = \sum_n e_n \mathbf{u}_n \quad (5.1)$$

Assuming that s is not a characteristic frequency, we have $\sigma_n \neq 0$ for all n . Inserting the above expansion into Maxwell's equations (3.3) then implies

$$\sum_n e_n \sigma_n \mathbf{v}_n = -\tilde{\mathbf{j}} \quad \Rightarrow \quad e_n = -\frac{1}{\sigma_n} (\tilde{\mathbf{j}}, \mathbf{v}_n) \quad (5.2)$$

which shows that the size of the expansion coefficients is determined by the singular values σ_n and the current density $\tilde{\mathbf{j}}$.

5.1 Estimate of the singular values

The singular value decomposition (4.25) is a decomposition of the differential operator $(\nabla + \mathbf{i}\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c$. This operator can be thought of as a perturbation of the vacuum operator,

$$(\nabla + \mathbf{i}\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c = \underbrace{(\nabla + \mathbf{i}\mathbf{k}) \times \mathbf{J} + s\mathbf{I}}_{\text{vacuum operator}} + \underbrace{s(\mathbf{M}_c - \mathbf{I})}_{\text{bounded perturbation}} \quad (5.3)$$

The singular values are eigenvalues of a self-adjoint operator,

$$\begin{pmatrix} \mathbf{0} & \mathcal{M} \\ \mathcal{M}^* & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{v}_n \\ \mathbf{u}_n \end{pmatrix} = \sigma_n \begin{pmatrix} \mathbf{v}_n \\ \mathbf{u}_n \end{pmatrix} \quad (5.4)$$

where $\mathcal{M} = (\nabla + i\mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c$. The perturbation of a self-adjoint operator by a bounded symmetric operator does not change the spectrum by more than the norm of the perturbing operator [7, Thm. V-4.10, p. 291], *i.e.*,

$$|\sigma_n - \sigma_{n0}| \leq \|s(\mathbf{M}_c - \mathbf{I})\| = \sup_{\mathbf{x} \in U} |s(\mathbf{M}_c(\mathbf{x}, s) - \mathbf{I})| \quad (5.5)$$

where σ_{n0} are the singular values corresponding to vacuum. Observe that when ordering the singular values according to their size, there is a natural pairing between the singular values for the perturbed and unperturbed operator [4, p. 30]. In Appendix A, Corollary A.1, the singular values for the vacuum operator are calculated as

$$\sigma_{n0} = \sqrt{|\operatorname{Re} s|^2 + (|\mathbf{k}_n + \mathbf{k}| \pm |\operatorname{Im} s|)^2} \geq |\mathbf{k}_n + \mathbf{k}| - |\operatorname{Im} s| \quad (5.6)$$

for the singular values corresponding to modes with zero divergence. Since the effect of $\mathbf{k}_n = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$ is to shift the origin to a different cell in the reciprocal lattice, and $\mathbf{k} \in U'$ can be written $\mathbf{k} = \beta_1\mathbf{b}_1 + \beta_2\mathbf{b}_2 + \beta_3\mathbf{b}_3$ where $|\beta_{1,2,3}| < 1/2$, the vector $\mathbf{k}_n + \mathbf{k}$ is always larger than the unit cell U' for $\mathbf{n} \neq \mathbf{0}$. This provides the estimate

$$|\mathbf{k}_n + \mathbf{k}| \geq \inf_{\mathbf{k}' \in \partial U'} |\mathbf{k}'| = \frac{D}{2a}, \quad |\mathbf{n}| > 0 \quad (5.7)$$

where D/a is the smallest diameter of the reciprocal unit cell U' . The factor $1/a$ originates in the scaling property $\mathbf{b}_{1,2,3} = a^{-1}\hat{\mathbf{b}}_{1,2,3}$, where the dimensionless vectors $\hat{\mathbf{b}}_{1,2,3}$ have the approximate length 2π . For a simple cubic lattice, $D = 2\pi$. This implies

$$\sigma_n \geq \sigma_{n0} - \|s(\mathbf{M}_c - \mathbf{I})\| \geq \frac{D}{2a} - |\operatorname{Im} s| - |s| \|\mathbf{M}_c - \mathbf{I}\| \geq \frac{D}{2a} - |s|(\|\mathbf{M}_c - \mathbf{I}\| + 1) \quad (5.8)$$

if $|\mathbf{n}| > 0$. This means that for each $C > 0$ we have

$$\sigma_n \geq \frac{C}{a}, \quad \text{if } |as| < \frac{D/2 - C}{\|\mathbf{M}_c - \mathbf{I}\| + 1}, \quad |\mathbf{n}| > 0 \quad (5.9)$$

independent of \mathbf{k} . For $\mathbf{n} = \mathbf{0}$, the corresponding estimate is

$$\sigma_n \geq |\mathbf{k}| - |s|(\|\mathbf{M}_c - \mathbf{I}\| + 1) \quad (5.10)$$

which cannot be used to bound the singular values σ_n from zero for all $\mathbf{k} \in U'$. Thus, by choosing the frequency bandwidth of the imposed current density $\tilde{\mathbf{j}}$ such that we may consider $|as| < (D/2 - C)/(\|\mathbf{M}_c - \mathbf{I}\| + 1)$, all singular values go to infinity at least as fast as C/a when $a \rightarrow 0$ except possibly for the six modes corresponding to $\mathbf{n} = \mathbf{0}$ and non-zero divergence. Introduce the index set I to denote these modes,

$$I = \{n : \inf_{\mathbf{k} \in U'} \sigma_n < \infty, a \rightarrow 0\} \quad (5.11)$$

Since the expansion coefficients e_n are proportional to $1/\sigma_n$, we have (for all $\mathbf{k} \in U'$)

$$n \notin I \quad \Rightarrow \quad e_n \rightarrow 0, \quad a \rightarrow 0 \quad (5.12)$$

which means only the six expansion coefficients e_m , $m \in I$, can survive in the limit $a \rightarrow 0$. In the following, we generally use the index m instead of n when referring to modes in the index set I .

6 Homogenized parameters

We state the following conjecture in spirit of the conjecture in [13].

Conjecture 1. For each $s \in \mathbb{C}$ for which the singular value decomposition can be defined, the modes corresponding to the six smallest singular values, indexed by the index set I , have the property that the mean values $\{\langle \mathbf{u}_m \rangle\}_{m \in I}$ are linearly independent, as well as the mean values $\{\langle \mathbf{v}_m \rangle\}_{m \in I}$.

The conjecture is supported by explicit results for the vacuum case, and is also necessary in order to be able to solve Maxwell's equations for small frequencies. However, it seems a rigorous proof is difficult, and we leave it as a conjecture.

We start with a lemma on linear algebra:

Lemma 6.1. For a set of linearly independent (constant) vectors $\{\mathbf{w}_m\}$, there exists $\alpha_{mm'} \in \mathbb{C}$, such that the orthogonality relations

$$\left[\sum_{m'} \alpha_{mm'} \mathbf{w}_{m'}^* \right] \cdot \mathbf{w}_{m''} = \delta_{mm''} \quad (6.1)$$

hold for $m, m'' \in I$, where $\delta_{mm''}$ is the Kronecker delta.

