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A FLOQUET–BLOCH DECOMPOSITION OF MAXWELL'S EQUATIONS APPLIED TO HOMOGENIZATION[*]

DANIEL SJÖBERG[†], CHRISTIAN ENGSTRÖM[†], GERHARD KRISTENSSON[†],
DAVID J. N. WALL[‡], AND NIKLAS WELLANDER[§]

Abstract. Using Bloch waves to represent the full solution of Maxwell's equations in periodic media, we study the limit where the material's period becomes much smaller than the wavelength. It is seen that for steady state fields, only a few of the Bloch waves contribute to the full solution. Effective material parameters can be explicitly represented in terms of dyadic products of the mean values of the nonvanishing Bloch waves, providing a new means of homogenization. The representation is valid for an arbitrary wave vector in the first Brillouin zone.

Key words. Bloch waves, Maxwell's equations, homogenization, eigenvalue problem

AMS subject classifications. 78A48, 78M40, 35P20, 35Q60

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1. Introduction. The behavior of the solutions of a PDE with rapidly oscillating coefficients, considered over distances large compared to the oscillations, is in several respects similar to the solutions of a PDE with slowly varying coefficients. The problem of homogenization is to find these slowly varying coefficients by an appropriate limit process of the rapidly oscillating ones. The results of homogenization apply to several types of PDEs that are used in the engineering sciences, such as heat conduction, elastic deformation, flow in porous media, acoustics, and, to a lesser extent, Maxwell's equations.

The objective of this paper is to give a rather complete analysis of solutions to Maxwell's equations in periodic media and study the limit when the unit cell becomes small. This is done by expanding the solution in Bloch waves, i.e., eigenmodes of the material, and it is seen that only a few Bloch waves contribute to the macroscopic field. This enables us to find explicit representations of the effective material parameters in terms of these waves, providing an alternative means of homogenization.

The observation that the macroscopic properties of a periodic material are obtained in the long-wavelength limit of the Bloch waves dates back at least to [5] and has recently been used in the physics literature to study optical activity [20]. The common approach to find effective material parameters for "div-grad"-type operators using Bloch waves is through differentiation of the principal eigenvalue with respect to the Bloch parameter $\boldsymbol{k}$, which represents the mismatch of the wave vector with the period of the lattice. In the case of electron dynamics in metals, this is the effective

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[†]Department of Electroscience, Lund Institute of Technology, P.O. Box 118, 221 00 Lund, Sweden (daniel.sjoberg@es.lth.se, christian.engstrom@es.lth.se, gerhard.kristensson@es.lth.se). The research of the first and third authors was supported by the Swedish Foundation for Strategic Research (SSF).

[‡]Department of Mathematics and Statistics, University of Canterbury, Private Bag 4800, Christchurch, New Zealand (david.wall@canterbury.ac.nz).

[§]Swedish Defence Research Agency, FOI, P.O. Box 1165, 581 11 Linköping, Sweden (niklas. wellander@foi.se). This author's research was partially supported by the Swedish Foundation for International Cooperation in Research and Higher Education (STINT) and by the Harald and Louise Ekman Foundation.

mass; see almost any book on solid state physics, for instance [17, p. 193]. A rigorous study on homogenization results by Bloch waves for a scalar equation was performed in the early 1980's [22]. The method has received recent interest from the mathematics community [21, 8, 7, 1, 13], where the effective material is found from studying the spectrum of the operator only.

Maxwell's equations are more difficult to analyze than the traditional scalar elliptic equations. They constitute a system of PDEs, where the "principal" eigenvalue is often degenerate, and it is not clear which one to differentiate when the degeneracy is lifted. In this paper, we circumvent this difficulty by expressing the homogenization primarily in terms of eigenvectors instead of eigenvalues. The main result is Theorem 6.2, a surprisingly simple representation of the homogenized matrix, which is applicable for any wave vector within the first Brillouin zone. It states that it is possible to define a homogenized material matrix for a given wave vector $\boldsymbol{k}$, and this matrix can be represented by calculating mean values of the Bloch waves. In order to prove this theorem, we need to make a conjecture in section 6.1.

The method used is based on constitutive relations where the permittivity and permeability are described by symmetric, positive definite matrices. With these constitutive relations, we can define differential operators which are self-adjoint, and we are able to apply classical spectral theorems. Conductivity and dispersive constitutive relations are at this stage not possible to include in this framework, since they lead to non-self-adjoint operators for which a more advanced spectral theory is needed; see, for instance, [19].

Finally, we remark that the homogenization results in this paper are ready for implementation, provided the mean values of the Bloch waves can be computed. This can be done analytically for some geometries such as laminates when $\boldsymbol{k} = \boldsymbol{0}$ (since this is just the standard homogenization case), but for arbitrary $\boldsymbol{k}$ we can so far perform only numerical calculations. Standard computational means exist for this task, such as photonic band gap techniques and finite elements [15, 10].

This paper is organized as follows. In section 2 we present the notation and the different function spaces used in this paper, and a variant of the famous Bloch theorem is given in section 3. Spectral properties for the curl operators in Maxwell's equations are given in section 4, and they are used in section 5 to give a representation of the general solution to Maxwell's equations in periodic media. Section 6 presents the scaling arguments needed in homogenization, where we show that only a few Bloch waves contribute to the macroscopic field. We show that the classical homogenization technique can be obtained as a limit of our formalism and present a new representation of the homogenized matrix for a finite wave vector. The results are discussed in section 7.

2. Basic equations and notation. We use scaled electric and magnetic fields and flux densities in this paper; i.e., the SI-unit fields $\boldsymbol{E}_{\mathrm{SI}}$, $\boldsymbol{H}_{\mathrm{SI}}$, $\boldsymbol{D}_{\mathrm{SI}}$, and $\boldsymbol{B}_{\mathrm{SI}}$ are related to the fields $\boldsymbol{E}$, $\boldsymbol{H}$, $\boldsymbol{D}$, and $\boldsymbol{B}$ used in this paper by

$$(2.1) \qquad \boldsymbol{E}_{\mathrm{SI}}(\boldsymbol{x}, t) = \epsilon_0^{-1/2} \boldsymbol{E}(\boldsymbol{x}, \tau), \qquad\qquad \boldsymbol{H}_{\mathrm{SI}}(\boldsymbol{x}, t) = \mu_0^{-1/2} \boldsymbol{H}(\boldsymbol{x}, \tau),$$

$$(2.2) \qquad \boldsymbol{D}_{\mathrm{SI}}(\boldsymbol{x}, t) = \epsilon_0^{1/2} \boldsymbol{D}(\boldsymbol{x}, \tau), \qquad\qquad \boldsymbol{B}_{\mathrm{SI}}(\boldsymbol{x}, t) = \mu_0^{1/2} \boldsymbol{B}(\boldsymbol{x}, \tau),$$

where the permittivity and permeability of vacuum are denoted ϵ_0 and μ_0, respectively. The time is scaled according to $\tau = c_0 t_{\mathrm{SI}}$, where c_0 is the speed of light in vacuum, so that both space and time have the physical dimension length. The corresponding relations for the current density $\boldsymbol{J}_{\mathrm{SI}}$ and the charge density ρ_{SI} are

(2.3) $$\boldsymbol{J}_{\mathrm{SI}}(\boldsymbol{x}, t) = \mu_0^{-1/2} \boldsymbol{J}(\boldsymbol{x}, \tau), \qquad \rho_{\mathrm{SI}}(\boldsymbol{x}, t) = \epsilon_0^{1/2} \rho(\boldsymbol{x}, \tau).$$

In these units, Maxwell's equations are

(2.4)
$$\begin{cases} \nabla \times \boldsymbol{E}(\boldsymbol{x}, \tau) = -\partial_\tau \boldsymbol{B}(\boldsymbol{x}, \tau), \\ \nabla \times \boldsymbol{H}(\boldsymbol{x}, \tau) = \boldsymbol{J}(\boldsymbol{x}, \tau) + \partial_\tau \boldsymbol{D}(\boldsymbol{x}, \tau), \end{cases}$$

and

(2.5)
$$\begin{cases} \nabla \cdot \boldsymbol{B}(\boldsymbol{x}, \tau) = 0, \\ \nabla \cdot \boldsymbol{D}(\boldsymbol{x}, \tau) = \rho(\boldsymbol{x}, \tau). \end{cases}$$

2.1. Six-dimensional vectors and differential operators. We adopt a six-dimensional notation. The fields are defined as

(2.6) $$\mathsf{e}(\boldsymbol{x}, \tau) = \begin{pmatrix} \boldsymbol{E}(\boldsymbol{x}, \tau) \\ \boldsymbol{H}(\boldsymbol{x}, \tau) \end{pmatrix}, \qquad \mathsf{d}(\boldsymbol{x}, \tau) = \begin{pmatrix} \boldsymbol{D}(\boldsymbol{x}, \tau) \\ \boldsymbol{B}(\boldsymbol{x}, \tau) \end{pmatrix},$$

and the material parameters are

(2.7) $$\mathsf{M}(\boldsymbol{x}) = \begin{pmatrix} \boldsymbol{\epsilon}(\boldsymbol{x}) & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\mu}(\boldsymbol{x}) \end{pmatrix},$$

where $\boldsymbol{\epsilon}(\boldsymbol{x})$ and $\boldsymbol{\mu}(\boldsymbol{x})$ are real, symmetric matrices with L^∞ entries, and the matrix satisfies

(2.8) $$c|\mathsf{e}|^2 \le \mathsf{e}^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{e} \le C|\mathsf{e}|^2$$

for all six-vectors e, with positive constants c and C independent of $\boldsymbol{x}$. We call such a matrix uniformly coercive. The constitutive relations between the fields are

(2.9) $$\mathsf{d}(\boldsymbol{x}, \tau) = \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{e}(\boldsymbol{x}, \tau).$$

This constitutive relation models only the instantaneous response of the material constituents and neglects any dispersive effects.

In the following, we define a number of spatial differential operators, where it helps to think of the nabla operator ∇ as a three-dimensional vector. Indeed, many natural, bounded operators occur in the following sections by simply replacing the ∇ symbol with a three-vector, often denoted $\boldsymbol{k}$. In many cases, the nabla operator is multiplied by $-\mathrm{i}$, in order to make the operator $-\mathrm{i}\nabla$ self-adjoint in a sesquilinear scalar product. Define the curl operator $\nabla \times \mathsf{J}$ in $\mathbb{C}^6$,

(2.10) $$\nabla \times \mathsf{J} = \begin{pmatrix} \mathbf{0} & -\nabla \times \mathbf{I} \\ \nabla \times \mathbf{I} & \mathbf{0} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & \partial_3 & -\partial_2 \\ 0 & 0 & 0 & -\partial_3 & 0 & \partial_1 \\ 0 & 0 & 0 & \partial_2 & -\partial_1 & 0 \\ 0 & -\partial_3 & \partial_2 & 0 & 0 & 0 \\ \partial_3 & 0 & -\partial_1 & 0 & 0 & 0 \\ -\partial_2 & \partial_1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where $\nabla = \hat{\boldsymbol{e}}_1 \partial_1 + \hat{\boldsymbol{e}}_2 \partial_2 + \hat{\boldsymbol{e}}_2 \partial_2$, with $\hat{\boldsymbol{e}}_{1,2,3}$ being the unit vectors in three orthogonal spatial directions and $\partial_{1,2,3}$ denoting differentiation in the corresponding variable, and $\mathbf{I}$ is the identity dyadic in $\mathbb{C}^3$. The matrix J is

(2.11) $$\mathsf{J} = \begin{pmatrix} \mathbf{0} & -\mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix},$$

and $\mathbf{0}$ is the zero dyadic in $\mathbb{C}^3$. The action on a six-dimensional vector is a new six-dimensional vector:

$$(2.12) \qquad \nabla \times \mathsf{J} \cdot \mathsf{e}(\boldsymbol{x}, \tau) = \begin{pmatrix} -\nabla \times \boldsymbol{H}(\boldsymbol{x}, \tau) \\ \nabla \times \boldsymbol{E}(\boldsymbol{x}, \tau) \end{pmatrix}.$$

The divergence of a six-dimensional vector is a two-dimensional vector:

$$(2.13) \qquad \nabla \cdot \mathsf{d}(\boldsymbol{x}, \tau) = \begin{pmatrix} \nabla \cdot \boldsymbol{D}(\boldsymbol{x}, \tau) \\ \nabla \cdot \boldsymbol{B}(\boldsymbol{x}, \tau) \end{pmatrix}.$$

The gradient of a two-scalar $\phi = (\phi^{\mathrm{e}}, \phi^{\mathrm{h}})^{\mathrm{T}}$ is also a six-vector:

$$(2.14) \qquad \nabla \phi = \begin{pmatrix} \nabla \phi^{\mathrm{e}} \\ \nabla \phi^{\mathrm{h}} \end{pmatrix}.$$

The usual differential orthogonalities are

$$(2.15) \qquad \nabla \cdot [\nabla \times \mathsf{J} \cdot \mathsf{e}(\boldsymbol{x}, \tau)] \equiv 0 \quad \text{and} \quad \nabla \times \mathsf{J} \cdot \nabla \phi \equiv \mathbf{0}.$$

Maxwell's equations can then be written (curl equations, six scalar equations)

$$(2.16) \qquad \nabla \times \mathsf{J} \cdot \mathsf{e}(\boldsymbol{x}, \tau) + \partial_\tau \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{e}(\boldsymbol{x}, \tau) + \mathsf{j}(\boldsymbol{x}, \tau) = \mathbf{0},$$

where $\mathsf{j} = (\boldsymbol{J}, \mathbf{0})^{\mathrm{T}}$, supplemented by the divergence equations (two scalar equations)

$$(2.17) \qquad \nabla \cdot [\mathsf{M}(\boldsymbol{x}) \cdot \mathsf{e}(\boldsymbol{x}, \tau)] = \varrho(\boldsymbol{x}, \tau),$$

where $\varrho = (\rho, 0)^{\mathrm{T}}$ is a two-scalar and satisfies $\int \varrho(\boldsymbol{y}) \, \mathrm{d}v_{\boldsymbol{y}} = 0$. The last condition means the total charge is zero, which is needed in the proofs below. Ignoring possible boundary effects, the material's response to an external field e_0 can be considered by using the polarization field $(\mathsf{M} - \mathsf{M}_0) \cdot \mathsf{e}_0$, where e_0 is a solution in a background medium M_0, by introducing sources $\mathsf{j} = \partial_\tau (\mathsf{M} - \mathsf{M}_0) \cdot \mathsf{e}_0$ and $\varrho = -\nabla \cdot [(\mathsf{M} - \mathsf{M}_0) \cdot \mathsf{e}_0]$.

