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2006

Link to publication

Citation for published version (APA):
Sjöberg, D. (2006). *Dispersive effective material parameters for Maxwell's equations.* (Technical Report LUTEDX/(TEAT-7146)/1-14/(2006); Vol. TEAT-7146). [Publisher information missing].

Total number of authors:
1

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CODEN:LUTEDX/(TEAT-7146)/1-14/(2006)

Dispersive effective material parameters for Maxwell's equations

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Editor: Gerhard Kristensson
© Daniel Sjöberg, Lund, March 24, 2006

Abstract

We study how effective material parameters can be defined for Maxwell's equations when taking dispersion into account. The reasoning is based on the concept of dispersion relations, and is consequently primarily concerned with lossless media. We essentially require that the effective material parameters should produce the same dispersion relations as the heterogeneous problem, which implies the effective material is primarily connected to the phase velocity of the waves. Material parameters which exhibit temporal dispersion only, can be defined if the propagation direction is fixed.

1 Introduction

It is common to model materials which are inhomogeneous on a very small scale compared to the wavelength with a homogeneous material. To find the proper value of this fictitious material, it is often assumed that the wavelength is infinitely large compared to the microstructure of the material, which permits the problem to be treated by means of classical homogenization, see for instance the books [1, 2, 8, 14, 18] and references therein. The result is, in brief, that the solution to the wave equation involving the heterogeneous material is approximated to an arbitrary degree by the solution to the wave equation involving the homogeneous material, if the homogeneous material is chosen correctly.

In reality, the microstructure is never infinitely small compared to the wavelength. The interplay between these two scales causes dispersive effects, *i.e.*, the solution to the wave equation depends on the frequency and propagation direction. This is usually modeled by a dispersion relation, which connects the temporal frequency ω and the spatial frequency (wave vector) $\boldsymbol{k}$ through a relation of the kind $\omega = W(\boldsymbol{k})$ [24, Ch. 11]. The idea we investigate in this paper is whether it is possible to define, in a reasonable way, a homogeneous material which has the same dispersion relation as the original heterogeneous material.

Various ways of taking the finite scale into account are presented in [3, 15, 16, 19, 20, 23]. A common feature in these approaches is that the effective medium typically depends on the wave vector $\boldsymbol{k}$ in some way, *i.e.*, we arrive at a spatially dispersive material. Physical interpretations of spatial dispersion can be found in, for instance, [12, pp. 358–371]. In this paper, we demonstrate that the effective permittivity for a non-magnetic material can be expressed through the phase velocity, found from the dispersion relation. On the philosophical side, a main result of this paper is that the effective material should be defined from the phase velocity $W(\boldsymbol{k})/k$, and not from the group velocity $W'(\boldsymbol{k})$, even though the group velocity is often deemed as the "physical" velocity relevant for a material. However, even though we use the phase velocity, signals propagating in the effective material will still travel at the group velocity, since we are defining a dispersive medium.

This paper is organized as follows. In Section 2 we introduce the notation necessary to describe fields in periodic media, which are used as a suitable model for heterogeneous materials. In periodic media, it is a well-defined procedure to set up

an eigenvalue problem defining the dispersion relation, which is discussed in Section 3. In Section 4 we compare the solution to a heterogeneous problem with the solution of a homogeneous problem, and identify the effective material parameters directly from the equations. This results in a spatially dispersive material, the implications of which are discussed in Section 5, and in Section 6 we show how to convert the spatial dispersion into a temporal dispersion, which is easier to handle with traditional numerical methods. En explicit example with a simple, stratified laminate geometry is discussed in Section 7, and some conclusions are given in Section 8.

2 Periodic media

In this paper, we study the time harmonic Maxwell's equations for nonmagnetic, anisotropic media, *i.e.*, (time convention $\mathrm{e}^{-\mathrm{i}\omega t}$)

$$\nabla \times \boldsymbol{E} - \mathrm{i}\omega\mu_0 \boldsymbol{H} = \boldsymbol{0} \tag{2.1}$$

$$\nabla \times \boldsymbol{H} + \mathrm{i}\omega\epsilon_0 \boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \boldsymbol{E} = \boldsymbol{0} \tag{2.2}$$

where the fields are given in SI units. The magnetic field can be eliminated to give

$$\nabla \times (\nabla \times \boldsymbol{E}) = c^{-2}\omega^2 \boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \boldsymbol{E} \tag{2.3}$$

where $c = 1/\sqrt{\epsilon_0\mu_0}$ is the speed of light in vacuum. We now assume the medium is periodic with unit cell U, *i.e.*, the permittivity matrix satisfies $\boldsymbol{\epsilon}(\boldsymbol{x} + \boldsymbol{x_n}) = \boldsymbol{\epsilon}(\boldsymbol{x})$, $\boldsymbol{n} \in \mathbb{Z}^3$, 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 with 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 [10]. We denote the typical length of the unit cell by a, *i.e.*, the physical vectors $\boldsymbol{a}_{1,2,3}$ and $\boldsymbol{b}_{1,2,3}$ can be expressed in dimensionless vectors $\hat{\boldsymbol{a}}_{1,2,3}$ and $\hat{\boldsymbol{b}}_{1,2,3}$ through the scaling $\boldsymbol{a}_{1,2,3} = a\hat{\boldsymbol{a}}_{1,2,3}$ and $\boldsymbol{b}_{1,2,3} = a^{-1}\hat{\boldsymbol{b}}_{1,2,3}$, where the dimensionless vectors $\hat{\boldsymbol{a}}_{1,2,3}$ have a typical length of 1.