Proof. Due to the linear independence of the vectors $\{\mathbf{w}_m\}$, the square matrix with entries $A_{m'm''} = \mathbf{w}_{m'}^* \cdot \mathbf{w}_{m''}$ is invertible. This means the equation $\sum_{m'} A_{m'm''} a_{m'} = b_{m''}$ has a unique solution $a_{m'}$ for each $b_{m''}$. Fixing m and choosing $b_{m''} = \delta_{mm''}$, this uniquely determines $\alpha_{mm'} = a_{m'}$. \square

6.1 Existence of homogenized matrix

In general, the homogenized matrix is defined by $\langle \mathbf{M}_c \cdot \tilde{\mathbf{e}} \rangle = \mathbf{M}_c^h \cdot \langle \tilde{\mathbf{e}} \rangle$. If $\tilde{\mathbf{e}} = \sum_{m \in I} e_m \mathbf{u}_m$, the homogenized matrix can be equivalently defined by

$$\langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle = \mathbf{M}_c^h \cdot \langle \mathbf{u}_m \rangle, \quad \forall m \in I \quad (6.2)$$

The following theorem proves existence for this kind of matrix.

Theorem 6.1. There exists homogenized matrices \mathbf{M}_c^h and \mathbf{N}_c^h such that

$$\langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle = \mathbf{M}_c^h \cdot \langle \mathbf{u}_m \rangle, \quad \langle \mathbf{M}_c^H \cdot \mathbf{v}_m \rangle = \mathbf{N}_c^h \cdot \langle \mathbf{v}_m \rangle \quad (6.3)$$

Proof. With $\{\langle \mathbf{u}_m \rangle\}_{m \in I}$ being linearly independent, there exists an orthogonality relation $[\sum_{m' \in I} \alpha_{mm'}^u \mathbf{u}_{m'}^*] \cdot \mathbf{u}_{m''} = \delta_{mm''}$ due to Lemma 6.1. We then have

$$\begin{aligned} \langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle &= \langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle \underbrace{\left[\sum_{m' \in I} \alpha_{mm'}^u \langle \mathbf{u}_{m'}^* \rangle \right]}_{=1} \cdot \langle \mathbf{u}_m \rangle \\ &= \left[\sum_{m', m'' \in I} \langle \mathbf{M}_c \cdot \mathbf{u}_{m''} \rangle \alpha_{m''m'}^u \langle \mathbf{u}_{m'}^* \rangle \right] \cdot \langle \mathbf{u}_m \rangle = \mathbf{M}_c^h \cdot \langle \mathbf{u}_m \rangle \quad (6.4) \end{aligned}$$

where we used the orthogonality relation to include the sum over m'' . In the same way, we have

$$\begin{aligned} \langle \mathbf{M}_c^H \cdot \mathbf{v}_m \rangle &= \langle \mathbf{M}_c^H \cdot \mathbf{v}_m \rangle \underbrace{\left[\sum_{m' \in I} \alpha_{mm'}^v \langle \mathbf{v}_{m'}^* \rangle \right]}_{=1} \cdot \langle \mathbf{v}_m \rangle \\ &= \left[\sum_{m', m'' \in I} \langle \mathbf{M}_c^H \cdot \mathbf{v}_{m''} \rangle \alpha_{m''m'}^v \langle \mathbf{v}_{m'}^* \rangle \right] \cdot \langle \mathbf{v}_m \rangle = \mathbf{N}_c^h \cdot \langle \mathbf{v}_m \rangle \end{aligned} \quad (6.5)$$

□

Remark 4. It is not *a priori* guaranteed that $\mathbf{N}_c^h = (\mathbf{M}_c^h)^H$.

6.2 Averaging the equations

Taking the mean value of the singular value decomposition (4.25) implies

$$\begin{cases} \mathbf{i}\mathbf{k} \times \mathbf{J} \cdot \langle \mathbf{u}_n \rangle + s \langle \mathbf{M}_c \cdot \mathbf{u}_n \rangle = \sigma_n \langle \mathbf{v}_n \rangle \\ -\mathbf{i}\mathbf{k} \times \mathbf{J} \cdot \langle \mathbf{v}_n \rangle + s^* \langle \mathbf{M}_c^H \cdot \mathbf{v}_n \rangle = \sigma_n \langle \mathbf{u}_n \rangle \end{cases} \quad (6.6)$$

Restricting ourselves to indices $m \in I$ and introducing the homogenized matrices implies

$$\begin{cases} (\mathbf{i}\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c^h) \cdot \langle \mathbf{u}_m \rangle = \sigma_m \langle \mathbf{v}_m \rangle \\ (-\mathbf{i}\mathbf{k} \times \mathbf{J} + s^*\mathbf{N}_c^h) \cdot \langle \mathbf{v}_m \rangle = \sigma_m \langle \mathbf{u}_m \rangle \end{cases} \quad (6.7)$$

From this we obtain the finite dimensional eigenvalue equations

$$\begin{cases} (-\mathbf{i}\mathbf{k} \times \mathbf{J} + s^*\mathbf{N}_c^h) \cdot (\mathbf{i}\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c^h) \cdot \langle \mathbf{u}_m \rangle = \sigma_m^2 \langle \mathbf{u}_m \rangle \\ (\mathbf{i}\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c^h) \cdot (-\mathbf{i}\mathbf{k} \times \mathbf{J} + s^*\mathbf{N}_c^h) \cdot \langle \mathbf{v}_m \rangle = \sigma_m^2 \langle \mathbf{v}_m \rangle \end{cases} \quad (6.8)$$

Since σ_m^2 is real and positive, the matrices in the left hand side must be symmetric, positive definite. This requires that $\mathbf{N}_c^h = (\mathbf{M}_c^h)^H$. This in turn implies

$$\begin{cases} (\mathbf{i}\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c^h) \cdot \langle \mathbf{u}_m \rangle = \sigma_m \langle \mathbf{v}_m \rangle \\ (-\mathbf{i}\mathbf{k} \times \mathbf{J} + s^*(\mathbf{M}_c^h)^H) \cdot \langle \mathbf{v}_m \rangle = \sigma_m \langle \mathbf{u}_m \rangle \end{cases} \quad (6.9)$$

Multiplying the first equation with $\langle \mathbf{v}_m^* \rangle$, the second with $\langle \mathbf{u}_m^* \rangle$ and taking the complex conjugate of the second equation, the left hand sides are equal. This means the scalar products $\langle \mathbf{u}_m^* \rangle \cdot \langle \mathbf{u}_m \rangle$ and $\langle \mathbf{v}_m^* \rangle \cdot \langle \mathbf{v}_m \rangle$ must be equal, and the mean values can be normalized.