For developing the representation of the solution to Maxwell's equations in section 5.1, we assume only the sources j and ϱ are square integrable in space. However, when discussing homogenization in section 6, we assume that the frequency spectrum of the sources is band limited. Since the sources are usually generated by some electronic equipment where we can control the time dependence, this is a reasonable assumption. A further discussion of the band limited frequency spectrum, and its consequences to homogenization, is found in Remark 5 in section 6.

2.2. Function spaces for periodic media. We further assume the medium is periodic. The unit cell is denoted by U, and the periodic material satisfies $\mathsf{M}(\boldsymbol{x}+\boldsymbol{x_n}) = \mathsf{M}(\boldsymbol{x})$, $\boldsymbol{n} \in \mathbb{Z}^3$, where $\boldsymbol{x_n} = n_1 \boldsymbol{a}_1 + n_2 \boldsymbol{a}_2 + n_3 \boldsymbol{a}_3$ and $\boldsymbol{a}_i$, $i = 1, 2, 3$, are the basis vectors for the lattice. The reciprocal unit cell is denoted by U', and a vector in the reciprocal lattice is $\boldsymbol{k_n} = n_1 \boldsymbol{b}_1 + n_2 \boldsymbol{b}_2 + n_3 \boldsymbol{b}_3$, where $\boldsymbol{b}_1 = \frac{2\pi}{|U|} \boldsymbol{a}_2 \times \boldsymbol{a}_3$, $\boldsymbol{b}_2 = \frac{2\pi}{|U|} \boldsymbol{a}_3 \times \boldsymbol{a}_1$, $\boldsymbol{b}_3 = \frac{2\pi}{|U|} \boldsymbol{a}_1 \times \boldsymbol{a}_2$, and $|U| = \boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$. This implies $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi \delta_{ij}$, 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 [17].

We need some standard function spaces defined as below, where $C_\#^\infty(U; \mathbb{C}^6)$ and $C_\#^\infty(U; \mathbb{C}^2)$ are the spaces of infinitely differentiable periodic functions on U with

values in $\mathbb{C}^6$ and $\mathbb{C}^2$, respectively:

(2.18) $L^2_\#(U; \mathbb{C}^6) = $ the completion of $C^\infty_\#(U; \mathbb{C}^6)$ in the L^2 norm,

(2.19) $L^2_\#(U; \mathbb{C}^2) = $ the completion of $C^\infty_\#(U; \mathbb{C}^2)$ in the L^2 norm,

(2.20) $H_\#(\mathrm{rot}) = \{\mathsf{v} \in L^2_\#(U; \mathbb{C}^6) : -\mathrm{i}\nabla \times \mathsf{J} \cdot \mathsf{v} \in L^2_\#(U; \mathbb{C}^6)\}$,

(2.21) $H^1_\#(U; \mathbb{C}^2) = \{\phi \in L^2_\#(U; \mathbb{C}^2) : -\mathrm{i}\nabla\phi \in L^2_\#(U; \mathbb{C}^6)\}$.

In sections 4.2 and 4.3, we also introduce the more specialized spaces $H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho})$ and $H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho})$, which are closed subspaces of $L^2_\#(U; \mathbb{C}^6)$.

Due to the periodic boundary conditions, these spaces contain functions which are constants. The L^2 spaces are equipped with either the ordinary L^2 scalar product

(2.22) $$(\mathsf{u}, \mathsf{v}) = \int_U \mathsf{u} \cdot \mathsf{v}^* \, dv_{\boldsymbol{x}}$$

and its induced norm or the weighted scalar product $(\mathsf{u}, \mathsf{M} \cdot \mathsf{v})$ and its induced norm. The norms are equivalent due to (2.8).

We often use the mean value of a quantity defined in the unit cell. This is the integral over the unit cell,

(2.23) $$\langle f \rangle \equiv \frac{1}{|U|} \int_U f(\boldsymbol{x}) \, dv_{\boldsymbol{x}}.$$

3. The Floquet–Bloch theorem. In this section we present a version of the celebrated Floquet–Bloch theorem, first given in a one-dimensional setting by Floquet [12] and later rediscovered by Bloch [4]. The proof is given since these references may be difficult to find, and we need to reference the explicit representations of the Bloch amplitude later in the paper.

THEOREM 3.1. *Any function $\mathsf{u}(\boldsymbol{x}) \in L^2(\mathbb{R}^3; \mathbb{C}^6)$ can be represented as*

(3.1) $$\mathsf{u}(\boldsymbol{x}) = \int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) \, dv_{\boldsymbol{k}},$$

where the Bloch amplitude $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})$ is U-periodic in $\boldsymbol{x}$ and has the representations

(3.2) $$\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) = \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \hat{\mathsf{u}}(\boldsymbol{k} + \boldsymbol{k_n}) \mathrm{e}^{\mathrm{i}\boldsymbol{k_n}\cdot\boldsymbol{x}} = \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathsf{u}(\boldsymbol{x} + \boldsymbol{x_n}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}+\boldsymbol{x_n})},$$

where $\hat{\mathsf{u}}(\boldsymbol{k})$ is the Fourier transform of $\mathsf{u}(\boldsymbol{x})$.

Proof. An L^2 function can be represented with its Fourier transform $\hat{\mathsf{u}}(\boldsymbol{k})$ according to

(3.3) $$\mathsf{u}(\boldsymbol{x}) = \int_{\mathbb{R}^3} \hat{\mathsf{u}}(\boldsymbol{k}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \, dv_{\boldsymbol{k}}.$$

The integral can be divided into blocks of U',

(3.4) $$\int_{\mathbb{R}^3} \hat{\mathsf{u}}(\boldsymbol{k}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \, dv_{\boldsymbol{k}} = \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \int_{\boldsymbol{k} \in U'} \hat{\mathsf{u}}(\boldsymbol{k} + \boldsymbol{k_n}) \mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{k_n})\cdot\boldsymbol{x}} \, dv_{\boldsymbol{k}}$$

$$= \int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \hat{\mathsf{u}}(\boldsymbol{k} + \boldsymbol{k_n}) \mathrm{e}^{\mathrm{i}\boldsymbol{k_n}\cdot\boldsymbol{x}} \, dv_{\boldsymbol{k}} = \int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) \, dv_{\boldsymbol{k}}.$$

This proves the first representation of the Bloch amplitude. The second is shown by using the Dirac delta distribution $\delta(\boldsymbol{k} - \boldsymbol{k}') = \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{x}+\boldsymbol{x_n})}$ (see Appendix A for a derivation), and the Bloch amplitude can be written

(3.5)

$$\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) = \int_{U'} \delta(\boldsymbol{k}-\boldsymbol{k}')\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}') \, \mathrm{d}v_{\boldsymbol{k}'} = \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \int_{U'} \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{x}+\boldsymbol{x_n})}\tilde{\mathsf{u}}(\boldsymbol{x}+\boldsymbol{x_n}, \boldsymbol{k}') \, \mathrm{d}v_{\boldsymbol{k}'}$$

$$= \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}+\boldsymbol{x_n})} \int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{x}+\boldsymbol{x_n})}\tilde{\mathsf{u}}(\boldsymbol{x}+\boldsymbol{x_n}, \boldsymbol{k}') \, \mathrm{d}v_{\boldsymbol{k}'}$$

$$= \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}+\boldsymbol{x_n})}\mathsf{u}(\boldsymbol{x}+\boldsymbol{x_n}),$$

where we used the periodicity of $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})$ in the first line. $\square$

By definition of the reciprocal lattice $\{\boldsymbol{k_n}\}$, we have $\langle \mathrm{e}^{\mathrm{i}\boldsymbol{k_n}\cdot\boldsymbol{x}} \rangle = 0$ for $\boldsymbol{k_n} \neq \boldsymbol{0}$. The relation $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) = \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \hat{\mathsf{u}}(\boldsymbol{k}+\boldsymbol{k_n})\mathrm{e}^{\mathrm{i}\boldsymbol{k_n}\cdot\boldsymbol{x}}$ then implies that the mean value of the Bloch amplitude is the Fourier amplitude of u for the corresponding wave vector,

(3.6)
$$\langle \tilde{\mathsf{u}}(\cdot, \boldsymbol{k}) \rangle = \hat{\mathsf{u}}(\boldsymbol{k}).$$

Using the Bloch representation implies that all derivatives are shifted by $\boldsymbol{k}$ in the following sense:

(3.7)
$$-\mathrm{i}\nabla \times \mathsf{J} \cdot (\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} \cdot \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}),$$

(3.8)
$$-\mathrm{i}\nabla \cdot (\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}(-\mathrm{i}\nabla + \boldsymbol{k}) \cdot \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}).$$

In the following, we continue to use the terms "curl" and "divergence" when we refer to the shifted differentials $(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} \cdot \tilde{\mathsf{u}}$ and $(-\mathrm{i}\nabla + \boldsymbol{k}) \cdot \tilde{\mathsf{u}}$.

One of our aims in this paper is to define expansion functions $\mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})$, called Bloch eigenmodes, such that they can be used to represent the Bloch amplitudes as

(3.9)
$$\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) = \sum_n u_n(\boldsymbol{k})\mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})$$

and at the same time diagonalize Maxwell's equations, in a manner to be made precise in section 5. Note that the expansion coefficients u_n in general depend on the wave vector $\boldsymbol{k}$.

4. Spectral properties of the curl operator.

4.1. The vacuum eigenvectors. We expect the eigenvectors in the material case to be similar to the vacuum case, which can be calculated explicitly. We study the unbounded operator

(4.1)
$$(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} : \; L^2_\#(U; \mathbb{C}^6) \to L^2_\#(U; \mathbb{C}^6)$$

with the dense domain $H_\#(\mathrm{rot})$. We require $\boldsymbol{k} \in U'$.

THEOREM 4.1. *The operator in* (4.1) *is self-adjoint.*

Proof. The operator is symmetric in the usual L^2 scalar product, and the equation $[(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} \pm \mathrm{i}\mathsf{I}] \cdot \mathsf{v} = \mathsf{w}$ is solvable for all $\mathsf{w} \in L^2_\#(U; \mathbb{C}^6)$. This is shown through expansion in Fourier series, where the operator is replaced by the matrix

$(\boldsymbol{k_n} + \boldsymbol{k}) \times \mathsf{J} \pm i\mathsf{I}$, which has an inverse bounded by $1/(1+|\boldsymbol{k_n} + \boldsymbol{k}|^2)^{1/2}$ for all $\boldsymbol{n} \in \mathbb{Z}^3$. Thus, the range of $(-i\nabla + \boldsymbol{k}) \times \mathsf{J} \pm i\mathsf{I}$ is all of $L^2_\#(U; \mathbb{C}^6)$, which is equivalent to the operator in (4.1) being self-adjoint; see, for instance, [24, p. 513].   □

THEOREM 4.2. *Represent the arbitrary function* $\mathsf{v} \in L^2_\#(U; \mathbb{C}^6)$ *with its Fourier series* $\mathsf{v}(\boldsymbol{x}) = \sum_{\boldsymbol{n}\in\mathbb{Z}^3} \hat{\mathsf{v}}_{\boldsymbol{n}} e^{i\boldsymbol{k_n}\cdot\boldsymbol{x}}$. *The eigenproblem in vacuum,*

$$(4.2) \qquad (-i\nabla + \boldsymbol{k}) \times \mathsf{J} \cdot \mathsf{v} = \omega\mathsf{v},$$

has the following (nonnormalized) solutions, where the index $\boldsymbol{n}' \in \mathbb{Z}^3$ *corresponds to an enumeration of the eigenvalues and* $\alpha_{\boldsymbol{n}}$ *and* $\beta_{\boldsymbol{n}}$ *are arbitrary constants:*

$$(4.3) \qquad \omega = 0: \qquad \hat{\mathsf{v}}_{\boldsymbol{n}} = \alpha_{\boldsymbol{n}} \begin{pmatrix} \boldsymbol{k_n} + \boldsymbol{k} \\ \boldsymbol{0} \end{pmatrix}, \qquad \hat{\mathsf{v}}_{\boldsymbol{n}} = \beta_{\boldsymbol{n}} \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{k_n} + \boldsymbol{k} \end{pmatrix},$$

$$(4.4) \qquad \omega_{\boldsymbol{n}'} = |\boldsymbol{k_{n'}} + \boldsymbol{k}|: \qquad \hat{\mathsf{v}}_{\boldsymbol{n}} = \delta_{\boldsymbol{n},\boldsymbol{n}'} \begin{pmatrix} \hat{\boldsymbol{l}} \\ \hat{\boldsymbol{m}} \end{pmatrix}, \qquad \hat{\mathsf{v}}_{\boldsymbol{n}} = \delta_{\boldsymbol{n},\boldsymbol{n}'} \begin{pmatrix} -\hat{\boldsymbol{m}} \\ \hat{\boldsymbol{l}} \end{pmatrix},$$

$$(4.5) \qquad \omega_{\boldsymbol{n}'} = -|\boldsymbol{k_{n'}} + \boldsymbol{k}|: \qquad \hat{\mathsf{v}}_{\boldsymbol{n}} = \delta_{\boldsymbol{n},\boldsymbol{n}'} \begin{pmatrix} \hat{\boldsymbol{l}} \\ -\hat{\boldsymbol{m}} \end{pmatrix}, \qquad \hat{\mathsf{v}}_{\boldsymbol{n}} = \delta_{\boldsymbol{n},\boldsymbol{n}'} \begin{pmatrix} \hat{\boldsymbol{m}} \\ \hat{\boldsymbol{l}} \end{pmatrix},$$

where $\delta_{\boldsymbol{n},\boldsymbol{n}'}$ *is the Kronecker delta, and* $\hat{\boldsymbol{l}}$ *and* $\hat{\boldsymbol{m}}$ *are unit three-vectors orthogonal to* $\boldsymbol{k_{n'}} + \boldsymbol{k}$, *which satisfy* $\hat{\boldsymbol{l}} \times \hat{\boldsymbol{m}} = (\boldsymbol{k_{n'}} + \boldsymbol{k})/|\boldsymbol{k_{n'}} + \boldsymbol{k}|$.