For the definition of suitable function spaces for Maxwell's equations in infinite periodic media, we refer to [20]. It is useful to employ a Floquet-Bloch representation of fields when studying periodic media [20, 23]. Using this representation, the electromagnetic field can be written

$$\boldsymbol{E}(\boldsymbol{x}) = \frac{1}{|U'|} \int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \widetilde{\boldsymbol{E}}(\boldsymbol{x}, \boldsymbol{k}) \, \mathrm{d}v_{\boldsymbol{k}} \tag{2.4}$$

The Bloch amplitude $\widetilde{\boldsymbol{E}}(\boldsymbol{x}, \boldsymbol{k})$ is a U-periodic function of $\boldsymbol{x}$, and $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\tilde{\mathsf{e}}(\boldsymbol{x}, \boldsymbol{k})$ is a U'-periodic function of $\boldsymbol{k}$. The advantage with this representation is that it separates the large scale behavior of the field, described by the $\boldsymbol{k}$ variable, from the small scale behavior, described by the $\boldsymbol{x}$ variable.

3 Dispersion relations and band diagrams

Using the Floquet-Bloch representation (2.4) in Maxwell's equations for a periodic medium, implies the following equation for the Bloch amplitude $\widetilde{\boldsymbol{E}}$:

$$(\nabla + \mathrm{i}\boldsymbol{k}) \times [(\nabla + \mathrm{i}\boldsymbol{k}) \times \widetilde{\boldsymbol{E}}(\boldsymbol{x}, \boldsymbol{k})] = c^{-2}\omega^2 \boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \widetilde{\boldsymbol{E}}(\boldsymbol{x}, \boldsymbol{k}), \quad \boldsymbol{k} \in U' \tag{3.1}$$

This is an eigenvalue problem, where the eigenvalue is $c^{-2}\omega^2$ and the eigenvector is $\widetilde{\boldsymbol{E}}$. Since $\boldsymbol{k}$ is a free parameter in the equation, this equation defines ω as a function of $\boldsymbol{k}$, $\omega = W(\boldsymbol{k})$, which is the dispersion relation. The general features of this eigenvalue problem and the function spaces necessary to properly formulate it are examined in [23], although there it is treated as a first order system for greater generality.

A particular feature is that for each $\boldsymbol{k} \in U'$, there are infinitely many solutions, meaning we should write

$$(\nabla + \mathrm{i}\boldsymbol{k}) \times [(\nabla + \mathrm{i}\boldsymbol{k}) \times \widetilde{\boldsymbol{E}}_n(\boldsymbol{x}, \boldsymbol{k})] = c^{-2}\omega_n^2 \boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \widetilde{\boldsymbol{E}}_n(\boldsymbol{x}, \boldsymbol{k}), \quad \boldsymbol{k} \in U' \tag{3.2}$$

where the eigenvalues $\{c^{-2}\omega_n^2\}_{n=1}^{\infty}$ form a nondecreasing sequence of positive numbers, and the modes $\{\widetilde{\boldsymbol{E}}_n\}_{n=1}^{\infty}$ are mutually orthogonal in the scalar product

$$(\widetilde{\boldsymbol{E}}_m, \widetilde{\boldsymbol{E}}_n)_{\boldsymbol{\epsilon}} = \int_U \widetilde{\boldsymbol{E}}_m(\boldsymbol{x}, \boldsymbol{k})^* \cdot \boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \widetilde{\boldsymbol{E}}_n(\boldsymbol{x}, \boldsymbol{k}) \, \mathrm{d}v_{\boldsymbol{x}} = \delta_{mn} \tag{3.3}$$

where $\delta_{mm} = 1$ and $\delta_{mn} = 0$ for $m \neq n$ is the Kronecker delta. Thus, the modes can be used as an orthonormal basis for the electric field when weighting the scalar product by $\boldsymbol{\epsilon}(\boldsymbol{x})$.

A typical plot of the dispersion relations is given in Figure 1. In order to obtain dimensionless quantities, we have normalized everything by the unit cell size a. As can be seen from the figure, for small enough frequencies ω, *i.e.*, below the band gap, there are only two eigenmodes contributing to the field. With the terminology used in [23], these are the acoustic modes, which are characterized by $\omega_n \to 0$ as $\boldsymbol{k} \to \boldsymbol{0}$. For the remaining modes ω_n is nonzero for $\boldsymbol{k} = \boldsymbol{0}$, and these are called the optical modes. In [23], it is shown that for an arbitrary unit cell geometry, with or without a band gap, there are only two modes contributing to the solution if the frequency is small enough. More precisely, it is shown that *four* modes contribute, but these are composed of both electric and magnetic fields. The extra two modes come from separately considering waves propagating in the positive or negative $\boldsymbol{k}$-direction. When studying the electric field alone, this reduces to two modes as in this paper.