6.3 Homogenization

Now, we identify (6.9) as a singular value decomposition of a finite dimensional matrix $i\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c^h$. This implies that $\{\langle \mathbf{u}_m \rangle\}_{m \in I}$ are mutually orthogonal, and the matrix formed by the sum

$$\mathbf{M}_c^h = \sum_{m \in I} \frac{\langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle \langle \mathbf{u}_m^* \rangle}{\langle \mathbf{u}_m^* \rangle \cdot \langle \mathbf{u}_m \rangle} \quad (6.10)$$

satisfies $\mathbf{M}_c^h \cdot \langle \mathbf{u}_m \rangle = \langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle$ for all $m \in I$, and is therefore a representation of the homogenized matrix. The same reasoning can be applied to the vectors $\{\langle \mathbf{v}_m \rangle\}_{m \in I}$, and we have the following representations of the homogenized matrix:

$$\mathbf{M}_c^h = \sum_{m \in I} \frac{\langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle \langle \mathbf{u}_m^* \rangle}{\langle \mathbf{u}_m^* \rangle \cdot \langle \mathbf{u}_m \rangle} \quad (6.11)$$

$$(\mathbf{M}_c^h)^H = \sum_{m \in I} \frac{\langle \mathbf{M}_c^H \cdot \mathbf{v}_m \rangle \langle \mathbf{v}_m^* \rangle}{\langle \mathbf{v}_m^* \rangle \cdot \langle \mathbf{v}_m \rangle} \quad (6.12)$$

which can be computed from the singular value decomposition (4.25).

7 Discussion

We have given a homogenization formula for dispersive materials, based on a singular value decomposition of non-selfadjoint partial differential operators. In this section, we discuss some loose ends and interesting possibilities.

7.1 Anything special about the index set I ?

An interesting question is “what happens if we change one of the functions in I ?”

Assume there are more than 6 u_n with non-zero mean value. Let I denote the “normal” index set of 6 linearly independent mean values, which we use in the paper. Let $n' \notin I$ be the index of one of the remaining modes with non-zero mean value. Then there is at least one index $m' \in I$ with the property $\langle \mathbf{u}_{m'}^* \rangle \cdot \langle \mathbf{u}_{n'} \rangle \neq 0$. Let I' denote the index set where m' is replaced by n' . All mean values $\langle \mathbf{u}_m \rangle$ with $m \in I'$ are mutually orthogonal, since they correspond to a singular value decomposition. Since I and I' differ only in one element, the mean values corresponding to these indices must be proportional to each other.

Thus, any index n which corresponds to non-zero mean values, can be considered as a “harmonic” of one of the six modes corresponding to the smallest singular values. However, it is likely that $\langle \mathbf{M}_c \cdot \mathbf{u}_{m'} \rangle \neq \langle \mathbf{M}_c \cdot \mathbf{u}_{n'} \rangle$, and consequently $\mathbf{M}_c^h \neq \mathbf{M}_c^{h'}$.

7.2 Non-existence of scale-invariant problem

Introduce dimension free quantities according to

$$\mathbf{x} = a\mathbf{y}, \quad \mathbf{k} = a^{-1}\boldsymbol{\eta}, \quad \tilde{\sigma}_n = a\sigma_n \quad (7.1)$$

where a is the physical size of the unit cell. The singular value decomposition (4.25) then becomes

$$\begin{cases} ((\nabla_{\mathbf{y}} + i\boldsymbol{\eta}) \times \mathbf{J} + as\mathbf{M}_c(s)) \cdot \mathbf{u}_n = \tilde{\sigma}_n \mathbf{v}_n \\ (- (\nabla_{\mathbf{y}} + i\boldsymbol{\eta}) \times \mathbf{J} + as^*(\mathbf{M}_c(s))^H) \cdot \mathbf{v}_n = \tilde{\sigma}_n \mathbf{u}_n \end{cases} \quad (7.2)$$

This demonstrates that for a dispersive material, where the matrix \mathbf{M}_c depends on the frequency s , we cannot get rid of the scale a completely in our calculations. It is instructive to take a look at the simplest case, symmetric optical response with conductivity, *i.e.*, $\mathbf{M}_c(s) = \mathbf{M} + \boldsymbol{\sigma}/s$. In this case, the equations are

$$\begin{cases} ((\nabla_{\mathbf{y}} + i\boldsymbol{\eta}) \times \mathbf{J} + as\mathbf{M} + a\boldsymbol{\sigma}) \cdot \mathbf{u}_n = \tilde{\sigma}_n \mathbf{v}_n \\ (- (\nabla_{\mathbf{y}} + i\boldsymbol{\eta}) \times \mathbf{J} + as^*\mathbf{M} + a\boldsymbol{\sigma}) \cdot \mathbf{v}_n = \tilde{\sigma}_n \mathbf{u}_n \end{cases} \quad (7.3)$$

From this formulation we see that we can only get a scale invariant problem, which defines $(\tilde{\sigma}_n, \mathbf{u}_n, \mathbf{v}_n)$, if as and $a\boldsymbol{\sigma}$ are kept constant as $a \rightarrow 0$. This shows that in general we need to make the material properties depend on the scale a if we want to define a scale-invariant unit cell problem.

7.3 Future investigations

There does not seem to exist any standard numerical tools to calculate the singular value decomposition for partial differential operators. One option is to do a finite element discretization of the equations, and do a singular value decomposition of the resulting matrix. Since we are only interested in a few of the singular vectors, a power method should be employed to extract only the smallest singular values we are interested in. The discretization can also be made with the fast Fourier transform, which promises to be a very efficient way to do the calculations.

The present method is an extension of the method presented in [13], where only symmetric, non-dispersive media could be treated. The strength of the method presented in this paper, as compared to classical homogenization methods, is that it is possible to calculate the material behavior for wavelengths not necessarily infinitely large compared to the unit cell. In this respect, some spatial dispersion effects can be captured. One possibility is to do a rigorous study of chiral media, where a coupling between electric and magnetic fields is created by, for instance, metallic inclusions such as small coils. This effect always vanishes in the extreme homogenization limit, where the unit cell is infinitely small compared to the wavelength.

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Appendix A Homogeneous, isotropic media

In this appendix we compute the singular values and the corresponding vectors for a homogeneous material with constitutive parameters

$$\mathbf{M}_c(s) = \begin{pmatrix} \epsilon_c(s)\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mu_c(s)\mathbf{I} \end{pmatrix} \quad (\text{A.1})$$

where $\epsilon_c(s)$ and $\mu_c(s)$ are scalars, constant in space but possibly functions of s . The most common case is $\epsilon_c = \epsilon + \sigma/s$ and $\mu_c = 1$, *i.e.*, a non-magnetic, lossy dielectric, which we occasionally mention the explicit result for. The equations (4.25) can then be Fourier transformed in space to read

$$\begin{cases} (\mathbf{i}(\mathbf{k}_n + \mathbf{k}) \times \mathbf{J} + s\mathbf{M}_c) \cdot \hat{\mathbf{u}}_{nn} = \sigma_n \hat{\mathbf{v}}_{nn} \\ (-\mathbf{i}(\mathbf{k}_n + \mathbf{k}) \times \mathbf{J} + s^* \mathbf{M}_c^H) \cdot \hat{\mathbf{v}}_{nn} = \sigma_n \hat{\mathbf{u}}_{nn} \end{cases} \quad (\text{A.2})$$

where $\mathbf{k}_n = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3$. In order to proceed, we need the singular value decomposition of a finite dimensional matrix. In the following, we skip the indices n and \mathbf{n} and write only \mathbf{k} instead of $\mathbf{k}_n + \mathbf{k}$, in order to reduce the notational complexity.