Proof. When substituting the Fourier series in the eigenvalue equation, the following algebraic eigenvalue problem is obtained for each Fourier coefficient $\mathsf{v}_{\boldsymbol{n}'}$ corresponding to a fixed wave vector $\boldsymbol{k_{n'}}$ in the reciprocal lattice:

$$(4.6) \qquad (\boldsymbol{k_{n'}} + \boldsymbol{k}) \times \mathsf{J} \cdot \hat{\mathsf{v}}_{\boldsymbol{n}'} = \omega\hat{\mathsf{v}}_{\boldsymbol{n}'}.$$

The eigenvectors and eigenvalues in the theorem are obviously the solution to this algebraic problem for every wave vector $\boldsymbol{k_{n'}}$ in the reciprocal lattice. Since every L^2 function is uniquely determined by its Fourier coefficients, the proof is complete.   □

Remark 1. Each nonzero eigenvalue has multiplicity two, whereas for $\omega = 0$ there are infinitely many undetermined constants $\alpha_{\boldsymbol{n}}$ and $\beta_{\boldsymbol{n}}$. This means the dimension of the kernel (null space) of $(-i\nabla + \boldsymbol{k}) \times \mathsf{J}$ is infinite.   □

4.2. Compactness of the vacuum resolvent. Instead of explicitly constructing the spectral properties of $(-i\nabla + \boldsymbol{k}) \times \mathsf{J}$, we can study its resolvent, $\mathsf{R}_0(z) = ((-i\nabla + \boldsymbol{k}) \times \mathsf{J} + z\mathsf{I})^{-1}$, where I is the identity operator in $\mathbb{C}^6$ and $z \in \mathbb{C}$ is chosen such that the resolvent exists as a bounded operator. The standard procedure is to prove that the resolvent is compact and use the spectral theorem for compact, self-adjoint operators. However, it can be shown that the resolvent $\mathsf{R}_0(z)$ is proportional to the identity operator on the kernel of $(-i\nabla + \boldsymbol{k}) \times \mathsf{J}$, corresponding to $\omega = 0$ in Theorem 4.2, which is obviously infinite-dimensional. Since the identity operator is compact if and only if the space is finite-dimensional, we need to work in a space smaller than $L^2_\#(U; \mathbb{C}^6)$ to prove compactness. We choose the space where all divergences are proportional to the Bloch amplitude $\tilde{\varrho}(\boldsymbol{x}, \boldsymbol{k}, \tau)$ of the charge distribution $\varrho(\boldsymbol{x}, \tau)$,

$$(4.7) \qquad H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho}) \equiv \{\mathsf{v} \in L^2_\#(U; \mathbb{C}^6) : \exists z \in \mathbb{C}, (-i\nabla + \boldsymbol{k}) \cdot \mathsf{v} = z\tilde{\varrho}\},$$

since, as we see in the following theorem, the kernel of $(-i\nabla + \boldsymbol{k}) \times \mathsf{J}$ is finite-dimensional in this space.

THEOREM 4.3. *The space $H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho})$ is a closed linear subspace of $L^2_\#(U; C^6)$; i.e., it is a Hilbert space with the standard L^2 scalar product. In this space, the kernel of $(-i\nabla + \boldsymbol{k}) \times \mathsf{J}$ has dimension 1 for $\boldsymbol{k} \neq \mathbf{0}$ and dimension 7 for $\boldsymbol{k} = \mathbf{0}$.*

Proof. The first part of the proof concerns the closedness of the space. Any function $\mathsf{v} \in L^2_\#(U; \mathbb{C}^6)$ can be decomposed according to $\mathsf{v} = \mathsf{v}_1 + \mathsf{v}_0$, where $(-i\nabla + \boldsymbol{k}) \cdot \mathsf{v}_1 = 0$ and $(\mathsf{v}_1, \mathsf{v}_0) = 0$. This is due to the fact that the null space of the divergence operator $(-i\nabla + \boldsymbol{k}) \cdot$ is characterized by

$$(4.8) \qquad \mathsf{v}_1 \in \ker((-i\nabla + \boldsymbol{k}) \cdot) \quad \Leftrightarrow \quad (\mathsf{v}_1, (-i\nabla + \boldsymbol{k})\phi) = 0 \quad \forall \phi \in H^1_\#(U; \mathbb{C}^2);$$

i.e., it is the orthogonal complement of the image of the gradient operator $(-i\nabla + \boldsymbol{k})$ acting on its natural domain $H^1_\#(U; \mathbb{C}^2)$. The orthogonal complement of any set is a closed subspace, and since $-i\nabla : H^1_\#(U; \mathbb{C}^2) \to L^2_\#(U; C^6)$ is a closed operator the image of $(-i\nabla + \boldsymbol{k})$ is also closed.

Any function v_0 which is orthogonal to v_1 can then be written as a gradient, $\mathsf{v}_0 = (-i\nabla + \boldsymbol{k})\phi_0$. Lax–Milgram's theorem can be used to show that for $\boldsymbol{k} \neq \mathbf{0}$ the equation $(-i\nabla + \boldsymbol{k}) \cdot (-i\nabla + \boldsymbol{k})\phi_0 = \tilde{\varrho}$ uniquely determines the function $\phi_0 \in H^1_\#(U; \mathbb{C}^2)$, including possible nonzero mean values of ϕ_0, and for $\boldsymbol{k} = \mathbf{0}$ the solution is unique if we require $\langle \phi_0 \rangle = 0$. In the latter case, the mean values are included in $\ker(-i\nabla \cdot)$. The space can then be written as

$$(4.9) \qquad\qquad H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho}) = \ker((-i\nabla + \boldsymbol{k}) \cdot) \oplus \overline{\{\mathsf{v}_0\}},$$

where $\overline{\{\mathsf{v}_0\}}$ is the linear hull of the unique function v_0. Thus, $H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho})$ is a direct sum of orthogonal, closed spaces and is therefore closed in $L^2_\#(U; \mathbb{C}^6)$.

The second part concerns the dimension of the kernel of $(-i\nabla + \boldsymbol{k}) \times \mathsf{J}$. In Appendix B, it is shown that

$$(4.10) \quad (-i\nabla + \boldsymbol{k}) \times \mathsf{J} \cdot \mathsf{v} = \mathbf{0} \quad \Rightarrow \quad \mathsf{v} = \langle \mathsf{v} \rangle + (-i\nabla + \boldsymbol{k})\phi, \quad \boldsymbol{k} \times \mathsf{J} \cdot \langle \mathsf{v} \rangle = \mathbf{0},$$
$$\langle \phi \rangle = 0, \quad \phi \in H^1_\#(U; \mathbb{C}^2).$$

For $\boldsymbol{k} \neq \mathbf{0}$, the condition $\boldsymbol{k} \times \mathsf{J} \cdot \langle \mathsf{v} \rangle = 0$ implies $\mathsf{v} = (-i\nabla + \boldsymbol{k})(\phi + \Phi)$, where Φ is a constant two-scalar. This corresponds precisely to the linear hull of the function v_0 defined above, that is, $\ker((-i\nabla + \boldsymbol{k}) \times \mathsf{J}) = \overline{\{\mathsf{v}_0\}}$, which has dimension 1.

For $\boldsymbol{k} = \mathbf{0}$, we have $\mathsf{v} \in \ker(-i\nabla \times \mathsf{J}) \Rightarrow \mathsf{v} = \langle \mathsf{v} \rangle - i\nabla\phi$, where $\langle \mathsf{v} \rangle \in \mathbb{C}^6$ without restrictions. The elliptic equation $-i\nabla \cdot [(\langle \mathsf{v} \rangle - i\nabla\phi)] = z\tilde{\varrho}$ then provides the solutions $\mathsf{v} = \langle \mathsf{v} \rangle - i\nabla z\phi_0$, where ϕ_0 solves $-\nabla^2\phi_0 = \tilde{\varrho}$. Since there are six degrees of freedom to choose the constant six-vector $\langle \mathsf{v} \rangle \in \mathbb{C}^6$ and we allow for all $z \in \mathbb{C}$, we conclude that for $\boldsymbol{k} = \mathbf{0}$ we have $\ker(-i\nabla \times \mathsf{J}) = \mathbb{C}^6 \oplus \overline{\{-i\nabla\phi_0\}}$, which has dimension 7. Note that for $\boldsymbol{k} = \mathbf{0}$, it is necessary to require $\langle \tilde{\varrho} \rangle = 0$, in order for the divergence condition to make sense, i.e., for a solution to exist. $\qquad \square$

THEOREM 4.4. *The resolvent operator*

$$(4.11) \qquad \mathsf{R}_0(z) = [(-i\nabla + \boldsymbol{k}) \times \mathsf{J} + z\mathsf{I}]^{-1} : H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho}) \to H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho})$$

is a compact operator for $z \in \rho((-i\nabla + \boldsymbol{k}) \times \mathsf{J})$. Furthermore, there exists $z' \in \mathbb{R}$ such that $\mathsf{R}_0(z')$ is a compact, self-adjoint operator in the standard L^2 scalar product.

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

$$(4.12) \qquad\qquad [(-i\nabla + \boldsymbol{k}) \times \mathsf{J} + z\mathsf{I}] \cdot \mathsf{v} = \mathsf{w} \quad \Leftrightarrow \quad \mathsf{v} = \mathsf{R}_0(z) \cdot \mathsf{w}.$$

Choosing $z = \mathrm{i}$ for simplicity and taking the Fourier transform of this equation, we have

(4.13)
$$[(\boldsymbol{k_n} + \boldsymbol{k}) \times \mathsf{J} + \mathrm{i}\mathsf{l}] \cdot \hat{\mathsf{v}}_{\boldsymbol{n}} = \hat{\mathsf{w}}_{\boldsymbol{n}}.$$

We introduce the decomposition $\hat{\mathsf{v}}_{\boldsymbol{n}} = \hat{\mathsf{v}}_{\boldsymbol{n}\perp} + \hat{\mathsf{v}}_{\boldsymbol{n}\|}$, where the index $\perp$ indicates components orthogonal to $\boldsymbol{k_n} + \boldsymbol{k}$. We then have

(4.14)
$$[(\boldsymbol{k_n} + \boldsymbol{k}) \times \mathsf{J} + \mathrm{i}\mathsf{l}] \cdot \hat{\mathsf{v}}_{\boldsymbol{n}\perp} = \hat{\mathsf{w}}_{\boldsymbol{n}\perp}, \quad \mathrm{i}\hat{\mathsf{v}}_{\boldsymbol{n}\|} = \hat{\mathsf{w}}_{\boldsymbol{n}\|},$$

which demonstrates that the resolvent is proportional to the identity operator for the $\|$ components. This is precisely the space $\overline{\{\mathsf{v}_0\}}$ (or $\mathbb{C}^6 \oplus \overline{\{\mathsf{v}_0\}}$ for $\boldsymbol{k} = \boldsymbol{0}$) used in 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

(4.15)
$$(|\boldsymbol{k_n} + \boldsymbol{k}|^2 + 1)|\hat{\mathsf{v}}_{\boldsymbol{n}\perp}|^2 = |\hat{\mathsf{w}}_{\boldsymbol{n}\perp}|^2.$$

Using the notation $\mathsf{w}_\perp = \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k_n} \cdot \boldsymbol{y}} \hat{\mathsf{w}}_{\boldsymbol{n}\perp}$, we have

(4.16)
$$\|\mathsf{R}_0(\mathrm{i}) \cdot \mathsf{w}_\perp\|_{L^2}^2 = \|\mathsf{v}_\perp\|_{L^2}^2 = \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \frac{|\hat{\mathsf{w}}_\perp|^2}{|\boldsymbol{k_n} + \boldsymbol{k}|^2 + 1}.$$

We define the operator S_N, which restricts the number of Fourier coefficients, as

(4.17)
$$[S_N \mathsf{v}](\boldsymbol{y}) = \sum_{|\boldsymbol{n}| \leq N} \hat{\mathsf{v}}_{\boldsymbol{n}} \mathrm{e}^{\mathrm{i}\boldsymbol{k_n} \cdot \boldsymbol{x}}.$$

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

(4.18)
$$\|(1 - S_N)\mathsf{R}_0(\mathrm{i}) \cdot \mathsf{w}_\perp\|_{L^2}^2 = \sum_{|\boldsymbol{n}| > N} \frac{|\hat{\mathsf{w}}_\perp|^2}{|\boldsymbol{k_n} + \boldsymbol{k}|^2 + 1} \leq \frac{\|\mathsf{w}_\perp\|^2}{|\boldsymbol{k}_N + \boldsymbol{k}|^2 + 1} \to 0$$

uniformly for all $\mathsf{w}_\perp$ of unit norm, as $N \to \infty$. This shows that $\mathsf{R}_0(\mathrm{i})$ is the limit of compact operators $S_N \mathsf{R}_0(\mathrm{i})$ in the operator norm and is therefore compact [24, p. 495]. Since any function $\mathsf{w} \in H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho})$ can be decomposed according to $\mathsf{w} = \mathsf{w}_\perp + \mathsf{w}_\|$ and the resolvent is compact on each associated subspace, it is compact on all $H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho})$.

Thus, the spectrum is a discrete subset of $\mathbb{C}$, which in turn implies that $\mathsf{R}_0(z)$ is compact for all z in the resolvent set; see, for instance, [24, p. 516]. Furthermore, there exists a number $z' \in \mathbb{R} \cap \rho((-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J})$, such that $\mathsf{R}_0(z')$ is a compact, self-adjoint operator.   □

4.3. Compact resolvent with a material. The spectral results from the vacuum case can be extended to the material case, where we are interested in the eigenproblem

(4.19)
$$\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} \cdot \mathsf{v}_n = \omega_n \mathsf{v}_n.$$

We put the material dependence on the left-hand side, so that the operator $\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J}$ is self-adjoint in the weighted scalar product $(\mathsf{u}, \mathsf{M} \cdot \mathsf{v})$. We use this scalar product in the space

(4.20)
$$H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho}) \equiv \{\mathsf{v} \in L_\#^2(U; \mathbb{C}^6) : \exists z \in \mathbb{C}, (-\mathrm{i}\nabla + \boldsymbol{k}) \cdot [\mathsf{M} \cdot \mathsf{v}] = z\tilde{\varrho}\},$$

which is a natural generalization of $H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho})$. The operator defined by multiplication with M,

$$(4.21) \qquad \mathsf{M} : H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho}) \to H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \tilde{\varrho}),$$

is a bijective mapping between these spaces. It is straightforward to show that Theorem 4.3 continues to hold for the space $H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho})$, and the following theorem generalizes Theorem 4.4.