4 Comparison with the solution of a homogeneous problem

From the presentation in the preceding section, it is seen that for small enough frequencies only two modes defined by the eigenvalue problem (3.2) contribute to

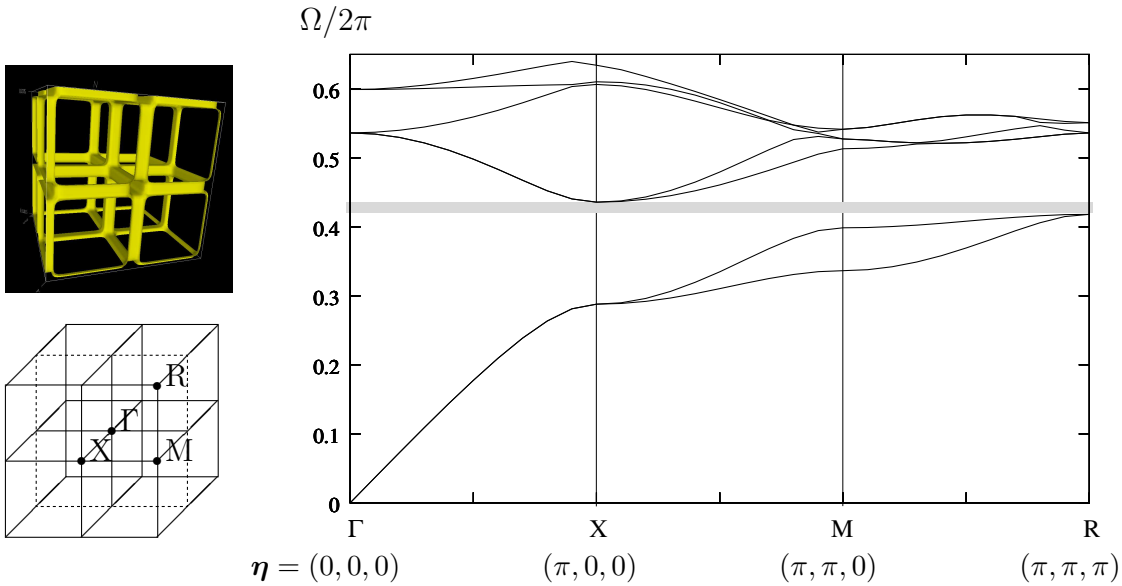

Figure 1: Plot of a typical band structure. The eigenvalues $\Omega_n = ac^{-1}\omega_n$ for the geometry in the upper left figure (normalized unit cell $a^{-1}U =]0,1[^3$) are depicted as functions of the normalized wave vector $\boldsymbol{\eta} = \boldsymbol{k}a$ in the reciprocal unit cell $aU' =]-\pi,\pi[^3$ in the lower left figure. 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, and for frequencies below this band gap, only two modes contribute to the electric field. The calculations are made with the program described in [9], and the scaffold geometry is taken from [4]. The thickness of the bars is 20% of the unit cell, and the permittivity in the bars is 12.96.

the electric field. This significantly reduces the information necessary to describe the electric field, *i.e.*, for a fixed wave vector $\boldsymbol{k}$ there are only two degrees of freedom left, corresponding to these two modes, which are propagating waves. The situation is similar to wave propagation in homogeneous media, where the two degrees of freedom correspond to the two possible polarizations orthogonal to the wave vector $\boldsymbol{k}$, *i.e.*, the TE and TM modes. It is natural to ask if it is possible to define a homogeneous material which has the same propagation characteristics, *i.e.*, the same dispersion relations, as the original heterogeneous one. If such a material can be defined, we call it the *effective permittivity*.

For homogeneous media, it is natural to represent the electric field $\boldsymbol{E}$ by its Fourier transform $\widehat{\boldsymbol{E}}$,

$$\boldsymbol{E}(\boldsymbol{x}) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\widehat{\boldsymbol{E}}(\boldsymbol{k})\,\mathrm{d}v_{\boldsymbol{k}}, \quad \text{where} \quad \widehat{\boldsymbol{E}}(\boldsymbol{k}) = \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\boldsymbol{E}(\boldsymbol{x})\,\mathrm{d}v_{\boldsymbol{x}} \tag{4.1}$$

We now aim to see if there exists a homogeneous permittivity $\boldsymbol{\epsilon}_{\mathrm{hom}}$, not depending on $\boldsymbol{x}$, such that solutions to Maxwell's equations with this permittivity, *i.e.*,

$$\mathrm{i}\boldsymbol{k}\times(\mathrm{i}\boldsymbol{k}\times\widehat{\boldsymbol{E}}_n(\boldsymbol{k})) = c^{-2}\omega_n^2\boldsymbol{\epsilon}_{\mathrm{hom}}\cdot\widehat{\boldsymbol{E}}_n(\boldsymbol{k}) \tag{4.2}$$

will exhibit the same dispersion relations $\omega_n = W_n(\boldsymbol{k})$ as in the heterogeneous case, at least for small frequencies corresponding to the first eigenvalues $n = 1, 2$. For a fixed $\boldsymbol{k}$ this is an algebraic eigenvalue problem with three eigenvalues $c^{-2}\omega_n^2$, one of which is always zero corresponding to eigenvectors $\widehat{\boldsymbol{E}}_n$ proportional to $\boldsymbol{k}$. The remaining two eigenvalues are uniquely determined once the matrix $\boldsymbol{\epsilon}_{\mathrm{hom}}$ is fixed.