Theorem A.1. *The singular value decomposition defined by the equations*

$$\begin{cases} (\mathbf{i}\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c) \cdot \hat{\mathbf{u}} = \sigma \hat{\mathbf{v}} \\ (-\mathbf{i}\mathbf{k} \times \mathbf{J} + s^* \mathbf{M}_c^H) \cdot \hat{\mathbf{v}} = \sigma \hat{\mathbf{u}} \end{cases} \quad (\text{A.3})$$

is given by the two singular values and their associated singular vectors

$$\sigma^2 = |s\epsilon_c|^2, \quad \hat{\mathbf{u}} = \begin{pmatrix} \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix}, \quad \hat{\mathbf{v}} = \frac{s\epsilon_c}{|s\epsilon_c|} \begin{pmatrix} \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix}, \quad (\text{A.4})$$

$$\sigma^2 = |s\mu_c|^2, \quad \hat{\mathbf{u}} = \begin{pmatrix} \mathbf{0} \\ \hat{\mathbf{k}} \end{pmatrix}, \quad \hat{\mathbf{v}} = \frac{s\mu_c}{|s\mu_c|} \begin{pmatrix} \mathbf{0} \\ \hat{\mathbf{k}} \end{pmatrix} \quad (\text{A.5})$$

and the four singular values (each is double)

$$\sigma_{\pm}^2 = k^2 + \frac{|s\epsilon_c|^2 + |s\mu_c|^2}{2} \pm \sqrt{\left(\frac{|s\epsilon_c|^2 - |s\mu_c|^2}{2}\right)^2 + k^2 |s\epsilon_c - s^* \mu_c^*|^2} \quad (\text{A.6})$$

and their associated singular vectors (with \mathbf{E}_{\perp} orthogonal to \mathbf{k} , hence two possible polarizations for each σ)

$$\hat{\mathbf{u}} = \begin{pmatrix} \hat{\mathbf{E}}_{\perp} \\ \frac{1}{\eta_{\pm}} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp} \end{pmatrix}, \quad \hat{\mathbf{v}} = \frac{1}{\sigma_{\pm}} \begin{pmatrix} (s\epsilon_c + \mathbf{i}k/\eta_{\pm}) \hat{\mathbf{E}}_{\perp} \\ (s\mu_c + \mathbf{i}k\eta_{\pm}) \frac{1}{\eta_{\pm}} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp} \end{pmatrix} \quad (\text{A.7})$$

with the wave impedance

$$\frac{1}{\eta_{\pm}} = \frac{|s\mu_c|^2 - |s\epsilon_c|^2}{2\mathbf{i}k(s^* \epsilon_c^* - s\mu_c)} \pm \frac{k|s\epsilon_c - s^* \mu_c^*|}{\mathbf{i}k(s^* \epsilon_c^* - s\mu_c)} \sqrt{\left(\frac{|s\epsilon_c|^2 - |s\mu_c|^2}{2k|s\epsilon_c - s^* \mu_c^*|}\right)^2 + 1} \quad (\text{A.8})$$

The characteristic frequencies, i.e., those s for which some $\sigma_n = 0$, are determined by the equation

$$k^2 = -\operatorname{Re}(s\epsilon_c s\mu_c) \left(1 \pm \sqrt{1 - \left| \frac{s\epsilon_c s\mu_c}{\operatorname{Re}(s\epsilon_c s\mu_c)} \right|^2} \right) \quad (\text{A.9})$$

For $\epsilon_c = \epsilon + \sigma/s$ and $\mu_c = \mu$, this is

$$s = -\frac{\sigma}{2\epsilon} \pm i\sqrt{\frac{k^2}{\epsilon\mu} - \left(\frac{\sigma}{2\epsilon}\right)^2} \quad (\text{A.10})$$

Proof. Is given by explicit calculations in the following subsections. \square

The singular vectors in the \mathbf{k} -direction correspond precisely to the subspaces of the function spaces X and Y which have non-zero divergence. Briefly returning to the indices n and \mathbf{n} , this means we should actually normalize them so that

$$\hat{\mathbf{u}}_{nn} = \frac{\mathbf{k}_n + \mathbf{k}}{|\mathbf{k}_n + \mathbf{k}|^2} \begin{pmatrix} \hat{\rho}_e(\mathbf{k}_n + \mathbf{k}) \\ 0 \end{pmatrix}, \quad \hat{\mathbf{v}}_{nn} = \frac{s\epsilon_c}{|s\epsilon_c|} \frac{\mathbf{k}_n + \mathbf{k}}{|\mathbf{k}_n + \mathbf{k}|^2} \begin{pmatrix} \hat{\rho}_e(\mathbf{k}_n + \mathbf{k}) \\ 0 \end{pmatrix} \quad (\text{A.11})$$

$$\hat{\mathbf{u}}_{nn} = \frac{\mathbf{k}_n + \mathbf{k}}{|\mathbf{k}_n + \mathbf{k}|^2} \begin{pmatrix} 0 \\ \hat{\rho}_h(\mathbf{k}_n + \mathbf{k}) \end{pmatrix}, \quad \hat{\mathbf{v}}_{nn} = \frac{s\mu_c}{|s\mu_c|} \frac{\mathbf{k}_n + \mathbf{k}}{|\mathbf{k}_n + \mathbf{k}|^2} \begin{pmatrix} 0 \\ \hat{\rho}_h(\mathbf{k}_n + \mathbf{k}) \end{pmatrix} \quad (\text{A.12})$$

but we do not go deeper into this. The singular values are not changed by this modification. The only singular vectors with non-zero mean values are the six vectors corresponding to $\mathbf{k}_n = \mathbf{0}$, which defines the index set I . It is shown in the following subsections that the homogenization formula

$$\mathbf{M}_c^h = \sum_{m \in I} \frac{\langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle \langle \mathbf{u}_m^* \rangle}{\langle \mathbf{u}_m \rangle \cdot \langle \mathbf{u}_m^* \rangle} = \begin{pmatrix} \epsilon_c \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mu_c \mathbf{I} \end{pmatrix} \quad (\text{A.13})$$

holds true with the explicit singular vectors defined in the above theorem. Before turning to the proof of this theorem, we give its corollary for the vacuum case, which is used in the estimate of the singular values in the paper.