THEOREM 4.5. *The resolvent operator*

$$(4.22) \quad \mathsf{R}(z) = [\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} + z\mathsf{I}]^{-1} : H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho}) \to H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho})$$

is a compact operator for $z \in \rho(\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J})$. Furthermore, there exists $z' \in \mathbb{R}$ such that $\mathsf{R}(z')$ is a compact, self-adjoint operator in the weighted L^2 scalar product $(\mathsf{u}, \mathsf{M} \cdot \mathsf{v})$.

Proof. The resolvent can be written using the vacuum resolvent $\mathsf{R}_0(z)$,

$$(4.23) \quad \mathsf{R}(z) = [\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} + z\mathsf{I}]^{-1} = [(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} + z\mathsf{I} + z(\mathsf{M} - \mathsf{I})]^{-1} \cdot \mathsf{M}$$

$$= [\mathsf{R}_0(z)^{-1} + z(\mathsf{M} - \mathsf{I})]^{-1} \cdot \mathsf{M} = [\mathsf{I} + z\mathsf{R}_0(z) \cdot (\mathsf{M} - \mathsf{I})]^{-1} \cdot \mathsf{R}_0(z) \cdot \mathsf{M}.$$

Since M is bounded, the operator $\mathsf{R}_0(z) \cdot \mathsf{M} : H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \varrho) \to H_\#(\mathrm{div}_{\boldsymbol{k}} \propto \varrho)$ is compact. It is multiplied by $[\mathsf{I} + z\mathsf{R}_0(z)(\mathsf{M} - \mathsf{I})]^{-1}$, which is bounded unless -1 is an eigenvalue of $z\mathsf{R}_0(z)(\mathsf{M} - \mathsf{I})$. This cannot occur, since from Theorem 4.2 the eigenvalues of $(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J}$ are real, and we can assume $\mathrm{Im}(z) \neq 0$. Thus, the resolvent $\mathsf{R}(z)$ is compact, which implies it has a discrete spectrum. Since the operator $\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J}$ is self-adjoint in $L^2_\#(U; \mathbb{C}^6)$ with the weighted scalar product $(\mathsf{u}, \mathsf{M} \cdot \mathsf{v})$, the arguments from the proof of Theorem 4.4 can be repeated. Thus, there exists a real number z' such that $\mathsf{R}(z')$ is compact and self-adjoint in this space. □

In conclusion, we have the following theorem.

THEOREM 4.6. *The set of eigenfunctions for the resolvent operator $\mathsf{R}(z')$ is countable and forms an orthogonal basis for the space $H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho})$ with the scalar product $(\mathsf{u}, \mathsf{M} \cdot \mathsf{v})$, and the only accumulation point for the real eigenvalues is 0. This set of eigenvectors is equivalent to the set of eigenvectors for the original operator $\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J}$, where the accumulation points for the real eigenvalues $\{\omega_n\}$ are $\pm\infty$.*

Proof. The proof follows from Theorem 4.5 and the spectral theorem for compact, self-adjoint operators. See also [24, p. 516]. □

Remark 2. The eigenvalues are continuous functions of the wave vector, i.e.,

$$(4.24) \qquad |\omega_n(\boldsymbol{k}) - \omega_n(\boldsymbol{k}_0)| \leq \frac{1}{c}|\boldsymbol{k} - \boldsymbol{k}_0|,$$

where c is defined in (2.8). This is clear from Theorem V-4.10 in [16], which states that when perturbing a self-adjoint operator with a bounded, symmetric operator, the change of the spectrum is bounded by the norm of the perturbing operator. In our case, the operator is

$$(4.25) \qquad \mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J} = \underbrace{\mathsf{M}^{-1} \cdot (-\mathrm{i}\nabla + \boldsymbol{k}_0) \times \mathsf{J}}_{\text{self-adjoint}} + \underbrace{\mathsf{M}^{-1} \cdot (\boldsymbol{k} - \boldsymbol{k}_0) \times \mathsf{J}}_{\text{bounded perturbation}},$$

the norm of the perturbing operator is

$$(4.26) \qquad \left\| \mathsf{M}^{-1} \cdot (\boldsymbol{k} - \boldsymbol{k}_0) \times \mathsf{J} \right\| \leq \left(\sup_{\boldsymbol{x} \in U} |\mathsf{M}^{-1}(\boldsymbol{x})| \right) |\boldsymbol{k} - \boldsymbol{k}_0|,$$

and $\sup_{\boldsymbol{x} \in U} |\mathsf{M}^{-1}(\boldsymbol{x})| \leq 1/c$. □

Remark 3. Since $(-i\nabla + \boldsymbol{k}) \cdot (-i\nabla + \boldsymbol{k}) \times \mathsf{J} \equiv 0$, we have

$$(4.27) \qquad \omega_n(\boldsymbol{k}) \neq 0 \quad \Rightarrow \quad (-i\nabla + \boldsymbol{k}) \cdot [\mathsf{M}(\boldsymbol{x}) \cdot \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})] = 0;$$

i.e., nonzero eigenvalues imply zero divergence after multiplication with M. Only modes with $\omega_n(\boldsymbol{k}) = 0$ can have nonzero divergence, which is exploited in the following section.   ☐

5. Bloch decomposition. The Bloch eigenmodes are defined from the following eigenvalue problem [2, 8, 7, 21]:

$$(5.1) \qquad (-i\nabla + \boldsymbol{k}) \times \mathsf{J} \cdot \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k}) = \omega_n(\boldsymbol{k})\mathsf{M}(\boldsymbol{x}) \cdot \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k}), \quad \boldsymbol{x} \in U,$$

with periodic boundary conditions and the normalization

$$(5.2) \qquad (\mathsf{v}_n, \mathsf{M} \cdot \mathsf{v}_n) = |U|.$$

Since M is dimensionless, this normalization means the functions $\{\mathsf{v}_n\}$ are dimensionless. The enumeration is chosen such that $n = 0$ corresponds to the unique function $\mathsf{v}_0(\boldsymbol{x}, \boldsymbol{k})$ satisfying $(-i\nabla + \boldsymbol{k}) \times \mathsf{J} \cdot \mathsf{v}_0 = \boldsymbol{0}$ and $(-i\nabla + \boldsymbol{k}) \cdot [\mathsf{M} \cdot \mathsf{v}_0] = z\tilde{\varrho}$ for some $z \in \mathbb{C}$ (where z is determined by the normalization of v_0). This means $\omega_0(\boldsymbol{k}) = 0$ for all $\boldsymbol{k} \in U'$. All other modes are enumerated by $n > 0$.

The following theorem is equivalent to a generalized Fourier series in Hilbert space, and a scalar version is given in [7]. See also [3, p. 619].

THEOREM 5.1. *Let* $\mathsf{u} \in L^2_\#(U; \mathbb{C}^6)$ *with* $\nabla \cdot \mathsf{u} = \varrho$. *The* nth *Bloch coefficient of* u *is defined as follows for all* $n \in \mathbb{Z}$ *and* $\boldsymbol{k} \in U'$:

$$(5.3) \qquad u_n(\boldsymbol{k}) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{u}(\boldsymbol{x}) \, dv_{\boldsymbol{x}}.$$

Then the following inverse formula holds:

$$(5.4) \qquad \mathsf{u}(\boldsymbol{x}) = \sum_{n \geq 0} \int_{U'} u_n(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k}) \, dv_{\boldsymbol{k}}.$$

Further, we have Parseval's identity:

$$(5.5) \qquad \int_{\mathbb{R}^3} \mathsf{u}(\boldsymbol{x})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{u}(\boldsymbol{x}) \, dv_{\boldsymbol{x}} = (2\pi)^3 \sum_{n \geq 0} \int_{U'} |u_n(\boldsymbol{k})|^2 \, dv_{\boldsymbol{k}}.$$

Finally, for all u *in the domain of* $\nabla \times \mathsf{J}$, *we have*

$$(5.6) \qquad \nabla \times \mathsf{J} \cdot \mathsf{u}(\boldsymbol{x}) = \sum_{n > 0} \int_{U'} i\omega_n(\boldsymbol{k}) u_n(\boldsymbol{k}) \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \, dv_{\boldsymbol{k}}.$$

Proof. With $\mathsf{u} \in L^2_\#(U; \mathbb{C}^6)$ and $\nabla \cdot \mathsf{u} = \varrho$, it is clear that the Bloch amplitude $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})$ defined in Theorem 3.1 is in $H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho})$. From Theorem 4.6 it is clear that for each $\boldsymbol{k} \in U'$ the spectral problem (5.1) admits a discrete sequence of real eigenvalues and a complete set of eigenvectors in the Hilbert space $H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \varrho)$. The general Fourier series expansion in Hilbert spaces guarantees that for all $\boldsymbol{k}$ the Bloch amplitude $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})$ can be expanded in the corresponding eigenvectors,

$$(5.7) \qquad \mathsf{u}(\boldsymbol{x}) = \int_{U'} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) \, dv_{\boldsymbol{k}} = \int_{U'} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \sum_n u_n(\boldsymbol{k}) \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k}) \, dv_{\boldsymbol{k}}$$

with

$$(5.8) \qquad u_n(\boldsymbol{k}) = \frac{(\mathsf{v}_n, \mathsf{M} \cdot \tilde{\mathsf{u}})}{(\mathsf{v}_n, \mathsf{M} \cdot \mathsf{v}_n)} = \frac{1}{|U|} \int_U \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) \, \mathrm{d}v_{\boldsymbol{x}}.$$

From Theorem 3.1 the Bloch amplitude can be written $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) = \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathsf{u}(\boldsymbol{x} + \boldsymbol{x_n}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{x} + \boldsymbol{x_n})}$, and the expansion coefficients are

$$(5.9) \quad u_n(\boldsymbol{k}) = \frac{1}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \int_U \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{u}(\boldsymbol{x} + \boldsymbol{x_n}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{x} + \boldsymbol{x_n})} \, \mathrm{d}v_{\boldsymbol{x}}$$

$$= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{u}(\boldsymbol{x}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \, \mathrm{d}v_{\boldsymbol{x}}.$$

The Parseval identity in the theorem is shown by using the Bloch representation of $\mathsf{u}(\boldsymbol{x})$,

$$(5.10)$$

$$\int_{\mathbb{R}^3} \mathsf{u}(\boldsymbol{x})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \mathsf{u}(\boldsymbol{x}) \, \mathrm{d}v_{\boldsymbol{x}}$$

$$= \int_{\boldsymbol{x} \in \mathbb{R}^3} \left[\iint_{\boldsymbol{k} \in U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) \, \mathrm{d}v_{\boldsymbol{k}} \right]^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \left[\iint_{\boldsymbol{k}' \in U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}' \cdot \boldsymbol{x}} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}') \, \mathrm{d}v_{\boldsymbol{k}'} \right] \mathrm{d}v_{\boldsymbol{x}}$$

$$= \int_{\boldsymbol{x} \in \mathbb{R}^3} \int_{\boldsymbol{k} \in U'} \int_{\boldsymbol{k}' \in U'} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}' - \boldsymbol{k}) \cdot \boldsymbol{x}} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}') \, \mathrm{d}v_{\boldsymbol{k}} \, \mathrm{d}v_{\boldsymbol{k}'} \, \mathrm{d}v_{\boldsymbol{x}}$$

$$= \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \int_{\boldsymbol{x} \in U} \int_{\boldsymbol{k} \in U'} \int_{\boldsymbol{k}' \in U'} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}' - \boldsymbol{k}) \cdot (\boldsymbol{x} + \boldsymbol{x_n})} \tilde{\mathsf{u}}(\boldsymbol{x} + \boldsymbol{x_n}, \boldsymbol{k})^*$$

$$\cdot \mathsf{M}(\boldsymbol{x} + \boldsymbol{x_n}) \cdot \tilde{\mathsf{u}}(\boldsymbol{x} + \boldsymbol{x_n}, \boldsymbol{k}') \, \mathrm{d}v_{\boldsymbol{k}} \, \mathrm{d}v_{\boldsymbol{k}'} \, \mathrm{d}v_{\boldsymbol{x}}$$

$$= \int_{\boldsymbol{x} \in U} \int_{\boldsymbol{k} \in U'} \int_{\boldsymbol{k}' \in U'} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}') \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}' - \boldsymbol{k}) \cdot (\boldsymbol{x} + \boldsymbol{x_n})} \, \mathrm{d}v_{\boldsymbol{k}} \, \mathrm{d}v_{\boldsymbol{k}'} \, \mathrm{d}v_{\boldsymbol{x}}$$

$$= \frac{(2\pi)^3}{|U|} \int_{\boldsymbol{x} \in U} \int_{\boldsymbol{k} \in U'} \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{M}(\boldsymbol{x}) \cdot \tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) \, \mathrm{d}v_{\boldsymbol{k}} \, \mathrm{d}v_{\boldsymbol{x}}$$

$$= (2\pi)^3 \sum_n \int_{\boldsymbol{k} \in U'} |u_n(\boldsymbol{k})|^2 \, \mathrm{d}v_{\boldsymbol{k}},$$

where we used the representation $\frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{\mathrm{i}(\boldsymbol{k} - \boldsymbol{k}') \cdot (\boldsymbol{x} + \boldsymbol{x_n})} = \delta(\boldsymbol{k} - \boldsymbol{k}')$ of the delta distribution, and the periodicity of $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k})$ and $\mathsf{M}(\boldsymbol{x})$. The last equality follows from the Parseval equality for a general Fourier series expansion in Hilbert spaces when expanding the Bloch amplitude $\tilde{\mathsf{u}}(\boldsymbol{x}, \boldsymbol{k}) = \sum_n u_n(\boldsymbol{k}) \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})$. The factor $|U|$ in the denominator in the last line vanishes due to the normalization $(\mathsf{v}_n, \mathsf{M} \cdot \mathsf{v}_n) = |U|$.