The heterogeneous problem (3.2) is quite close in form to the problem (4.2). It is often the case that we can only observe the electric field on a specific scale, which may be modeled by a smoothing procedure represented by a convolution, $\boldsymbol{E}_{\mathrm{smooth}} = \zeta * \boldsymbol{E}$. This is a standard mollifying technique [5], where the smoothing function $\zeta(\boldsymbol{x})$ is nonnegative, has unit integral and is nonzero only in a region corresponding to the observation scale. Choosing an observation scale larger than the unit cell U, and applying the smoothing procedure on the Floquet-Bloch representation (2.4) implies

$$\boldsymbol{E}_{\mathrm{smooth}}(\boldsymbol{x}) = [\zeta * \boldsymbol{E}](\boldsymbol{x}) = \frac{1}{|U'|}\int_{U'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\hat{\zeta}(\boldsymbol{k})\,\langle\widetilde{\boldsymbol{E}}(\cdot,\boldsymbol{k})\rangle\,\mathrm{d}v_{\boldsymbol{k}} \tag{4.3}$$

where $\hat{\zeta}$ is the Fourier transform of ζ and

$$\langle\widetilde{\boldsymbol{E}}(\cdot,\boldsymbol{k})\rangle = \frac{1}{|U|}\int_U \widetilde{\boldsymbol{E}}(\boldsymbol{x},\boldsymbol{k})\,\mathrm{d}v_{\boldsymbol{x}} \tag{4.4}$$

is the mean value over the unit cell U. We refer to the appendix in [21] for detailed calculations. For the purpose of this paper, we only wish to indicate that taking the mean value of the Bloch amplitude corresponds to a smoothing procedure, and we will not use the mollifier ζ any further.

By taking the mean value of (3.2) we obtain an equation for the mean value of the Bloch amplitude, which represents the smooth part of the solution to the heterogeneous problem,

$$\mathrm{i}\boldsymbol{k}\times(\mathrm{i}\boldsymbol{k}\times\langle\widetilde{\boldsymbol{E}}_n(\cdot,\boldsymbol{k})\rangle) = c^{-2}W_n(\boldsymbol{k})^2\,\langle\boldsymbol{\epsilon}(\cdot)\cdot\widetilde{\boldsymbol{E}}_n(\cdot,\boldsymbol{k})\rangle \tag{4.5}$$

Note that we have used that the mean value of a derivative of a periodic function is zero, *i.e.*, $\langle \nabla \times \widetilde{\boldsymbol{E}} \rangle = \mathbf{0}$. Now, if we can find a matrix $\boldsymbol{\epsilon}_{\text{eff}}$ independent of n, such that

$$\langle \boldsymbol{\epsilon} \cdot \widetilde{\boldsymbol{E}}_n \rangle = \boldsymbol{\epsilon}_{\text{eff}} \cdot \langle \widetilde{\boldsymbol{E}}_n \rangle \tag{4.6}$$

then (4.5) is obviously the same eigenvalue problem as (4.2) if we choose $\boldsymbol{\epsilon}_{\text{hom}} = \boldsymbol{\epsilon}_{\text{eff}}$. Using (4.5) and the fact that $\mathrm{i}\boldsymbol{k} \times (\mathrm{i}\boldsymbol{k} \times \mathbf{I}) = k^2[\mathbf{I} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}}]$ we obtain

$$\langle \boldsymbol{\epsilon} \cdot \widetilde{\boldsymbol{E}}_n \rangle = \frac{1}{c^{-2} W_n(\boldsymbol{k})^2} \mathrm{i}\boldsymbol{k} \times (\mathrm{i}\boldsymbol{k} \times \langle \widetilde{\boldsymbol{E}}_n \rangle) = \frac{c^2 k^2}{W_n(\boldsymbol{k})^2} [\mathbf{I} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}}] \cdot \langle \widetilde{\boldsymbol{E}}_n \rangle \tag{4.7}$$

Introduce the notation $[\mathbf{I} - \hat{\boldsymbol{k}}\hat{\boldsymbol{k}}] \cdot \langle \widetilde{\boldsymbol{E}}_n \rangle = \langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle$. It is shown in [23] that the vectors $\{\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle\}_{n=1}^2$ are orthogonal, and can be used as a basis in the space orthogonal to $\boldsymbol{k}$. This leads to the representation

$$\boldsymbol{\epsilon}_{\text{eff}} = \sum_{n=1}^{2} \frac{c^2 k^2}{W_n(\boldsymbol{k})^2} \frac{\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle \langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle^*}{|\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle|^2} \tag{4.8}$$

which demonstrates that the principal values of the effective permittivity matrix are given by $c^2k^2/W_n(\boldsymbol{k})^2$, $n = 1, 2$. Using this definition of the effective permittivity, we obtain the same dispersion relations $W_n(\boldsymbol{k})$ for both the heterogeneous problem and the homogeneous problem. The downside is that in deriving this formula, we had to fix the wave vector $\boldsymbol{k}$, and in doing so we arrive at a spatially dispersive effective medium, *i.e.*, $\boldsymbol{\epsilon}_{\text{eff}} = \boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k})$. This is a problem when studying the application of the effective permittivity, as discussed in the next section.