Corollary A.1. *In the vacuum case, $\mathbf{M}_c = \mathbf{I}$, the singular value decomposition is given by the two singular values and their associated singular vectors*

$$\sigma^2 = |s|^2, \quad \hat{\mathbf{u}} = \begin{pmatrix} \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix}, \quad \hat{\mathbf{v}} = \frac{s}{|s|} \begin{pmatrix} \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix}, \quad (\text{A.14})$$

$$\sigma^2 = |s|^2, \quad \hat{\mathbf{u}} = \begin{pmatrix} \mathbf{0} \\ \hat{\mathbf{k}} \end{pmatrix}, \quad \hat{\mathbf{v}} = \frac{s}{|s|} \begin{pmatrix} \mathbf{0} \\ \hat{\mathbf{k}} \end{pmatrix} \quad (\text{A.15})$$

and the four singular values (each is double)

$$\sigma_{\pm}^2 = |\operatorname{Re} s|^2 + (k \pm |\operatorname{Im} s|)^2 \quad (\text{A.16})$$

and their associated singular vectors (with \mathbf{E}_\perp orthogonal to \mathbf{k} , hence two possible polarizations for each σ)

$$\hat{\mathbf{u}} = \begin{pmatrix} \hat{\mathbf{E}}_\perp \\ \frac{1}{\eta_\pm} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_\perp \end{pmatrix}, \quad \hat{\mathbf{v}} = \frac{1}{\sigma_\pm} \begin{pmatrix} (s + ik/\eta_\pm) \hat{\mathbf{E}}_\perp \\ (s + ik\eta_\pm) \frac{1}{\eta_\pm} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_\perp \end{pmatrix} \quad (\text{A.17})$$

with the wave impedance

$$\frac{1}{\eta_\pm} = \pm \text{sign}(\text{Im } s) \quad (\text{A.18})$$

The characteristic frequencies, i.e., those s for which some $\sigma_n = 0$, are determined by

$$s = \pm ik \quad (\text{A.19})$$

A.1 Singular values

We now turn to the proof of Theorem A.1. Starting with

$$\begin{cases} (i\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c) \cdot \hat{\mathbf{u}} = \sigma \hat{\mathbf{v}} \\ (-i\mathbf{k} \times \mathbf{J} + s^* \mathbf{M}_c^H) \cdot \hat{\mathbf{v}} = \sigma \hat{\mathbf{u}} \end{cases} \quad (\text{A.20})$$

the singular values are determined by the equation

$$(-i\mathbf{k} \times \mathbf{J} + s^* \mathbf{M}_c^H) \cdot (i\mathbf{k} \times \mathbf{J} + s\mathbf{M}_c) \cdot \hat{\mathbf{u}} = \sigma^2 \hat{\mathbf{u}} \quad (\text{A.21})$$

This is expanded as

$$(\mathbf{k} \times \mathbf{J} \cdot \mathbf{k} \times \mathbf{J} + |s|^2 \mathbf{M}_c^H \cdot \mathbf{M}_c - i\mathbf{k} \times \mathbf{J} \cdot s\mathbf{M}_c + s^* \mathbf{M}_c^H \cdot i\mathbf{k} \times \mathbf{J}) \cdot \hat{\mathbf{u}} = \sigma^2 \hat{\mathbf{u}} \quad (\text{A.22})$$

and since $\mathbf{k} \times \mathbf{J} \cdot \mathbf{k} \times \mathbf{J} = k^2 \mathbf{I} - \mathbf{k}\mathbf{k}$ this is

$$\begin{pmatrix} (k^2 + |s\epsilon_c|^2) \mathbf{I} - \mathbf{k}\mathbf{k} & -(s^* \epsilon_c^* - s\mu_c) i\mathbf{k} \times \mathbf{I} \\ -(s\epsilon_c - s^* \mu_c^*) i\mathbf{k} \times \mathbf{I} & (k^2 + |s\mu_c|^2) \mathbf{I} - \mathbf{k}\mathbf{k} \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \sigma^2 \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} \quad (\text{A.23})$$

There are two immediate solutions:

$$\hat{\mathbf{u}} = \begin{pmatrix} \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix} \Rightarrow \sigma^2 = |s\epsilon_c|^2, \quad \hat{\mathbf{v}} = \frac{s\epsilon_c}{|s\epsilon_c|} \begin{pmatrix} \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix} \quad (\text{A.24})$$

$$\hat{\mathbf{u}} = \begin{pmatrix} \mathbf{0} \\ \hat{\mathbf{k}} \end{pmatrix} \Rightarrow \sigma^2 = |s\mu_c|^2, \quad \hat{\mathbf{v}} = \frac{s\mu_c}{|s\mu_c|} \begin{pmatrix} \mathbf{0} \\ \hat{\mathbf{k}} \end{pmatrix} \quad (\text{A.25})$$

The other solutions are orthogonal to \mathbf{k} . They can be written

$$\hat{\mathbf{u}} = \begin{pmatrix} \hat{\mathbf{E}}_\perp \\ \frac{1}{\eta} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_\perp \end{pmatrix} \Rightarrow \hat{\mathbf{v}} = \frac{1}{\sigma} \begin{pmatrix} (s\epsilon_c + ik/\eta) \hat{\mathbf{E}}_\perp \\ (s\mu_c + ik\eta) \frac{1}{\eta} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_\perp \end{pmatrix} \quad (\text{A.26})$$

where η is the (so far unknown) wave impedance. Using this ansatz, the equations become

$$[k^2 + |s\epsilon_c|^2 + \frac{ik}{\eta}(s^*\epsilon_c^* - s\mu_c)]\hat{\mathbf{E}}_{\perp} = \sigma^2\hat{\mathbf{E}}_{\perp} \quad (\text{A.27})$$

$$[-ik(s\epsilon_c - s^*\mu_c^*) + \frac{1}{\eta}(k^2 + |s\mu_c|^2)]\hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp} = \sigma^2\frac{1}{\eta}\hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp} \quad (\text{A.28})$$

or

$$k^2 + |s\epsilon_c|^2 + ik(s^*\epsilon_c^* - s\mu_c)/\eta = \sigma^2 \quad (\text{A.29})$$

$$k^2 + |s\mu_c|^2 - ik(s\epsilon_c - s^*\mu_c^*)\eta = \sigma^2 \quad (\text{A.30})$$

For temporary use, we introduce the notation $\alpha = ik(s^*\epsilon_c^* - s\mu_c)$,

$$k^2 + |s\epsilon_c|^2 + \alpha/\eta = \sigma^2 \quad (\text{A.31})$$

$$k^2 + |s\mu_c|^2 + \alpha^*\eta = \sigma^2 \quad (\text{A.32})$$

We eliminate $\alpha/\eta = \sigma^2 - k^2 - |s\epsilon_c|^2$ from the first equation, and use $\alpha^*\eta = |\alpha|^2\eta/\alpha$ to find

$$k^2 + |s\mu_c|^2 + |\alpha|^2\frac{1}{\sigma^2 - k^2 - |s\epsilon_c|^2} = \sigma^2 \quad (\text{A.33})$$