The final part of the theorem, the representation of the curl operator (5.6), is an immediate consequence of the definition of the eigenvectors. The summation is only over $n > 0$ due to the multiplication with ω_n.   □

Remark 4. Since the eigenvectors are undetermined by an arbitrary phase $\mathrm{e}^{\mathrm{i}\theta}$, the expansion does not really make sense; i.e., the expansion coefficients $u_n(\boldsymbol{k})$ may not be continuous or even measurable as a function of $\boldsymbol{k}$. However, in our final results the phase always cancels, and we assume there exists a structured way of dealing with this problem; see [27] for further details.   □

5.1. Consequences for solutions of Maxwell's equations. The solution $\mathsf{e}(\boldsymbol{x}, \tau)$ of Maxwell's equations, $(\nabla \times \mathsf{J} + \partial_\tau \mathsf{M}) \cdot \mathsf{e} + \mathsf{j} = \mathbf{0}$ and $\nabla \cdot [\mathsf{M} \cdot \mathsf{e}] = \varrho$, is expanded in the Bloch waves as

$$(5.11) \qquad \mathsf{e}(\boldsymbol{x}, \tau) = \sum_{n \geq 0} \int_{U'} e_n(\boldsymbol{k}, \tau) \mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k}) \, \mathrm{d}v_{\boldsymbol{k}}.$$

The following theorem demonstrates that the expansion coefficients $e_n(\boldsymbol{k}, \tau)$ can be controlled by choosing the time dependence of the generating current suitably. This is exploited in the following section.

THEOREM 5.2. *The time-depending expansion coefficients $e_n(\boldsymbol{k}, \tau)$ are given by*

$$(5.12) \; e_n(\boldsymbol{k}, \tau) = -\mathrm{e}^{-\mathrm{i}\omega_n(\boldsymbol{k})\tau} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \int_{-\infty}^{\tau} \mathrm{e}^{\mathrm{i}\omega_n(\boldsymbol{k})\tau'} \mathsf{j}(\boldsymbol{x}, \tau') \, \mathrm{d}\tau' \, \mathrm{d}v_{\boldsymbol{x}}.$$

Proof. First, we multiply Maxwell's equations $(\nabla \times \mathsf{J} + \partial_\tau \mathsf{M}) \cdot \mathsf{e} + \mathsf{j} = \mathbf{0}$ with $(\mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k}))^* / (2\pi)^3$ and integrate over $\mathbb{R}^3$. Using (5.3) and (5.6), we see that the time-depending expansion coefficients $e_n(\boldsymbol{k}, \tau)$ must satisfy

$$(5.13) \qquad (\mathrm{i}\omega_n(\boldsymbol{k}) + \partial_\tau)e_n(\boldsymbol{k}, \tau) = -\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \mathsf{j}(\boldsymbol{x}, \tau) \, \mathrm{d}v_{\boldsymbol{x}},$$

that is,

$$(5.14) \; e_n(\boldsymbol{k}, \tau) = -\mathrm{e}^{-\mathrm{i}\omega_n(\boldsymbol{k})\tau} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \int_{-\infty}^{\tau} \mathrm{e}^{\mathrm{i}\omega_n(\boldsymbol{k})\tau'} \mathsf{j}(\boldsymbol{x}, \tau') \, \mathrm{d}\tau' \, \mathrm{d}v_{\boldsymbol{x}},$$

where we assumed $e_n(\boldsymbol{k}, \tau) \to 0$, $\tau \to -\infty$. This is the standard convolution solution of a time-invariant differential equation.   □

6. Homogenization. We now assume that the unit cell U is much smaller than the typical wavelength. The electromagnetic field is represented with its spatial Fourier transform

$$(6.1) \quad \mathsf{e}(\boldsymbol{x}, \tau) = \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \hat{\mathsf{e}}(\boldsymbol{k}, \tau) \, \mathrm{d}v_{\boldsymbol{k}} = \int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \hat{\mathsf{e}}(\boldsymbol{k}, \tau) \, \mathrm{d}v_{\boldsymbol{k}} + \int_{\mathbb{R}^3 \setminus U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \hat{\mathsf{e}}(\boldsymbol{k}, \tau) \, \mathrm{d}v_{\boldsymbol{k}}.$$

As the unit cell U shrinks to zero, the reciprocal cell U' fills $\mathbb{R}^3$, and since $\hat{\mathsf{e}} \in L^2(\mathbb{R}^3; \mathbb{C}^6)$ the integral over $\mathbb{R}^3 \setminus U'$ must vanish in this limit. Thus, only Fourier amplitudes $\hat{\mathsf{e}}(\boldsymbol{k}, \tau)$ with $\boldsymbol{k} \in U'$ contribute to the field when the unit cell is small. But as shown in section 3, these Fourier amplitudes are precisely the mean values of the corresponding Bloch amplitudes, $\hat{\mathsf{e}}(\boldsymbol{k}, \tau) = \langle \tilde{\mathsf{e}}(\cdot, \boldsymbol{k}, \tau) \rangle$, and we have

$$(6.2) \qquad \mathsf{e}(\boldsymbol{x}, \tau) \to \int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x}} \langle \tilde{\mathsf{e}}(\cdot, \boldsymbol{k}, \tau) \rangle \, \mathrm{d}v_{\boldsymbol{k}}, \quad |U| \to 0.$$

This suggests that the mean value of the Bloch amplitude carries the relevant information for the solution when the unit cell becomes small. To capture the effect of the microstructure, we introduce the dimensionless variables $\boldsymbol{y}$ and $\boldsymbol{\eta}$ as

$$(6.3) \qquad \boldsymbol{x} = a\boldsymbol{y}, \quad \boldsymbol{k} = a^{-1}\boldsymbol{\eta},$$
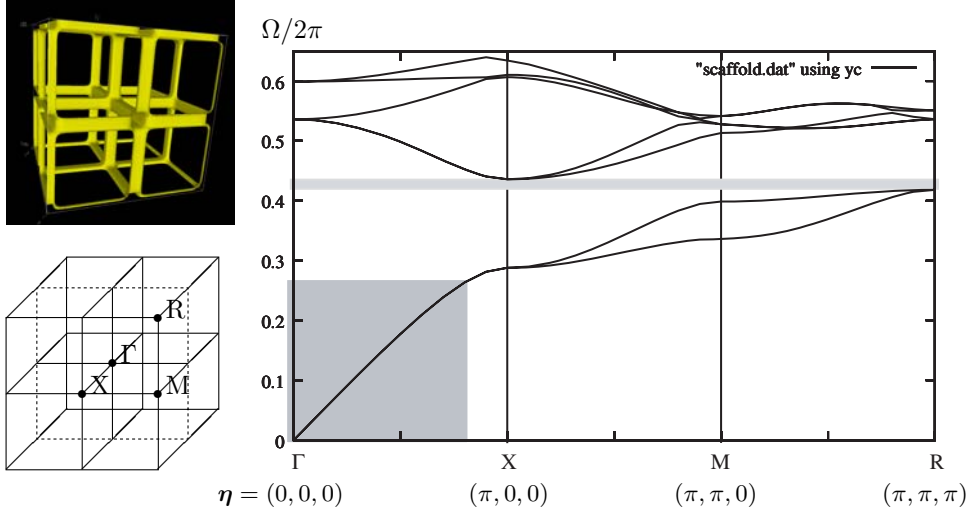
FIG. 6.1. *Plot of a typical band structure. The eigenvalues Ω_n for the geometry in the upper left figure (unit cell $U =]0, 1[^3$) are depicted as functions of the wave vector $\boldsymbol{\eta}$ in the reciprocal unit cell $U' =]-\pi, \pi[^3$ in the lower left figure. The shaded area in the lower left part of the diagram indicates the approximate validity range of classical homogenization [23]. The thin grey strip is a band gap, where there are no eigenvalues regardless of the wave vector. Thus, in this frequency interval there can exist no fixed frequency solutions to Maxwell's equations. In this plot, the optical modes are above the band gap, and the acoustic modes are below. There are only two acoustic modes, since we do not plot the negative frequencies corresponding to propagation in the negative $\boldsymbol{\eta}$-direction. The calculations are made with the program described in [15], and the scaffold geometry is taken from [9]. The thickness of the bars is 20% of the unit cell, and the permittivity in the bars is 12.96.*

where a is a typical size of the unit cell. Using this scaling, the eigenvalue problem can be represented in dimensionless variables as

$$(6.4) \qquad (-\mathrm{i}\nabla_{\boldsymbol{y}} + \boldsymbol{\eta}) \times \mathsf{J} \cdot \underbrace{\mathsf{v}_n(a\boldsymbol{y}, a^{-1}\boldsymbol{\eta})}_{\mathsf{u}_n(\boldsymbol{y}, \boldsymbol{\eta})} = \underbrace{a\omega_n(a^{-1}\boldsymbol{\eta})}_{\Omega_n(\boldsymbol{\eta})} \underbrace{\mathsf{M}(a\boldsymbol{y})}_{\mathsf{M}_0(\boldsymbol{y})} \cdot \underbrace{\mathsf{v}_n(a\boldsymbol{y}, a^{-1}\boldsymbol{\eta})}_{\mathsf{u}_n(\boldsymbol{y}, \boldsymbol{\eta})}.$$

From this formulation we conclude that the eigenvectors $\mathsf{u}_n(\boldsymbol{y}, \boldsymbol{\eta})$ and eigenvalues $\Omega_n(\boldsymbol{\eta})$ can be calculated independent of the physical size a of the unit cell. A typical plot of the eigenvalues as functions of the wave vector is given in Figure 6.1.

From (6.4) it is seen that the eigenvalues scale with the size of the unit cell as

$$(6.5) \qquad \qquad \omega_n(\boldsymbol{k}) = \frac{\Omega_n(a\boldsymbol{k})}{a}.$$

For eigenvalues with $\Omega_n(\boldsymbol{\eta}) \neq 0$ for all $\boldsymbol{\eta}$, this means $|\omega_n(\boldsymbol{k})| \to \infty$ when $a \to 0$. Apart from $\omega_0(\boldsymbol{k})$, which is identically zero, only eigenvalues corresponding to the index set

$$(6.6) \qquad \qquad I = \{n > 0; \ |\Omega_n(a\boldsymbol{k})|/a < \infty, \ a \to 0\}$$

remain bounded when $a \to 0$. The modes with $n \in I$ are often called the acoustic branch in the physics literature on lattice vibrations, and $n \notin I \cup \{0\}$ are the optical branch; see, for instance, [17, p. 88] or [18, p. 210]. Observe that $n = 0$ is not included in I, which means that $n \in I \Rightarrow (-\mathrm{i}\nabla + \boldsymbol{k}) \cdot [\mathsf{M} \cdot \mathsf{v}_n] \equiv 0$.

The following theorem shows that the steady state response to a band limited current can consist only of acoustic modes in the limit $a \to 0$.

THEOREM 6.1. *Denote the temporal Fourier transform of the current density by*

$$(6.7) \qquad \hat{\jmath}(\boldsymbol{x}, \omega) = \int_{-\infty}^{\infty} e^{i\omega\tau} \mathsf{j}(\boldsymbol{x}, \tau)\, \mathrm{d}\tau.$$

Let $\hat{\jmath}(\boldsymbol{x}, \omega) = 0$ for $|\omega| > \omega_0$, where $\omega_0 > 0$ is a given constant. The steady state electromagnetic field in the limit $a \to 0$ is then

$$(6.8) \qquad \lim_{\tau \to \infty} \mathsf{e}(\boldsymbol{x}, \tau) = \sum_{n \in I} \int_{U'} e_n(\boldsymbol{k}) e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_n(\boldsymbol{k})\tau)} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})\, \mathrm{d}v_{\boldsymbol{k}},$$

where

$$(6.9) \qquad e_n(\boldsymbol{k}) = -\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \hat{\jmath}(\boldsymbol{x}, \omega_n(\boldsymbol{k}))\, \mathrm{d}v_{\boldsymbol{x}}.$$

Proof. The steady state expansion coefficients are calculated by taking the limit $\tau \to \infty$ in (5.12),

$$(6.10)$$
$$\lim_{\tau \to \infty} e_n(\boldsymbol{k}, \tau) e^{i\omega_n(\boldsymbol{k})\tau} = -\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \int_{-\infty}^{\infty} e^{i\omega_n(\boldsymbol{k})\tau'} \mathsf{j}(\boldsymbol{x}, \tau')\, \mathrm{d}\tau'\, \mathrm{d}v_{\boldsymbol{x}}$$
$$= -\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})^* \cdot \hat{\jmath}(\boldsymbol{x}, \omega_n(\boldsymbol{k}))\, \mathrm{d}v_{\boldsymbol{x}}.$$

Since $\omega_n(\boldsymbol{k}) = \Omega_n(a\boldsymbol{k})/a$, only the eigenvalues $\omega_n(\boldsymbol{k})$ corresponding to $n \in I \cup \{0\}$ can satisfy $|\omega_n(\boldsymbol{k})| \leq \omega_0$ when $a \to 0$. Since $\mathsf{v}_0(\boldsymbol{x}, \boldsymbol{k})$ can be written as $(-i\nabla + \boldsymbol{k})\phi(\boldsymbol{x}, \boldsymbol{k})$, the expansion coefficient for $n = 0$ is ($\omega_0(\boldsymbol{k}) = 0$)

$$(6.11) \quad \lim_{\tau \to \infty} e_0(\boldsymbol{k}, \tau) = -\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} [(-i\nabla + \boldsymbol{k})\phi(\boldsymbol{x}, \boldsymbol{k})]^* \cdot \hat{\jmath}(\boldsymbol{x}, 0)\, \mathrm{d}v_{\boldsymbol{x}}$$
$$= -\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} [-i\nabla(e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\phi(\boldsymbol{x}, \boldsymbol{k}))]^* \cdot \hat{\jmath}(\boldsymbol{x}, 0)\, \mathrm{d}v_{\boldsymbol{x}}.$$