As is seen from (4.8), the effective permittivity is computed from knowledge of $ck/W_n(\boldsymbol{k})$, *i.e.*, the ratio between the speed of light in vacuum c and the phase velocity $W(\boldsymbol{k})/k$, which is associated with the propagation speed of the carrier wave. It is sometimes argued that the effective permittivity should be calculated according to the effective mass approximation, see for instance [19],

$$(\boldsymbol{\epsilon}_{\text{eff}}^{-1})_{ij} = \frac{1}{2} \frac{\partial^2 [c^{-2} W(\boldsymbol{k})^2]}{\partial k_i \partial k_j} \tag{4.9}$$

at least in the limit $\boldsymbol{k} \to \mathbf{0}$, $W(\boldsymbol{k}) \to 0$, which implies

$$\begin{aligned}
(\boldsymbol{\epsilon}_{\text{eff}}^{-1})_{ij} &= \frac{1}{2} \left. \frac{\partial^2 [c^{-2} W(\boldsymbol{k})^2]}{\partial k_i \partial k_j} \right|_{\boldsymbol{k}=\mathbf{0}} \\
&= \frac{1}{2} \left(2 \frac{\partial [c^{-1} W(\boldsymbol{k})]}{\partial k_i} \frac{\partial [c^{-1} W(\boldsymbol{k})]}{\partial k_j} + 2c^{-1} W(\boldsymbol{k}) \frac{\partial^2 [c^{-1} W(\boldsymbol{k})]}{\partial k_i \partial k_j} \right)_{\boldsymbol{k}=\mathbf{0}} \\
&= \left. \frac{\partial [c^{-1} W(\boldsymbol{k})]}{\partial k_i} \frac{\partial [c^{-1} W(\boldsymbol{k})]}{\partial k_j} \right|_{\boldsymbol{k}=\mathbf{0}}
\end{aligned} \tag{4.10}$$

where we used $W(\mathbf{0}) = 0$. This corresponds to defining the effective mass from the group velocity $W'(\boldsymbol{k})$, which is associated with the propagation speed of energy. In a handwaving manner, it would seem more appropriate to define the effective

material parameters from the propagation of energy or signals, corresponding to the group velocity [24, Ch. 11]. However, since (4.8) defines a *dispersive* medium with the same dispersion relation as the heterogeneous medium, it will still have the same group velocity as the original heterogeneous medium. Thus, by defining our effective medium based on the phase velocity as in (4.8), we retain the same physical properties of the solution as in the original problem. In the limit $\boldsymbol{k} \to \mathbf{0}$, the two definitions provide the same results.

5 Why is spatial dispersion a problem?

In the previous section, we saw that the effective material depends on the wave vector, $\boldsymbol{\epsilon}_{\text{eff}} = \boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k})$, which defines a spatially dispersive medium. The problem with spatial dispersion is that it changes the conditions for Maxwell's equations. There are no problems as long as we stay in the Fourier domain, since

$$\mathrm{i}\boldsymbol{k} \times (\mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{E}}) = c^{-2}\omega^2 \boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k}) \cdot \widehat{\boldsymbol{E}} \tag{5.1}$$

is an algebraic problem and is easily solved. However, many methods are designed for operating in the time-space domain, where we would have

$$\nabla \times (\nabla \times \boldsymbol{E}(\boldsymbol{x}, t)) = -c^{-2}\partial_t^2 [\check{\boldsymbol{\epsilon}}_{\text{eff}} * \boldsymbol{E}](\boldsymbol{x}, t) \tag{5.2}$$

where $*$ denotes spatial convolution and $\check{\boldsymbol{\epsilon}}_{\text{eff}}(\boldsymbol{x})$ is the inverse Fourier transform of $\boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k})$. Thus, the constitutive relation mapping $\boldsymbol{E}$ to $\boldsymbol{D}$ becomes nonlocal in space, and it is difficult to provide conditions under which the convolution in the right hand side will not destroy fundamental physical properties of Maxwell's equations.

These problems originate in the fact that in order to calculate the electric flux density $\boldsymbol{D} = \epsilon_0 \check{\boldsymbol{\epsilon}}_{\text{eff}} * \boldsymbol{E}$ at a specific point $\boldsymbol{x}$ in space, the spatial convolution requires samples of the electric field $\boldsymbol{E}$ from a region surrounding $\boldsymbol{x}$. The size of the region is determined from the support of $\check{\boldsymbol{\epsilon}}_{\text{eff}}$. This has two major effects: 1) values of $\boldsymbol{E}$ outside the light cone are permitted to influence the value of $\boldsymbol{D}$, which implies a formal propagation speed larger than the speed of light in vacuum, and 2) it is difficult to implement sensible boundary conditions, since the calculation of $\boldsymbol{D}$ close to the boundary would require samples of $\boldsymbol{E}$ on the wrong side of the boundary. These shortcomings are in effect even if the support of $\check{\boldsymbol{\epsilon}}_{\text{eff}}$ is extremely small, so that the convolution can be represented by differential operators.

As a striking example, assume $\boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k})$ can be written as a power series in $\boldsymbol{k}$, for instance as $\boldsymbol{\epsilon}_{\text{eff}}(\mathbf{0}) + (\alpha_1 k + \alpha_2 k^2 + \alpha_3 k^3)\mathbf{I}$, where $\alpha_{1,2,3}$ are small. Even if α_3 is small, the inverse Fourier transform of k^3 results in a third order spatial differential operator, which fundamentally changes the principal part of Maxwell's equations, *i.e.*, the highest order derivatives. This is the part of the equations that governs the important mathematical results concerning existence and uniqueness of solutions, as well as the formulation of boundary conditions, which means that even though $\alpha_3 k^3$ is meant to have a very small effect on the solution, it now has a fundamental impact even on the very existence of a solution.