With $\sigma^2 - k^2 = A$, we can write

$$|s\mu_c|^2(A - |s\epsilon_c|^2) + |\alpha|^2 = A(A - |s\epsilon_c|^2) \quad (\text{A.34})$$

or

$$A^2 - A(|s\epsilon_c|^2 + |s\mu_c|^2) + |s\epsilon_c|^2|s\mu_c|^2 - |\alpha|^2 = 0 \quad (\text{A.35})$$

with the solution

$$\begin{aligned} A &= \frac{|s\epsilon_c|^2 + |s\mu_c|^2}{2} \pm \sqrt{\left(\frac{|s\epsilon_c|^2 + |s\mu_c|^2}{2}\right)^2 - |s\epsilon_c|^2|s\mu_c|^2 + |\alpha|^2} \\ &= \frac{|s\epsilon_c|^2 + |s\mu_c|^2}{2} \pm \sqrt{\left(\frac{|s\epsilon_c|^2 - |s\mu_c|^2}{2}\right)^2 + |\alpha|^2} \end{aligned} \quad (\text{A.36})$$

Expanding the expressions for A and α we have

$$\sigma^2 = k^2 + \frac{|s\epsilon_c|^2 + |s\mu_c|^2}{2} \pm \sqrt{\left(\frac{|s\epsilon_c|^2 - |s\mu_c|^2}{2}\right)^2 + k^2|s\epsilon_c - s^*\mu_c^*|^2} \quad (\text{A.37})$$

Since the singular value $\sigma \geq 0$ by definition, this provides two solutions for the singular values for each $\hat{\mathbf{E}}_{\perp}$. Since there are two degrees of freedom to choose the vector $\hat{\mathbf{E}}_{\perp}$, corresponding to TE or TM polarization, this means each solution is double.

Summing up our results, for each fixed $k = |\mathbf{k}|$ and s , we have six singular values σ , with mutually orthogonal vectors $\hat{\mathbf{u}}$. It is relevant to note that $k^2 \rightarrow \infty \Rightarrow \sigma^2 \rightarrow$

∞ for the singular values corresponding to polarizations orthogonal to $\hat{\mathbf{k}}$, whereas the singular values corresponding to polarizations parallel to $\hat{\mathbf{k}}$ do not change with k .

We note that in vacuum the result is

$$\sigma^2 = k^2 + |s|^2 \pm k|s - s^*| = |\operatorname{Re} s|^2 + (k \pm |\operatorname{Im} s|)^2 \quad (\text{A.38})$$

A.2 Wave impedance

With $\alpha/\eta = \sigma^2 - k^2 - |s\epsilon_c|^2$, the wave impedance is

$$\frac{\alpha}{\eta} = \frac{|s\mu_c|^2 - |s\epsilon_c|^2}{2} \pm \sqrt{\left(\frac{|s\epsilon_c|^2 - |s\mu_c|^2}{2}\right)^2 + k^2|s\epsilon_c - s^*\mu_c^*|^2} \quad (\text{A.39})$$

or, with $\alpha = ik(s^*\epsilon_c^* - s\mu_c)$,

$$\frac{1}{\eta} = \frac{|s\mu_c|^2 - |s\epsilon_c|^2}{2ik(s^*\epsilon_c^* - s\mu_c)} \pm \frac{k|s\epsilon_c - s^*\mu_c^*|}{ik(s^*\epsilon_c^* - s\mu_c)} \sqrt{\left(\frac{|s\epsilon_c|^2 - |s\mu_c|^2}{2k|s\epsilon_c - s^*\mu_c^*|}\right)^2 + 1} \quad (\text{A.40})$$

This expression can be written

$$\frac{1}{\eta} = e^{-i\phi}(g \pm \sqrt{1 + g^2}) \quad (\text{A.41})$$

where $\phi = \arg(ik(s^*\epsilon_c^* - s\mu_c)) = \arg(\alpha)$, and

$$g = \frac{|s\mu_c|^2 - |s\epsilon_c|^2}{2k|s\epsilon_c - s^*\mu_c^*|} \quad (\text{A.42})$$

is a real number.

We note that in vacuum we have $g = 0$ and $\alpha = ik(-2i \operatorname{Im} s) = 2k \operatorname{Im} s$, which implies $\phi = \arg(\alpha) = 0$ when $\operatorname{Im} s > 0$ and $\phi = \pi$ when $\operatorname{Im} s < 0$. This means

$$\frac{1}{\eta} = e^{-i\phi}(0 \pm \sqrt{1 + 0}) = \pm \operatorname{sign}(\operatorname{Im} s) \quad (\text{A.43})$$

A.3 Characteristic values

Setting $\sigma = 0$ implies the equation

$$\left(k^2 + \frac{|s\epsilon_c|^2 + |s\mu|^2}{2}\right)^2 = \left(\frac{|s\epsilon_c|^2 - |s\mu_c|^2}{2}\right)^2 + k^2|s\epsilon_c - s^*\mu_c^*|^2 \quad (\text{A.44})$$

This is a dispersion relation, which is satisfied by a finite number of complex values s , which are the characteristic values of Maxwell's equations. The above equation implies

$$k^4 - k^2 \underbrace{(|s\epsilon_c - s^*\mu_c^*|^2 - |s\epsilon_c|^2 - |s\mu_c|^2)}_{2 \operatorname{Re}(s\epsilon_c s\mu_c)} + |s\epsilon_c|^2 |s\mu_c|^2 = 0 \quad (\text{A.45})$$

with the solution

$$k^2 = -\operatorname{Re}(s\epsilon_c s\mu_c) \pm \sqrt{(\operatorname{Re}(s\epsilon_c s\mu_c))^2 - |s\epsilon_c|^2 |s\mu_c|^2} \quad (\text{A.46})$$

$$= -\operatorname{Re}(s\epsilon_c s\mu_c) \left(1 \pm \sqrt{1 - \left| \frac{s\epsilon_c s\mu_c}{\operatorname{Re}(s\epsilon_c s\mu_c)} \right|^2} \right) \quad (\text{A.47})$$

Since k^2 is real, this obviously requires $s\epsilon_c s\mu$ to be real. Writing $s = \eta + i\omega$, $\epsilon_c = \epsilon + \sigma/s$, and $\mu_c = \mu$, we have

$$s\epsilon_c s\mu_c = (s\epsilon + \sigma)s\mu = (\eta^2 - \omega^2)\epsilon\mu + \sigma\eta\mu + 2i\eta\omega\epsilon\mu + i\sigma\omega\mu \quad (\text{A.48})$$

For the imaginary part to be zero, we require $\eta = -\sigma/2\epsilon$. The equation for ω is then

$$\begin{aligned} k^2 = -\operatorname{Re}((s\epsilon + \sigma)s\mu) &= -((\eta^2 - \omega^2)\epsilon\mu + \sigma\eta\mu) = -\left(\left(\frac{\sigma^2}{4\epsilon^2} - \omega^2 \right) \epsilon\mu - \sigma \frac{\sigma}{2\epsilon} \mu \right) \\ &= \left(\frac{\sigma^2}{4\epsilon^2} + \omega^2 \right) \epsilon\mu \end{aligned} \quad (\text{A.49})$$

which determines ω as a function of \mathbf{k} . The characteristic values are then

$$s = -\frac{\sigma}{2\epsilon} \pm i\sqrt{\frac{k^2}{\epsilon\mu} - \left(\frac{\sigma}{2\epsilon} \right)^2} \quad (\text{A.50})$$

We see that $|s|^2 = k^2/\epsilon\mu$, and for the case of zero conductivity we obtain the standard dispersion relation $\omega = \pm k/\sqrt{\epsilon\mu}$, corresponding to waves propagating in the positive or negative $\hat{\mathbf{k}}$ -direction.