But Maxwell's equations imply the time-harmonic continuity equation $\nabla \cdot \hat{\jmath}(\boldsymbol{x}, \omega) = i\omega\hat{\varrho}(\boldsymbol{x}, \omega)$, and for $\omega = 0$ this implies $\nabla \cdot \hat{\jmath}(\boldsymbol{x}, 0) = 0$, which is equivalent to $\hat{\jmath}(\boldsymbol{x}, 0)$ being orthogonal to all gradients. This means $\lim_{\tau \to \infty} e_0(\boldsymbol{k}, \tau) = 0$, and all expansion coefficients with $n \notin I$ are zero in the limit $\tau \to \infty$. The steady state field is then

$$(6.12) \qquad \lim_{\tau \to \infty} \mathsf{e}(\boldsymbol{x}, \tau) = \sum_{n \in I} \int_{U'} e_n(\boldsymbol{k}) e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_n(\boldsymbol{k})\tau)} \mathsf{v}_n(\boldsymbol{x}, \boldsymbol{k})\, \mathrm{d}v_{\boldsymbol{k}},$$

where $e_n(\boldsymbol{k}) = \lim_{\tau \to \infty} e_n(\boldsymbol{k}, \tau) e^{i\omega_n(\boldsymbol{k})\tau}$.   □

Remark 5. The limits $a \to 0$ and $\tau \to \infty$ in the above theorem do not have to be taken literally. In some respect they are complementary, depending on whether the current is limited in time or in frequency. If the current density $\mathsf{j}(\boldsymbol{x}, \tau)$ is zero after some time T, the limit $\tau \to \infty$ is reached as soon as $\tau > T$. But, as a consequence, the Fourier transform $\hat{\jmath}(\boldsymbol{x}, \omega)$ is small but not zero for large ω (due to the "uncertainty principle" for Fourier transform pairs), which requires an infinitesimal a in order to make $\hat{\jmath}(\boldsymbol{x}, \omega_n(\boldsymbol{k}))$ small enough. On the other hand, if the current is band limited in frequency (as in the theorem), there is a finite A such that $|\omega_n(\boldsymbol{k})| = |\Omega_n(a\boldsymbol{k})|/a > \omega_0$

for all $n \notin I \cup \{0\}$ as soon as $a < A$, which implies $\hat{\jmath}(\boldsymbol{x}, \omega_n(\boldsymbol{k})) = 0$. But a current limited in frequency is small but not zero for large times, requiring $\tau \to \infty$. In practice, a tradeoff is made between these requirements, choosing τ large enough and a small enough, but we do not go into detail here. The fact that, for currents band limited as in the theorem, $a < A$ is a sufficient condition for Theorem 6.1 to hold indicates that the homogenization results presented below are actually valid for a finite microscopic scale a, although we still phrase the results in terms of the limit $a \to 0$. □

We are now ready to state the main result of this paper, where the index $\perp$ denotes components perpendicular to $\hat{\boldsymbol{k}} = \boldsymbol{k}/|\boldsymbol{k}|$, which is the unit vector in the $\boldsymbol{k}$-direction.

THEOREM 6.2. *Define the homogenized matrix* $\mathsf{M}^{\mathrm{h}}_{\perp}(\boldsymbol{k})$ *as*

$$(6.13) \qquad \lim_{\substack{\tau \to \infty \\ a \to 0}} \langle \tilde{\mathsf{d}}(\cdot, \boldsymbol{k}, \tau) \rangle = \lim_{\substack{\tau \to \infty \\ a \to 0}} \langle \mathsf{M}(\cdot) \cdot \tilde{\mathsf{e}}(\cdot, \boldsymbol{k}, \tau) \rangle = \mathsf{M}^{\mathrm{h}}_{\perp}(\boldsymbol{k}) \cdot \lim_{\substack{\tau \to \infty \\ a \to 0}} \langle \tilde{\mathsf{e}}(\cdot, \boldsymbol{k}, \tau) \rangle .$$

For every nonzero $\boldsymbol{k} \in U'$, *this matrix has the representation*

$$(6.14) \qquad \mathsf{M}^{\mathrm{h}}_{\perp}(\boldsymbol{k}) = \sum_{m \in I} \frac{\langle \mathsf{M} \cdot \mathsf{v}_m \rangle \langle \mathsf{v}^*_m \cdot \mathsf{M} \rangle}{\langle \mathsf{v}^*_m \cdot \mathsf{M} \rangle \cdot \langle \mathsf{v}_{m\perp} \rangle} .$$

Proof. Theorem 6.1 ensures that only modes with $m \in I$ survive in the limit $\tau \to \infty$, $a \to 0$. Since $(-\mathrm{i}\nabla + \boldsymbol{k}) \cdot [\mathsf{M} \cdot \mathsf{v}_m] = 0$ for $m \in I$, we have $\hat{\boldsymbol{k}} \cdot \langle \mathsf{M} \cdot \mathsf{v}_m \rangle = 0$, which implies $\hat{\boldsymbol{k}} \cdot \langle \tilde{\mathsf{d}} \rangle = 0$. The proof is complete if we can find a matrix $\mathsf{M}^{\mathrm{h}}_{\perp}(\boldsymbol{k})$ such that $\langle \mathsf{M} \cdot \mathsf{v}_m \rangle = \mathsf{M}^{\mathrm{h}}_{\perp} \cdot \langle \mathsf{v}_m \rangle$ for all $m \in I$. That such a matrix exists and has the above representation is proven in Theorem 6.5. The proof is based on a conjecture. □

6.1. Proof of the homogenization theorem. Some of the properties of the mean values which are needed in this paper seem intuitively reasonable but difficult to prove. Therefore, we state the following conjecture.

CONJECTURE 1. *For each nonzero* $\boldsymbol{k} \in U'$, *precisely four eigenvectors correspond to the index set* I *defined in* (6.6). *The mean values* $\{\langle \mathsf{v}_{m\perp} \rangle\}_{m \in I}$ *are linearly independent; i.e., the components orthogonal to* $\hat{\boldsymbol{k}}$ *constitute a basis in the four-dimensional space* $\{\mathsf{v} \in \mathbb{C}^6 : \hat{\boldsymbol{k}} \cdot \mathsf{v} = 0\}$.

Remark 6. That I consists only of four indices and not six (the dimension of the zero-divergence kernel of $(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J}$ at $\boldsymbol{k} = \boldsymbol{0}$) might seem counterintuitive. This kernel consists of six functions of the form $\langle \mathsf{v} \rangle - \nabla \phi$, and it is reasonable to believe that all these could be continued as eigenvectors for $\boldsymbol{k} \neq \boldsymbol{0}$. The intuitive explanation is of a geometric nature. We first note that of the four eigenvectors corresponding to I, two of them are associated with propagation in the $-\boldsymbol{k}$ direction. These can be found from the other two by reversing the direction of the electric or the magnetic field. This leaves two fundamentally independent modes, often named transverse electric and transverse magnetic modes, for each propagation direction $\boldsymbol{k}$. In three-dimensional space we have three fundamental directions, which are indistinguishable at $\boldsymbol{k} = \boldsymbol{0}$. This leaves us with $3 \times 2 = 6$ independent modes corresponding to I, which is precisely the dimension of the zero-divergence kernel of $(-\mathrm{i}\nabla + \boldsymbol{k}) \times \mathsf{J}$ at $\boldsymbol{k} = \boldsymbol{0}$. □

The conjecture is supported by the explicit representation of the eigenvectors in the vacuum case (Theorem 4.2) and experience from numerical calculations. Also, since the mean values of Bloch amplitudes correspond to the Fourier amplitudes, $\langle \tilde{\mathsf{e}} \rangle = \hat{\mathsf{e}}(\boldsymbol{k})$, the conjecture describes the expected behavior of the electromagnetic field at small wavenumbers.

To proceed we need a lemma on linear algebra.

LEMMA 6.3. *For a set of linearly independent (constant) vectors $\{\mathsf{w}_m\}$, there exists $\alpha_{mm'} \in \mathbb{C}$, such that the orthogonality relations*

$$(6.15) \qquad \left[\sum_{m' \in I} \alpha_{mm'} \mathsf{w}_{m'}^*\right] \cdot \mathsf{w}_{m''} = \delta_{mm''}$$

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

Proof. Due to the linear independence of the vectors $\{\mathsf{w}_m\}$, the square matrix with entries $A_{m'm''} = \mathsf{w}_{m'}^* \cdot \mathsf{w}_{m''}$ 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 $a_{m'} = \alpha_{mm'}$.   □

LEMMA 6.4. *There exists a matrix $\mathsf{M}_\perp^{\mathrm{h}}(\boldsymbol{k})$, not depending on the space variable $\boldsymbol{x}$ or the index m, such that*

$$(6.16) \qquad \langle \mathsf{M}(\cdot) \cdot \mathsf{v}_m(\cdot, \boldsymbol{k}) \rangle = \mathsf{M}_\perp^{\mathrm{h}}(\boldsymbol{k}) \cdot \langle \mathsf{v}_{m\perp}(\cdot, \boldsymbol{k}) \rangle$$

for every $m \in I$.

Proof. With $\{\langle \mathsf{v}_{m\perp} \rangle\}_{m \in I}$ being linearly independent, there exist orthogonality relations $[\sum_{m' \in I} \alpha_{mm'} \langle \mathsf{v}_{m'\perp} \rangle] \cdot \langle \mathsf{v}_{m''\perp} \rangle = \delta_{mm''}$ due to Lemma 6.3. We then have

$$(6.17) \quad \langle \mathsf{M} \cdot \mathsf{v}_m \rangle = \langle \mathsf{M} \cdot \mathsf{v}_m \rangle \underbrace{\left[\sum_{m' \in I} \alpha_{mm'} \langle \mathsf{v}_{m'\perp} \rangle\right] \cdot \langle \mathsf{v}_{m\perp} \rangle}_{=1}$$

$$= \left[\sum_{m', m'' \in I} \langle \mathsf{M} \cdot \mathsf{v}_{m''} \rangle \, \alpha_{m''m'} \langle \mathsf{v}_{m'\perp} \rangle\right] \cdot \langle \mathsf{v}_{m\perp} \rangle = \mathsf{M}_\perp^{\mathrm{h}} \cdot \langle \mathsf{v}_{m\perp} \rangle,$$

where we used the orthogonality to include the sum over m''.   □

As alluded to above, Theorem 6.2 is a consequence of the following theorem, which concludes the proof of Theorem 6.2.

THEOREM 6.5. *The homogenized matrix is hermitian symmetric and positive definite, and it has the representation*

$$(6.18) \qquad \mathsf{M}_\perp^{\mathrm{h}}(\boldsymbol{k}) = \sum_{m \in I} \frac{\langle \mathsf{M} \cdot \mathsf{v}_m \rangle \langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle}{\langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle \cdot \langle \mathsf{v}_{m\perp} \rangle}.$$

In addition, the orthogonality relations

$$(6.19) \qquad \frac{\langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle \cdot \langle \mathsf{v}_{m'\perp} \rangle}{\langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle \cdot \langle \mathsf{v}_{m\perp} \rangle} = \delta_{mm'}$$

hold for each $m, m' \in I$.

Proof. Taking the mean value of (5.1), we find

$$(6.20) \qquad \hat{\boldsymbol{k}} \times \mathsf{J} \cdot \langle \mathsf{v}_m \rangle = \frac{\omega_m}{|\boldsymbol{k}|} \langle \mathsf{M} \cdot \mathsf{v}_m \rangle,$$

where $\hat{\boldsymbol{k}} = \boldsymbol{k}/|\boldsymbol{k}|$ is the unit vector in the $\boldsymbol{k}$-direction. Introducing the homogenized matrix $\mathsf{M}_\perp^{\mathrm{h}}$ and observing $\hat{\boldsymbol{k}} \times \mathsf{J} \cdot \langle \mathsf{v}_m \rangle = \hat{\boldsymbol{k}} \times \mathsf{J} \cdot \langle \mathsf{v}_{m\perp} \rangle$, we have the algebraic generalized eigenvalue problem

$$(6.21) \qquad \hat{\boldsymbol{k}} \times \mathsf{J} \cdot \langle \mathsf{v}_{m\perp} \rangle = \frac{\omega_m}{|\boldsymbol{k}|} \mathsf{M}_\perp^{\mathrm{h}} \cdot \langle \mathsf{v}_{m\perp} \rangle,$$

also known as the simultaneous diagonalization of $\hat{\boldsymbol{k}} \times \mathsf{J}$ and $\mathsf{M}_\perp^{\mathrm{h}}$. Since $\hat{\boldsymbol{k}} \times \mathsf{J}$ is a real, symmetric matrix and all eigenvalues $\omega_m/|\boldsymbol{k}|$ are real, the matrix $\mathsf{M}_\perp^{\mathrm{h}}$ must be hermitian symmetric, which is also clear from the symmetry of $\mathsf{M}(\boldsymbol{x})$. Using the eigenvalue problem, we find

$$(6.22) \quad \langle \mathsf{v}_{m'\perp}^* \rangle \cdot \mathsf{M}_\perp^{\mathrm{h}} \cdot \langle \mathsf{v}_{m\perp} \rangle = \frac{|\boldsymbol{k}|}{\omega_m} \langle \mathsf{v}_{m'\perp}^* \rangle \cdot \hat{\boldsymbol{k}} \times \mathsf{J} \cdot \langle \mathsf{v}_{m\perp} \rangle = \frac{\omega_{m'}}{\omega_m} \langle \mathsf{v}_{m'\perp}^* \rangle \cdot \mathsf{M}_\perp^{\mathrm{h}} \cdot \langle \mathsf{v}_{m\perp} \rangle,$$

which implies the eigenvectors $\langle \mathsf{v}_{m\perp} \rangle$ are mutually orthogonal over $\mathsf{M}_\perp^{\mathrm{h}}$ since generally we have $\omega_{m'} \neq \omega_m$ for $m \neq m'$. We ignore the technical problem of multiple eigenvalues; these occur in macroscopically isotropic media and can be removed by considering the medium as a limit of macroscopically anisotropic media, which have distinct eigenvalues. Noting that $\mathsf{M}_\perp^{\mathrm{h}} \cdot \langle \mathsf{v}_{m\perp} \rangle = \langle \mathsf{M} \cdot \mathsf{v}_{m\perp} \rangle$, we have the orthogonality relations

$$(6.23) \qquad\qquad \frac{\langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle \cdot \langle \mathsf{v}_{m'\perp} \rangle}{\langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle \cdot \langle \mathsf{v}_{m\perp} \rangle} = \delta_{mm'}.$$

This means the matrix

$$(6.24) \qquad\qquad \mathsf{A} = \sum_{m \in I} \frac{\langle \mathsf{M} \cdot \mathsf{v}_m \rangle \langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle}{\langle \mathsf{v}_m^* \cdot \mathsf{M} \rangle \cdot \langle \mathsf{v}_{m\perp} \rangle}$$

satisfies $\mathsf{A} \cdot \langle \mathsf{v}_{m\perp} \rangle = \langle \mathsf{M} \cdot \mathsf{v}_m \rangle$, and therefore $\mathsf{A} = \mathsf{M}_\perp^{\mathrm{h}}$. This matrix is hermitian symmetric and positive definite by construction. □

Remark 7. The homogenized matrix is computed from the mean values of the acoustic modes only. The representation is valid for any nonzero $\boldsymbol{k} \in U'$, irrespective of the scale of the unit cell. In the space $\{\mathsf{v} \in \mathbb{C}^6; \ \hat{\boldsymbol{k}} \cdot \mathsf{v} = 0\}$, the matrix $\mathsf{M}_\perp^{\mathrm{h}}$ is hermitian, positive definite by construction. □

6.2. Interpretation of the homogenized matrix. We first comment that there is no information on the $\hat{\boldsymbol{k}}\hat{\boldsymbol{k}}$ part of the homogenized matrix corresponding to static fields. This is not surprising, since we are studying the limit of wave propagation in a periodic medium. In wave propagation, there is no interaction with static fields, unless nonlinear effects are taken into account. This part of the homogenized matrix could possibly be recovered from the divergence condition built into the function space $H_\#(\mathrm{div}_{\boldsymbol{k}} \mathsf{M} \propto \tilde{\varrho})$, but we do not proceed along those lines in this paper.