In contrast, had $\boldsymbol{\epsilon}_{\text{eff}}$ depended only on ω instead of $\boldsymbol{k}$, the resulting convolution in (5.2) would be in the time variable instead, and the constitutive relation would be local in space. It is then much easier to give conditions under which the resulting equations can actually be solved, see for instance [6]. In fact, this is a very common model taking into account that materials behave differently for different frequencies, *i.e.*, temporal dispersion. This motivates us to look for cases where it is possible to convert the spatial dispersion into temporal dispersion.

We end this section by emphasizing that we do not claim that spatial dispersion is a bad model, since many physical phenomena can be effectively discussed and interpreted in such a model, for instance chirality and optical activity. Our point is that it is difficult to use spatial dispersion when calculating a *numerical* solution to Maxwell's equations. For further discussion on spatial dispersion, we refer to [12, pp. 358–371]. Some recent contributions to the question of boundary conditions for spatially dispersive media can be found in [7, 17].

6 Converting spatial dispersion to temporal dispersion

In this section we present a few cases where at least a partial conversion of spatial to temporal dispersion can be achieved. In principle, we need to invert the dispersion relation $\omega = W(\boldsymbol{k})$ to give $\boldsymbol{k} = W^{-1}(\omega)$. However, since $\omega = W(\boldsymbol{k})$ defines a surface in U' for a fixed ω, the map W does not have a unique inverse. Even worse, for each fixed $\boldsymbol{k} \in U'$ we have two dispersion relations to keep track of, which are usually not identical.

6.1 Single mode with fixed propagation direction

Assuming that only one mode is excited in the heterogeneous material, and that this mode is constrained to a fixed propagation direction $\hat{\boldsymbol{k}}$, implies that we only need to consider the dispersion relation associated with this mode, denoted $\omega = W(\boldsymbol{k}) = W(k\hat{\boldsymbol{k}}) = W_{\hat{\boldsymbol{k}}}(k)$, which has a well-defined inverse. This means we only consider the principal value of the effective permittivity, which is

$$\epsilon_{\text{eff}}^{\hat{\boldsymbol{k}}}(k) = \frac{c^2k^2}{W(k\hat{\boldsymbol{k}})^2} = \frac{c^2k^2}{W_{\hat{\boldsymbol{k}}}(k)^2} = \frac{c^2[W_{\hat{\boldsymbol{k}}}^{-1}(\omega)]^2}{\omega^2} = \epsilon_{\text{eff}}^{\hat{\boldsymbol{k}}}(\omega) \tag{6.1}$$

This is the intuitive result which defines the temporally dispersive permittivity. This result could be used in a situation where the interior of a domain is governed by a spatially dispersive material $\boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k})$ according to (4.8), but in a region close to the boundary (close meaning on the scale of the support of $\check{\boldsymbol{\epsilon}}_{\text{eff}}(\boldsymbol{x})$), we replace the spatially dispersive medium with a temporally dispersive medium $\epsilon_{\text{eff}}^{\hat{\boldsymbol{k}}}(\omega)$ where the fixed propagation direction $\hat{\boldsymbol{k}}$ is chosen in the normal direction.

6.2 Fixed polarization eigenmodes

We continue to write $\boldsymbol{k} = k\hat{\boldsymbol{k}}$, keeping $\hat{\boldsymbol{k}}$ fixed. If the vectors $\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle$ have constant direction for each k, we may treat each mode individually. This provides

$$\boldsymbol{\epsilon}_{\text{eff}}^{\hat{\boldsymbol{k}}}(k) = \sum_{n=1}^{2} \frac{c^2 k^2}{W_n(k\hat{\boldsymbol{k}})^2} \frac{\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle \langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle^*}{|\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle|^2} = \sum_{n=1}^{2} \frac{c^2 [W_{n\hat{\boldsymbol{k}}}^{-1}(\omega)]^2}{\omega^2} \frac{\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle \langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle^*}{|\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle|^2} = \boldsymbol{\epsilon}_{\text{eff}}^{\hat{\boldsymbol{k}}}(\omega) \tag{6.2}$$

The reason we may treat the modes individually, is that if the vectors $\langle \widetilde{\boldsymbol{E}}_n \rangle$ have fixed direction, there is a unique dispersion relation applying to the corresponding Cartesian component of $\boldsymbol{E}$.