To calculate the root vectors corresponding to this frequency, we must determine the wave impedance. A key ingredient is the factor

$$s^*\epsilon + \sigma - s\mu = \frac{\sigma\epsilon}{2\epsilon} + \frac{\sigma\mu}{2\epsilon} \mp i(\epsilon + \mu)\sqrt{\frac{k^2}{\epsilon\mu} - \left(\frac{\sigma}{2\epsilon} \right)^2} = -(\epsilon + \mu)s \quad (\text{A.51})$$

Since $s\epsilon + \sigma = -s^*\epsilon$, we have

$$g = \frac{|s\mu|^2 - |s\epsilon + \sigma|^2}{2k|s\epsilon + \sigma - s^*\mu|} = |s| \frac{\mu^2 - \epsilon^2}{2k(\epsilon + \mu)} = \frac{\mu - \epsilon}{2\sqrt{\epsilon\mu}} \quad (\text{A.52})$$

and $\phi = \arg(ik(s^*\epsilon + \sigma - s\mu)) = \arg(-is) = -\arg(is^*)$. Now, it is important to remember that the \pm in (A.41) is not the same \pm as in this subsection. In fact, only the minus sign in (A.41) is appropriate for $\sigma = 0$ to hold. Thus, with $|s|^2 = k^2/\epsilon\mu$,

the wave impedance is given by

$$\begin{aligned}
\frac{1}{\eta} &= e^{-i\phi}(g - \sqrt{1+g^2}) = e^{i\arg(is^*)} \left(\frac{\mu - \epsilon}{2\sqrt{\epsilon\mu}} - \sqrt{1 + \left(\frac{\mu - \epsilon}{2\sqrt{\epsilon\mu}} \right)^2} \right) \\
&= \frac{is^*}{|s|} \left(\frac{\mu - \epsilon}{2\sqrt{\epsilon\mu}} - \sqrt{1 + \frac{(\mu - \epsilon)^2}{4\epsilon\mu}} \right) = \frac{is^*}{|s|} \left(\frac{\mu - \epsilon}{2\sqrt{\epsilon\mu}} - \sqrt{\frac{(\mu + \epsilon)^2}{4\epsilon\mu}} \right) \\
&= \frac{is^*}{|s|} \left(\frac{\mu - \epsilon}{2\sqrt{\epsilon\mu}} - \frac{\mu + \epsilon}{2\sqrt{\epsilon\mu}} \right) = \frac{is^*}{|s|} \sqrt{\epsilon/\mu} = \left(-i \frac{\sigma \sqrt{\mu/\epsilon}}{2k} \pm \sqrt{1 - \left(\frac{\sigma \sqrt{\mu/\epsilon}}{2k} \right)^2} \right) \sqrt{\epsilon/\mu} \\
&= -i \frac{\sigma}{2k} \pm \sqrt{\frac{\epsilon}{\mu} - \left(\frac{\sigma}{2k} \right)^2} \quad (\text{A.53})
\end{aligned}$$

Setting the conductivity to zero, we obtain the standard wave impedance $\eta = \pm \sqrt{\mu/\epsilon}$, corresponding to waves propagating in the positive or negative $\hat{\mathbf{k}}$ -direction.

In vacuum, the characteristic values and impedances are

$$s = \pm ik, \quad \frac{1}{\eta} = \pm 1 \quad (\text{A.54})$$

A.4 Homogenization

The index set I obviously corresponds to the six singular values for $\mathbf{n} = \mathbf{0}$, since all the other vectors have mean value zero. The homogenized matrix is

$$\mathbf{M}_c^h = \sum_{m \in I} \frac{\langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle \langle \mathbf{u}_m^* \rangle}{\langle \mathbf{u}_m \rangle \cdot \langle \mathbf{u}_m^* \rangle} \quad (\text{A.55})$$

The two vectors in (A.24) and (A.25) (ignoring the complication of normalization from equations (A.11) and (A.12)) give the contributions

$$\frac{\begin{pmatrix} \epsilon_c \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix} \begin{pmatrix} \hat{\mathbf{k}} \\ \mathbf{0} \end{pmatrix}}{\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}} = \begin{pmatrix} \epsilon_c \hat{\mathbf{k}} \hat{\mathbf{k}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \frac{\begin{pmatrix} \mathbf{0} \\ \mu_c \hat{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ \hat{\mathbf{k}} \end{pmatrix}}{\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mu_c \hat{\mathbf{k}} \hat{\mathbf{k}} \end{pmatrix} \quad (\text{A.56})$$

The contributions from the remaining four vectors can be written on the form

$$\begin{aligned}
&\frac{\begin{pmatrix} \epsilon_c \hat{\mathbf{E}}_{\perp m} \\ \frac{\mu_c}{\eta_m} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp m} \end{pmatrix} \begin{pmatrix} \hat{\mathbf{E}}_{\perp m}^* \\ \frac{1}{\eta_m^*} \hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp m}^* \end{pmatrix}}{(1 + 1/|\eta_m|^2) |\hat{\mathbf{E}}_{\perp m}|^2} \\
&= \frac{1}{(1 + \frac{1}{|\eta_m|^2}) |\hat{\mathbf{E}}_{\perp m}|^2} \begin{pmatrix} \epsilon_c \hat{\mathbf{E}}_{\perp m} \hat{\mathbf{E}}_{\perp m}^* & \frac{\epsilon_c}{\eta_m^*} \hat{\mathbf{E}}_{\perp m} (\hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp m}^*) \\ \frac{\mu_c}{\eta_m} (\hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp m}) \hat{\mathbf{E}}_{\perp m}^* & \frac{\mu_c}{|\eta_m|^2} (\hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp m}) (\hat{\mathbf{k}} \times \hat{\mathbf{E}}_{\perp m}^*) \end{pmatrix} \quad (\text{A.57})
\end{aligned}$$