Theorem 6.2 is a statement on the mean value of the Bloch amplitudes, i.e., $\langle \tilde{\mathsf{d}}(\cdot, \boldsymbol{k}, \tau) \rangle = \mathsf{M}_\perp^{\mathrm{h}}(\boldsymbol{k}) \cdot \langle \tilde{\mathsf{e}}(\cdot, \boldsymbol{k}, \tau) \rangle$, or, equivalently, the Fourier amplitudes $\hat{\mathsf{d}}(\boldsymbol{k}, \tau) = \mathsf{M}_\perp^{\mathrm{h}}(\boldsymbol{k}) \cdot \hat{\mathsf{e}}(\boldsymbol{k}, \tau)$, $\boldsymbol{k} \in U'$. But what does this mean in the spatial domain? If the entire spectral content of $\hat{\mathsf{e}}(\boldsymbol{k})$ is contained in the first Brillouin zone U' we can at least formally invert the Fourier transform to find

$$(6.25) \qquad\qquad \mathsf{d}(\boldsymbol{x}, \tau) = [\mathcal{F}_3^{-1} \mathsf{M}_\perp^{\mathrm{h}}(\boldsymbol{k})] * \mathsf{e}(\boldsymbol{x}, \tau),$$

where $*$ indicates spatial convolution and $\mathcal{F}_3^{-1}$ is a three-dimensional inverse Fourier transform. This is a nonlocal constitutive relation, which shows that, at least formally, the constitutive relation exhibits spatial dispersion.

7. Discussion and conclusions. We have presented a method to compute effective material parameters for electromagnetic waves propagating in a periodic medium. The result is an explicit representation in terms of mean values of the Bloch eigenvectors, which can be computed with standard photonic band gap computational

techniques, such as described in [15], or a general finite element program [10]. There are very few results in the literature regarding qualitative results on mean values of eigenvectors, which indicates there is more work to be done in this field before a proper evaluation of this new method can be done.

In spite of the latter point, we can speculate whether this new formulation of homogenization seems to have any potential advantages compared to existing methods. We recall that the major step in classical homogenization consists in solving an elliptic equation of the form $\nabla \cdot [\boldsymbol{\epsilon}(\boldsymbol{x}) \cdot (\mathbf{I} - \nabla\boldsymbol{\chi})] = 0$. In [6, 11], the accuracy and computational time of solving the local, elliptic problem is compared to solving the eigenvalue problem with the corresponding operator and differentiating the eigenvalue (effective mass homogenization). It is found that there is no significant difference between the two methods from a numerical point of view, neither in accuracy nor in computational time.

It is shown in [6] that the "Bloch approximation," which expresses the homogenized solution in terms of the first Bloch eigenvector and thus has similarities with the method presented in this paper, is a better approximation to the exact solution than the classical first-order corrector method, at least in the smooth coefficient case. In our case, the first Bloch eigenvector corresponds to the acoustic modes, $m \in I$. As we can see from Theorem 6.1, we can actually represent the *full* solution using only acoustic modes under certain conditions, even when the wavelength is not necessarily infinitely large compared to the unit cell.

One drawback of the Bloch wave method is that the spectral results deal only with real, symmetric material matrices. This means dispersion effects and a finite conductivity cannot be handled with this method, unless additional analysis is performed to guarantee the existence and suitable properties of eigenvalues and eigenvectors. The finite conductivity was a vital component of the derivation of the local problem in [26], which demonstrates that, at least at the present understanding, the two methods live in somewhat different worlds. On the other hand, one advantage of the Bloch wave expansion is that it represents the full solution of the electromagnetic problem in periodic media. This makes it possible to estimate the range of validity for the homogenized result, where some first steps have been taken in [23].

Appendix A. A representation of the Dirac delta distribution. The following representation of the delta distribution is proven here since the authors have not succeeded in finding a suitable reference when the basis vectors $\boldsymbol{a}_{1,2,3}$ are not necessarily mutually orthogonal.

LEMMA A.1. *The Dirac delta distribution can be represented by a sum over the lattice points*

$$\text{(A.1)} \qquad \delta(\boldsymbol{k}) = \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x_n}}, \quad \boldsymbol{k} \in U',$$

where $\boldsymbol{x_n} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$, $n_{1,2,3} \in \mathbb{Z}$, and $\boldsymbol{a}_{1,2,3}$ are the basis vectors for the lattice.

Proof. Represent the vector $\boldsymbol{k} \in U'$ as $\boldsymbol{k} = k_1\boldsymbol{b}_1 + k_2\boldsymbol{b}_2 + k_3\boldsymbol{b}_3$, $|k_{1,2,3}| \leq 1/2$, where the reciprocal vectors $\boldsymbol{b}_{1,2,3}$ satisfy $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$ and δ_{ij} is the Kronecker delta. The sum can be written

(A.2)
$$\sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x_n}} = \left(\sum_{n_1 \in \mathbb{Z}} \mathrm{e}^{\mathrm{i}2\pi k_1 n_1}\right)\left(\sum_{n_2 \in \mathbb{Z}} \mathrm{e}^{\mathrm{i}2\pi k_2 n_2}\right)\left(\sum_{n_3 \in \mathbb{Z}} \mathrm{e}^{\mathrm{i}2\pi k_3 n_3}\right) = \delta(k_1)\delta(k_2)\delta(k_3),$$

where we used the standard representation of the one-dimensional delta distribution $\delta(a) = \sum_{n \in \mathbb{Z}} \mathrm{e}^{\mathrm{i}2\pi an}$, $|a| < 1$. Now, identifying (k_1, k_2, k_3) as Cartesian coordinates for a dimensionless vector $\boldsymbol{\eta}$ in $\mathbb{R}^3$, we identify $\delta(k_1)\delta(k_2)\delta(k_3)$ as the three-dimensional delta distribution $\delta(\boldsymbol{\eta})$. The physical vector $\boldsymbol{k}$ is a smooth mapping $\boldsymbol{k}(\boldsymbol{\eta})$, and we have the standard scaling for delta distributions composed of smooth maps $\delta(\boldsymbol{k}(\boldsymbol{\eta})) = |\det \boldsymbol{k}'(\boldsymbol{\eta})|^{-1}\delta(\boldsymbol{\eta})$; see, for instance, [14, p. 136]. Since $\det \boldsymbol{k}'(\boldsymbol{\eta}) = \boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)$ is the volume of the reciprocal unit cell U', it can also be written $\det \boldsymbol{k}'(\boldsymbol{\eta}) = |U'| = (2\pi)^3/|U|$, and we have

$$(\text{A.3}) \qquad \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x_n}} = \delta(\boldsymbol{\eta}) = \frac{(2\pi)^3}{|U|}\delta(\boldsymbol{k}),$$

which completes the proof. $\square$

COROLLARY A.2. *The Dirac delta distribution can be represented as*

$$(\text{A.4}) \qquad \delta(\boldsymbol{k}) = \frac{|U|}{(2\pi)^3} \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}+\boldsymbol{x_n})}, \quad \boldsymbol{k} \in U'.$$

Proof. The proof follows from the lemma since $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\delta(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\boldsymbol{0}\cdot\boldsymbol{x}}\delta(\boldsymbol{k}) = \delta(\boldsymbol{k})$. $\square$

Appendix B. The null space of the curl operator. The following lemma is well known and is proved in, for instance, [26].

LEMMA B.1. *Let $\boldsymbol{f} \in H^1_{\#}(U; \mathbb{R}^3)$, and assume that $\nabla \times \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$. Then there exists a unique function $\phi \in H^2_{\#}(U)/\mathbb{R}$ such that*

$$(\text{B.1}) \qquad \boldsymbol{f}(\boldsymbol{x}) = \langle \boldsymbol{f}(\boldsymbol{x}) \rangle + \nabla\phi(\boldsymbol{x}).$$

The following lemma generalizes this result for the shifted curl operator.

LEMMA B.2. *Let $\boldsymbol{f} \in H^1_{\#}(U; \mathbb{C}^3)$. Assume that $(-\mathrm{i}\nabla + \boldsymbol{k}) \times \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$, where $\boldsymbol{k} \in \mathbb{R}^3$. Then there exists a vector $\boldsymbol{k_{n_0}}$ in the reciprocal lattice and a unique function $\phi \in H^2_{\#}(U)$ such that*

$$(\text{B.2}) \qquad \boldsymbol{f}(\boldsymbol{x}) = \big\langle \mathrm{e}^{-\mathrm{i}\boldsymbol{k_{n_0}}\cdot\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}) \big\rangle \mathrm{e}^{\mathrm{i}\boldsymbol{k_{n_0}}\cdot\boldsymbol{x}} + (-\mathrm{i}\nabla + \boldsymbol{k})\phi(\boldsymbol{y})$$

and $\langle \mathrm{e}^{-\mathrm{i}\boldsymbol{k_{n_0}}\cdot\boldsymbol{x}}\phi(\boldsymbol{x}) \rangle = 0$. Furthermore, $(\boldsymbol{k_{n_0}} + \boldsymbol{k}) \times \langle \mathrm{e}^{-\mathrm{i}\boldsymbol{k_{n_0}}\cdot\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}) \rangle = \boldsymbol{0}$.

Proof. The periodicity of the function $\boldsymbol{f} \in H^1_{\#}(U; \mathbb{R}^3)$ implies that $\boldsymbol{f}$ has a Fourier expansion

$$(\text{B.3}) \qquad \boldsymbol{f}(\boldsymbol{x}) = \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \hat{\boldsymbol{f}}_{\boldsymbol{n}}\mathrm{e}^{\mathrm{i}\boldsymbol{k_n}\cdot\boldsymbol{x}}.$$

The sequence $\hat{\boldsymbol{f}}_{\boldsymbol{n}}$ belongs to $(\ell^2_1)^3$. Due to the condition $(-\mathrm{i}\nabla + \boldsymbol{k}) \times \boldsymbol{f} = \boldsymbol{0}$, the coefficients $\hat{\boldsymbol{f}}_{\boldsymbol{n}}$ also satisfy

$$(\text{B.4}) \qquad (\boldsymbol{k_n} + \boldsymbol{k}) \times \hat{\boldsymbol{f}}_{\boldsymbol{n}} = \boldsymbol{0} \quad \forall \boldsymbol{n} \in \mathbb{Z}^3.$$

Construct the function $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}) - \langle \mathrm{e}^{-\mathrm{i}\boldsymbol{k_{n_0}}\cdot\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}) \rangle \mathrm{e}^{\mathrm{i}\boldsymbol{k_{n_0}}\cdot\boldsymbol{x}}$, where $\boldsymbol{n}_0$ is determined from

$$(\text{B.5}) \qquad |\boldsymbol{k_{n_0}} + \boldsymbol{k}| = \min_{\boldsymbol{n} \in \mathbb{Z}^3} |\boldsymbol{k_n} + \boldsymbol{k}|.$$

This new function has zero Fourier component for $\boldsymbol{n} = \boldsymbol{n}_0$, i.e., $\hat{\boldsymbol{g}}_{\boldsymbol{n}_0} = \boldsymbol{0}$. The other components satisfy $(\boldsymbol{k_n} + \boldsymbol{k}) \times \hat{\boldsymbol{g}}_{\boldsymbol{n}} = \boldsymbol{0}$, where now $|\boldsymbol{k_n} + \boldsymbol{k}|$ is clearly bounded from zero. Therefore, we can write $\boldsymbol{g_n}$ in the form

$$\text{(B.6)} \qquad\qquad \hat{\boldsymbol{g}}_{\boldsymbol{n}} = (\boldsymbol{k_n} + \boldsymbol{k}) \hat{\phi}_{\boldsymbol{n}} \quad \forall \boldsymbol{n} \neq \boldsymbol{n}_0.$$