For a highly symmetrical structure like the one in Figure 1, it is tempting to fix the propagation direction $\hat{\boldsymbol{k}}$ along an axis of symmetry, say $\hat{\boldsymbol{x}}_1$. Using (6.2), we would then define a temporally dispersive permittivity $\boldsymbol{\epsilon}_{\text{eff}}^{\hat{\boldsymbol{x}}_1}(\omega)$, which is isotropic, *i.e.*, both principal values are identical due to the symmetry axis. Repeating the procedure for $\hat{\boldsymbol{x}}_2$ and $\hat{\boldsymbol{x}}_3$, we would obtain the same result, *i.e.*, the principal values of $\boldsymbol{\epsilon}_{\text{eff}}^{\hat{\boldsymbol{x}}_1}(\omega)$, $\boldsymbol{\epsilon}_{\text{eff}}^{\hat{\boldsymbol{x}}_2}(\omega)$, and $\boldsymbol{\epsilon}_{\text{eff}}^{\hat{\boldsymbol{x}}_3}(\omega)$ are all equal, and conclude that the effective permittivity $\boldsymbol{\epsilon}_{\text{eff}}(\omega) = c^2[W_{n\hat{\boldsymbol{x}}_i}^{-1}(\omega)]^2/\omega^2 \mathbf{I}$ for any $n = 1, 2$ or $i = 1, 2, 3$. But we also see from Figure 1 that there is clearly a difference between the modes when $\boldsymbol{k}$ is not along a symmetry axis, for instance for $\boldsymbol{\eta} = \boldsymbol{k}a = (\pi, \pi, 0)$. This demonstrates that even if measurements along three principal axes of the material provide the same results, indicating an isotropic material, the finite scale may still provide anisotropic effects. This is called optical anisotropy, first studied by H. A. Lorentz in 1878 [12, p. 366].

6.3 Identical dispersion relations

There is at least one special, although unlikely, case where we may free ourselves from the requirement of fixing the propagation direction $\hat{\boldsymbol{k}}$. If the dispersion relations are all identical and independent of the propagation direction, *i.e.*, $\omega = W_1(\boldsymbol{k}) = W_2(\boldsymbol{k}) = W(k)$, we have

$$\boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k}) = \sum_{n=1}^{2} \frac{c^2 k^2}{W_n(\boldsymbol{k})^2} \frac{\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle \langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle^*}{|\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle|^2} = \frac{c^2 k^2}{W(k)^2} \sum_{n=1}^{2} \frac{\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle \langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle^*}{|\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle|^2} \tag{6.3}$$

In [23] it is discussed that the $\hat{\boldsymbol{k}}\hat{\boldsymbol{k}}$ part of $\boldsymbol{\epsilon}_{\text{eff}}$ is fundamentally undetermined by the Bloch formalism employed in this paper. This is not a problem, since this component only deals with static fields and we are only interested in propagating waves. However, this does provide the interesting possibility of adding the dyadic product $\hat{\boldsymbol{k}}\hat{\boldsymbol{k}}$ to the sum in the above equation without changing the effect of the effective permittivity, *i.e.*,

$$\boldsymbol{\epsilon}_{\text{eff}}(\boldsymbol{k}) = \frac{c^2 k^2}{W(k)^2} \left(\hat{\boldsymbol{k}}\hat{\boldsymbol{k}} + \sum_{n=1}^{2} \frac{\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle \langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle^*}{|\langle \widetilde{\boldsymbol{E}}_{n\perp} \rangle|^2} \right) = \frac{c^2 [W^{-1}(\omega)]^2}{\omega^2} \mathbf{I} = \boldsymbol{\epsilon}_{\text{eff}}(\omega) \tag{6.4}$$

As previously indicated, this is indeed an unlikely case to occur, since in general the dispersion relations are not only unequal but also fundamentally depend on the propagation direction $\hat{\boldsymbol{k}}$, in addition to the magnitude of the wave vector k.

6.4 Chiral media

Although we only study non-magnetic models in this paper, we wish to mention that in the special case of chiral media, a complete conversion from a spatially dispersive medium to a temporally dispersive medium can be achieved, *i.e.*, we do not have to fix a propagation direction. The Drude-Born-Fedorov model for chiral media is

$$\widehat{\boldsymbol{D}} = \epsilon_0(\epsilon\widehat{\boldsymbol{E}} + \beta \mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{E}}) \tag{6.5}$$

$$\widehat{\boldsymbol{B}} = \mu_0(\mu\widehat{\boldsymbol{H}} + \beta \mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{H}}) \tag{6.6}$$

Inserting these expressions into the Fourier transformed Maxwell's equations imply

$$\mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{E}} = \mathrm{i}\omega\widehat{\boldsymbol{B}} = \mathrm{i}\omega\mu_0(\mu\widehat{\boldsymbol{H}} + \beta \mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{H}}) \tag{6.7}$$

$$\mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{H}} = -\mathrm{i}\omega\widehat{\boldsymbol{D}} = -\mathrm{i}\omega\epsilon_0(\epsilon\widehat{\boldsymbol{E}} + \beta \mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{E}}) \tag{6.8}$$

From the combination of these equations we solve for $\mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{E}}$ and $\mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{H}}$ to find

$$\mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{E}} = \mathrm{i}\omega\mu_0 \left(\frac{\mu}{1 - c^{-2}\omega^2\beta^2}\widehat{\boldsymbol{H}} + \frac{-\mathrm{i}\omega\epsilon_0\epsilon\beta}{1 - c^{-2}\omega^2\beta^2}\widehat{\boldsymbol{E}} \right) = \mathrm{i}\omega\widehat{\boldsymbol{B}} \tag{6.9}$$

$$\mathrm{i}\boldsymbol{k} \times \widehat{\boldsymbol{H}} = -\mathrm{i}\omega\epsilon_0 \left(\frac{\epsilon}{1 - c^{-2}\omega^2\beta^2}\widehat{\boldsymbol{E}} + \frac{\mathrm{i}\omega\mu_0\mu\beta}{1 - c^{-2}\omega^2\beta^2}\widehat{\boldsymbol{H}} \right) = -\mathrm{i}\omega\widehat{\boldsymbol{D}} \tag{6.10}$$

where we used $\epsilon_0\mu_0 = c^{-2}$. This demonstrates that a new set of constitutive relations can be formulated, with only temporal dispersion. However, the derivation depended heavily on the special form of the Drude-Born-Fedorov constitutive relations. For further discussion on chiral media, we refer to [11, 13].