Introduce the unit three-vectors $\hat{\mathbf{m}}$ and $\hat{\mathbf{l}}$ according to $\hat{\mathbf{m}} \times \hat{\mathbf{l}} = \hat{\mathbf{k}}$. The sum can then be written using the wave impedances η_{\pm} as

$$\begin{aligned} \mathbf{M}_c^h = & \begin{pmatrix} \epsilon_c \hat{\mathbf{k}} \hat{\mathbf{k}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mu_c \hat{\mathbf{k}} \hat{\mathbf{k}} \end{pmatrix} \\ & + \frac{1}{1 + \frac{1}{|\eta_+|^2}} \begin{pmatrix} \epsilon_c \hat{\mathbf{m}} \hat{\mathbf{m}} & \frac{\epsilon_c}{\eta_+^*} \hat{\mathbf{m}} \hat{\mathbf{l}} \\ \frac{\mu_c}{\eta_+} \hat{\mathbf{l}} \hat{\mathbf{m}} & \frac{\mu_c}{|\eta_+|^2} \hat{\mathbf{l}} \hat{\mathbf{l}} \end{pmatrix} + \frac{1}{1 + \frac{1}{|\eta_-|^2}} \begin{pmatrix} \epsilon_c \hat{\mathbf{m}} \hat{\mathbf{m}} & \frac{\epsilon_c}{\eta_-^*} \hat{\mathbf{m}} \hat{\mathbf{l}} \\ \frac{\mu_c}{\eta_-} \hat{\mathbf{l}} \hat{\mathbf{m}} & \frac{\mu_c}{|\eta_-|^2} \hat{\mathbf{l}} \hat{\mathbf{l}} \end{pmatrix} \\ & + \frac{1}{1 + \frac{1}{|\eta_+|^2}} \begin{pmatrix} \epsilon_c \hat{\mathbf{l}} \hat{\mathbf{l}} & -\frac{\epsilon_c}{\eta_+^*} \hat{\mathbf{l}} \hat{\mathbf{m}} \\ -\frac{\mu_c}{\eta_+} \hat{\mathbf{m}} \hat{\mathbf{l}} & \frac{\mu_c}{|\eta_+|^2} \hat{\mathbf{m}} \hat{\mathbf{m}} \end{pmatrix} + \frac{1}{1 + \frac{1}{|\eta_-|^2}} \begin{pmatrix} \epsilon_c \hat{\mathbf{l}} \hat{\mathbf{l}} & -\frac{\epsilon_c}{\eta_-^*} \hat{\mathbf{l}} \hat{\mathbf{m}} \\ -\frac{\mu_c}{\eta_-} \hat{\mathbf{m}} \hat{\mathbf{l}} & \frac{\mu_c}{|\eta_-|^2} \hat{\mathbf{m}} \hat{\mathbf{m}} \end{pmatrix} \quad (\text{A.58}) \end{aligned}$$

When adding these terms, we must determine the sums

$$\begin{aligned} & \frac{1}{1 + 1/|\eta_+|^2} + \frac{1}{1 + 1/|\eta_-|^2}, \quad \frac{1/\eta_+}{1 + 1/|\eta_+|^2} + \frac{1/\eta_-}{1 + 1/|\eta_-|^2}, \\ & \frac{1/\eta_+^*}{1 + 1/|\eta_+|^2} + \frac{1/\eta_-^*}{1 + 1/|\eta_-|^2}, \quad \text{and} \quad \frac{1/|\eta_+|^2}{1 + 1/|\eta_+|^2} + \frac{1/|\eta_-|^2}{1 + 1/|\eta_-|^2} \quad (\text{A.59}) \end{aligned}$$

With $1/\eta_{\pm} = e^{-i\phi}(g \pm \sqrt{1+g^2})$, we have $1/|\eta_{\pm}|^2 = 1 + 2g^2 \pm 2g\sqrt{1+g^2}$ and

$$\begin{aligned} & \frac{1}{1 + 1/|\eta_+|^2} + \frac{1}{1 + 1/|\eta_-|^2} = \frac{1}{1 + 1 + 2g^2 + 2g\sqrt{1+g^2}} + \frac{1}{1 + 1 + 2g^2 - 2g\sqrt{1+g^2}} \\ & = \frac{2(2 + 2g^2)}{(2(1 + g^2))^2 - (2g\sqrt{1+g^2})^2} = \frac{4(1 + g^2)}{4(1 + g^2)^2 - 4g^2(1 + g^2)} \\ & = \frac{1}{1 + g^2 - g^2} = 1 \quad (\text{A.60}) \end{aligned}$$

and (ignoring the factor $e^{-i\phi}$)

$$\begin{aligned} & \frac{e^{i\phi}/\eta_+}{1 + 1/|\eta_+|^2} + \frac{e^{i\phi}/\eta_-}{1 + 1/|\eta_-|^2} = \frac{g + \sqrt{1+g^2}}{1 + 1 + 2g^2 + 2g\sqrt{1+g^2}} + \frac{g - \sqrt{1+g^2}}{1 + 1 + 2g^2 - 2g\sqrt{1+g^2}} \\ & = g + \sqrt{1+g^2} \frac{-4g\sqrt{1+g^2}}{(2(1 + g^2))^2 - (2g\sqrt{1+g^2})^2} = g - \frac{4g(1 + g^2)}{4(1 + g^2)^2 - 4g^2(1 + g^2)} \\ & = g - \frac{g}{1 + g^2 - g^2} = 0 \quad (\text{A.61}) \end{aligned}$$

and

$$\begin{aligned} & \frac{1/|\eta_+|^2}{1 + 1/|\eta_+|^2} + \frac{1/|\eta_-|^2}{1 + 1/|\eta_-|^2} = \frac{1 + 2g^2 + 2g\sqrt{1+g^2}}{1 + 1 + 2g^2 + 2g\sqrt{1+g^2}} + \frac{1 + 2g^2 - 2g\sqrt{1+g^2}}{1 + 1 + 2g^2 - 2g\sqrt{1+g^2}} \\ & = 1 + 2g^2 + 2g\sqrt{1+g^2} \frac{-4g\sqrt{1+g^2}}{(2(1 + g^2))^2 - (2g\sqrt{1+g^2})^2} = 1 + 2g^2 - \frac{8g^2(1 + g^2)}{4(1 + g^2)^2 - 4g^2(1 + g^2)} \\ & = 1 + 2g^2 - \frac{2g^2}{1 + g^2 - g^2} = 1 \quad (\text{A.62}) \end{aligned}$$

Finally, this means that the homogenized matrix is

$$\mathbf{M}_c^h = \sum_{m \in I} \frac{\langle \mathbf{M}_c \cdot \mathbf{u}_m \rangle \langle \mathbf{u}_m^* \rangle}{\langle \mathbf{u}_m \rangle \cdot \langle \mathbf{u}_m^* \rangle} = \begin{pmatrix} \epsilon_c \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mu_c \mathbf{I} \end{pmatrix} \quad (\text{A.63})$$

which demonstrates that the homogenization theorem works as planned for homogeneous, isotropic media.

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