The coefficients $\hat{\phi}_{\boldsymbol{n}}$ are in ℓ_2^2 and

$$\text{(B.7)} \qquad\qquad \boldsymbol{g}(\boldsymbol{x}) = \sum_{\boldsymbol{n} \neq \boldsymbol{n}_0} (\boldsymbol{k_n} + \boldsymbol{k}) \hat{\phi}_{\boldsymbol{n}} \mathrm{e}^{\mathrm{i}\boldsymbol{k_n} \cdot \boldsymbol{x}} = (-\mathrm{i}\nabla + \boldsymbol{k}) \phi(\boldsymbol{x}, \boldsymbol{k}),$$

where

$$\text{(B.8)} \qquad\qquad \phi(\boldsymbol{x}, \boldsymbol{k}) = \sum_{\boldsymbol{n} \neq \boldsymbol{n}_0} \hat{\phi}_{\boldsymbol{n}} \mathrm{e}^{\mathrm{i}\boldsymbol{k_n} \cdot \boldsymbol{x}} \in H_{\#}^2(U).$$

Using this construction in the original equation, we find

$$
\begin{aligned}
\boldsymbol{0} &= (-\mathrm{i}\nabla + \boldsymbol{k}) \times \boldsymbol{f}(\boldsymbol{x}) \\
&= (-\mathrm{i}\nabla + \boldsymbol{k}) \times \left(\left\langle \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_{\boldsymbol{n}_0} \cdot \boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x}) \right\rangle \mathrm{e}^{\mathrm{i}\boldsymbol{k}_{\boldsymbol{n}_0} \cdot \boldsymbol{x}} + (-\mathrm{i}\nabla + \boldsymbol{k}) \phi(\boldsymbol{x}, \boldsymbol{k}) \right) \\
\text{(B.9)} \qquad &= \mathrm{e}^{\mathrm{i}\boldsymbol{k}_{\boldsymbol{n}_0} \cdot \boldsymbol{x}} (\boldsymbol{k}_{\boldsymbol{n}_0} + \boldsymbol{k}) \times \left\langle \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_{\boldsymbol{n}_0} \cdot \boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x}) \right\rangle,
\end{aligned}
$$

which completes the proof.   □

COROLLARY B.3. *If $\boldsymbol{k} \in U'$, the index $\boldsymbol{n}_0$ is $\boldsymbol{0}$. Thus, if $(-\mathrm{i}\nabla + \boldsymbol{k}) \times \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$, we have*

$$\text{(B.10)} \qquad\qquad \boldsymbol{f}(\boldsymbol{x}) = \langle \boldsymbol{f}(\cdot) \rangle + (-\mathrm{i}\nabla + \boldsymbol{k}) \phi(\boldsymbol{x}, \boldsymbol{k})$$

with $\langle \phi \rangle = 0$. Furthermore, $\boldsymbol{k} \times \langle \boldsymbol{f}(\cdot) \rangle = \boldsymbol{0}$.

Appendix C. Classical homogenization. We show that the classical formulas for the homogenized material matrix (see, for instance, [25, 26]) can be obtained from the Bloch expansion for zero wave vector $\boldsymbol{k}$.

THEOREM C.1. *For $\boldsymbol{k} = \boldsymbol{0}$, we can find six functions $\mathsf{v}_m \in H_\#(\mathrm{div}\, \mathsf{M} \propto \tilde{\varrho})$ and a homogenized matrix M^{h} such that*

$$\text{(C.1)} \qquad\qquad \langle \mathsf{M}(\cdot) \cdot \mathsf{v}_m(\cdot, \boldsymbol{0}) \rangle = \mathsf{M}^{\mathrm{h}} \cdot \langle \mathsf{v}_m(\cdot, \boldsymbol{0}) \rangle,$$

where the functions v_m are in the kernel of $\nabla \times \mathsf{J}$ and

$$\text{(C.2)} \quad \mathsf{M}^{\mathrm{h}} = \langle \mathsf{M}(\cdot) \cdot (\mathsf{I} - \nabla \chi(\cdot)) \rangle = \left\langle \begin{pmatrix} \boldsymbol{\epsilon}(\cdot) & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\mu}(\cdot) \end{pmatrix} \cdot \begin{pmatrix} \mathbf{I} - \nabla \boldsymbol{\chi}^{\mathrm{e}}(\cdot) & \boldsymbol{0} \\ \boldsymbol{0} & \mathbf{I} - \nabla \boldsymbol{\chi}^{\mathrm{h}}(\cdot) \end{pmatrix} \right\rangle$$

and the six-vector potential $\chi(\boldsymbol{x}) = [\boldsymbol{\chi}^{\mathrm{e}}(\boldsymbol{x}), \boldsymbol{\chi}^{\mathrm{h}}(\boldsymbol{x})]^{\mathrm{T}}$ satisfies the elliptic equation

$$\text{(C.3)} \qquad\qquad \nabla \cdot [\mathsf{M}(\boldsymbol{x}) \cdot (\mathsf{I} - \nabla \chi(\boldsymbol{x}))] = 0$$

with periodic boundary conditions.

Proof. For $\boldsymbol{k} = \boldsymbol{0}$ the modes in the kernel satisfy $\nabla \times \mathsf{J} \cdot \mathsf{v}_m(\boldsymbol{x}, \boldsymbol{0}) = \boldsymbol{0}$, which implies that (see Appendix B)

$$\text{(C.4)} \qquad\qquad \mathsf{v}_m(\boldsymbol{x}, \boldsymbol{0}) = \langle \mathsf{v}_m \rangle - \nabla \phi_m(\boldsymbol{x}),$$

where $\phi_m(\boldsymbol{x})$ is a two-scalar with zero mean, and $\langle \mathsf{v}_m \rangle$ is an arbitrary constant six-vector. From Theorem 4.3 it is clear that there exists seven independent functions satisfying

$$(\text{C.5}) \qquad \nabla \cdot [\mathsf{M}(\boldsymbol{x}) \cdot (\langle \mathsf{v}_m \rangle - \nabla \phi_m(\boldsymbol{x}))] = z_m \tilde{\varrho}, \quad m = 0, 1, 2, \ldots, 6.$$

Choose $z_0 = 1$ and $\langle \mathsf{v}_0 \rangle = \boldsymbol{0}$. The potential ϕ_0 is then uniquely determined by the elliptic equation $-\nabla \cdot [\mathsf{M} \cdot \nabla \phi_0] = \tilde{\varrho}$, and the requirement $\langle \phi_0 \rangle = 0$. In order for the seven functions to be linearly independent, we must set $z_m = 0$ for $m = 1, 2, \ldots, 6$. The remaining six functions are then determined by the zero divergence condition

$$(\text{C.6}) \qquad \nabla \cdot [\mathsf{M}(\boldsymbol{x}) \cdot (\langle \mathsf{v}_m \rangle - \nabla \phi_m(\boldsymbol{x}))] = 0, \quad m = 1, 2, \ldots, 6.$$

This elliptic problem is uniquely solvable for ϕ_m in terms of the mean value $\langle \mathsf{v}_m \rangle$, and the solution can be represented as

$$(\text{C.7}) \qquad \nabla \phi_m(\boldsymbol{x}) = \begin{pmatrix} \nabla \phi_m^{\mathrm{e}}(\boldsymbol{x}) \\ \nabla \phi_m^{\mathrm{h}}(\boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} \nabla \boldsymbol{\chi}^{\mathrm{e}}(\boldsymbol{x}) & \boldsymbol{0} \\ \boldsymbol{0} & \nabla \boldsymbol{\chi}^{\mathrm{h}}(\boldsymbol{x}) \end{pmatrix} \cdot \langle \mathsf{v}_m \rangle = \nabla \chi \cdot \langle \mathsf{v}_m \rangle,$$

where the six-vector $\chi(\boldsymbol{x})$ is independent of m. Since the mean values $\langle \mathsf{v}_m \rangle$ can be chosen to span $\mathbb{C}^6$, $\chi(\boldsymbol{x})$ must satisfy

$$(\text{C.8})$$
$$\nabla \cdot [\mathsf{M}(\boldsymbol{x}) \cdot (\mathsf{I} - \nabla \chi)] = \nabla \cdot \left[\begin{pmatrix} \boldsymbol{\epsilon}(\boldsymbol{x}) & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\mu}(\boldsymbol{x}) \end{pmatrix} \cdot \begin{pmatrix} \mathbf{I} - \nabla \boldsymbol{\chi}^{\mathrm{e}}(\boldsymbol{x}) & \boldsymbol{0} \\ \boldsymbol{0} & \mathbf{I} - \nabla \boldsymbol{\chi}^{\mathrm{h}}(\boldsymbol{x}) \end{pmatrix} \right] = \boldsymbol{0},$$

which are 2×3 scalar equations that together with periodic boundary conditions determine the solution $\chi(\boldsymbol{x}) = [\boldsymbol{\chi}^{\mathrm{e}}(\boldsymbol{x}), \boldsymbol{\chi}^{\mathrm{h}}(\boldsymbol{x})]^{\mathrm{T}}$. We get

$$(\text{C.9}) \qquad \mathsf{v}_m(\boldsymbol{x}, \boldsymbol{0}) = (\mathsf{I} - \nabla \chi(\boldsymbol{x})) \cdot \langle \mathsf{v}_m \rangle.$$

The homogenized matrix is then

$$(\text{C.10}) \qquad \langle \mathsf{M}(\cdot) \cdot \mathsf{v}_m(\cdot, \boldsymbol{0}) \rangle = \underbrace{\langle \mathsf{M}(\cdot) \cdot (\mathsf{I} - \nabla \chi(\cdot)) \rangle}_{\mathsf{M}^{\mathrm{h}}} \cdot \langle \mathsf{v}_m(\cdot, \boldsymbol{0}) \rangle,$$

which completes the proof.   □

REFERENCES

[1] G. ALLAIRE AND C. CONCA, *Bloch wave homogenization and spectral asymptotic analysis*, J. Math. Pures Appl. (9), 77 (1998), pp. 153–208.

[2] A. BABIN AND A. FIGOTIN, *Nonlinear photonic crystals:* I. *Quadratic nonlinearity*, Waves Random Media, 11 (2001), pp. R31–R102.

[3] A. BENSOUSSAN, J. L. LIONS, AND G. PAPANICOLAOU, *Asymptotic Analysis for Periodic Structures*, Stud. Math. Appl. 5, North-Holland, Amsterdam, 1978.

[4] F. BLOCH, *Über die Quantenmechanik der Electronen in Kristallgittern*, Z. Phys., 52 (1928), pp. 555–600.

[5] M. BORN AND K. HUANG, *Dynamical Theory of Crystal Lattices*, Oxford University Press, Oxford, UK, 1954.

[6] C. CONCA AND S. NATESAN, *Numerical methods for elliptic partial differential equations with rapidly oscillating coefficients*, Comput. Methods Appl. Mech. Engrg., 192 (2003), pp. 47–76.

[7] C. CONCA, R. ORIVE, AND M. VANNINATHAN, *Bloch approximation in homogenization and applications*, SIAM J. Math. Anal., 33 (2002), pp. 1166–1198.

[8] C. Conca and M. Vanninathan, *Homogenization of periodic structures via Bloch decomposition*, SIAM J. Appl. Math., 57 (1997), pp. 1639–1659.

[9] D. C. Dobson, J. Gopalakrishnan, and J. E. Pasciak, *An efficient method for band structure calculations in 3D photonic crystals*, J. Comput. Phys., 161 (2000), pp. 668–679.

[10] P. Dular, C. Geuzaine, F. Henrotte, and W. Legros, *A general environment for the treatment of discrete problems and its application to the finite element method*, IEEE Trans. Magnetics, 34 (1998), pp. 3395–3398.

[11] C. Engström and D. Sjöberg, *A Comparison of Two Numerical Methods for Homogenization of Maxwell's Equations*, Tech. Report LUTEDX/(TEAT-7121)/1–10/(2004), Lund Institute of Technology, Department of Electroscience, Lund, Sweden, 2004, http://www.es.lth.se.

[12] G. Floquet, *Sur les équations différentielles linéaries à coefficients périodique*, Ann. École Norm. Sup., 12 (1883), pp. 47–88.

[13] S. Guenneau and F. Zolla, *Homogenization of three-dimensional finite photonic crystals*, Progress in Electromagnetics Research, 27 (2000), pp. 91–127.

[14] L. Hörmander, *The Analysis of Linear Partial Differential Operators* I, Grundlehren Math. Wiss. 256, Springer-Verlag, Berlin, Heidelberg, 1983.

[15] S. G. Johnson and J. D. Joannopoulos, *Block-iterative frequency-domain methods for Maxwell's equations in a planewave basis*, Opt. Express, 8 (2001), pp. 173–190.

[16] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin, 1980.

[17] C. Kittel, *Introduction to Solid State Physics*, 6th ed., John Wiley & Sons, New York, 1986.

[18] L. D. Landau and E. M. Lifshitz, *Statistical Physics, Part* 1, 3rd ed., Butterworth-Heinemann, Linacre House, Jordan Hill, Oxford, UK, 1980.

[19] M. Lassas, *The essential spectrum of the nonself-adjoint Maxwell operator in a bounded domain*, J. Math. Anal. Appl., 224 (1998), pp. 201–217.

[20] S. Ponti, J. A. Reyes, and C. Oldano, *Homogeneous models for bianisotropic crystals*, J. Phys.–Condensed Matter, 14 (2002), pp. 10173–10182.

[21] F. Santosa and W. W. Symes, *A dispersive effective medium for wave propagation in periodic composites*, SIAM J. Appl. Math., 51 (1991), pp. 984–1005.

[22] E. V. Sevost'yanova, *Asymptotic expansion of the solution of a second-order elliptic equation with periodic rapidly oscillating coefficients*, Mat. Sb. (N.S.), 115 (1981), pp. 204–222 (in Russian); Math. USSR-Sb., 43 (1982), pp. 181–198 (in English).

[23] D. Sjöberg, G. Kristensson, and C. Engström, *Validity of homogenization using Bloch waves*, in Proceedings of the International Conference on Electromagnetics in Advanced Applications, Torino, Italy, 2003, pp. 455–458.

[24] M. E. Taylor, *Partial Differential Equations* I: *Basic Theory*, Springer-Verlag, New York, 1996.

[25] N. Wellander, *Homogenization of the Maxwell equations: Case* I. *Linear theory*, Appl. Math., 46 (2001), pp. 29–51.

[26] N. Wellander and G. Kristensson, *Homogenization of the Maxwell equations at fixed frequency*, SIAM J. Appl. Math., 64 (2003), pp. 170–195.

[27] C. H. Wilcox, *Theory of Bloch waves*, J. Analyse Math., 33 (1978), pp. 146–167.