7 Calculations for a laminated geometry

In [22], exact and asymptotic dispersion relations for a two-phase laminated geometry were derived. The unit cell is assumed to have width a in the z-direction, and is arbitrary in the x and y directions. The microscopic geometry is defined as

$$\epsilon(z) = \begin{cases} \epsilon_1 & 0 < z < a_1 \\ \epsilon_2 & a_1 < z < a \end{cases} \tag{7.1}$$

and the volume fractions of the materials are $f_1 = a_1/a$ and $f_2 = (a - a_1)/a$, where $f_1 + f_2 = 1$. Defining the propagation direction by the angle θ between the propagation direction and the z-axis, the asymptotic expressions for the effective permittivity is

$$\epsilon_{\text{eff}}(k, \theta) = f_1\epsilon_1 + f_2\epsilon_2 + \frac{1}{12}\frac{(\epsilon_1 - \epsilon_2)^2(f_1 f_2)^2}{f_1\epsilon_1 + f_2\epsilon_2}(ka)^2 + \mathrm{O}((ka)^4) \tag{7.2}$$

for fields parallel to the material interfaces (in the xy plane, *i.e.*, the TE mode), and

$$\epsilon_{\text{eff}}(k,\theta) = \frac{1}{\left(\frac{f_1}{\epsilon_1}+\frac{f_2}{\epsilon_2}\right)\sin^2\theta + \frac{\cos^2\theta}{f_1\epsilon_1+f_2\epsilon_2}} + \frac{1}{12}\frac{(\epsilon_1-\epsilon_2)^2(f_1f_2)^2}{f_1\epsilon_1+f_2\epsilon_2}\left(\frac{\frac{(f_1\epsilon_1+f_2\epsilon_2)^2}{\epsilon_1\epsilon_2}\sin^2\theta-\cos^2\theta}{\left(\frac{f_1}{\epsilon_1}+\frac{f_2}{\epsilon_2}\right)(f_1\epsilon_1+f_2\epsilon_2)\sin^2\theta+\cos^2\theta}\right)^2 (ka)^2 + \mathrm{O}((ka)^4) \quad (7.3)$$

for fields with a non-zero z-component, *i.e.*, the TM mode. This is a typical case of the situation discussed in Section 6.2. The inverse of the dispersion relations are

$$(ka)^2 = (f_1\epsilon_1+f_2\epsilon_2)(c^{-1}\omega a)^2 + \mathrm{O}((c^{-1}\omega a)^4) \quad (7.4)$$

for the TE mode and

$$(ka)^2 = \frac{1}{\left(\frac{f_1}{\epsilon_1}+\frac{f_2}{\epsilon_2}\right)\sin^2\theta+\frac{\cos^2\theta}{f_1\epsilon_1+f_2\epsilon_2}}(c^{-1}\omega a)^2 + \mathrm{O}((c^{-1}\omega a)^4) \quad (7.5)$$

for the TM mode. This implies

$$\epsilon_{\text{eff}}(\omega,\theta) = (f_1\epsilon_1+f_2\epsilon_2)\left(1+\frac{1}{12}\frac{(\epsilon_1-\epsilon_2)^2(f_1f_2)^2}{f_1\epsilon_1+f_2\epsilon_2}(c^{-1}\omega a)^2\right) + \mathrm{O}((c^{-1}\omega a)^4) \quad (7.6)$$

for the TE mode, which is seen to be independent of the propagation direction θ, and

$$\epsilon_{\text{eff}}(\omega,\theta) = \frac{1}{\left(\frac{f_1}{\epsilon_1}+\frac{f_2}{\epsilon_2}\right)\sin^2\theta+\frac{\cos^2\theta}{f_1\epsilon_1+f_2\epsilon_2}} \times \left[1+\frac{1}{12}\frac{(\epsilon_1-\epsilon_2)^2(f_1f_2)^2}{f_1\epsilon_1+f_2\epsilon_2}\left(\frac{\frac{(f_1\epsilon_1+f_2\epsilon_2)^2}{\epsilon_1\epsilon_2}\sin^2\theta-\cos^2\theta}{\left(\frac{f_1}{\epsilon_1}+\frac{f_2}{\epsilon_2}\right)(f_1\epsilon_1+f_2\epsilon_2)\sin^2\theta+\cos^2\theta}\right)^2 (c^{-1}\omega a)^2\right] + \mathrm{O}((c^{-1}\omega a)^4) \quad (7.7)$$

for the TM mode. Apparently, the expressions (7.6) and (7.7) are equal for $\theta = 0$. A graph of the expression in square brackets in (7.7) is shown in Figure 2.

8 Conclusions

We have demonstrated that it is possible to define effective material parameters, which do not vary in space, modelling the macroscopic behavior of heterogeneous problems varying on a small scale. Our reasoning is based on the idea that both the heterogeneous and the homogenized problem should have the same dispersion relations. This leads to identifying the effective material parameters from the phase

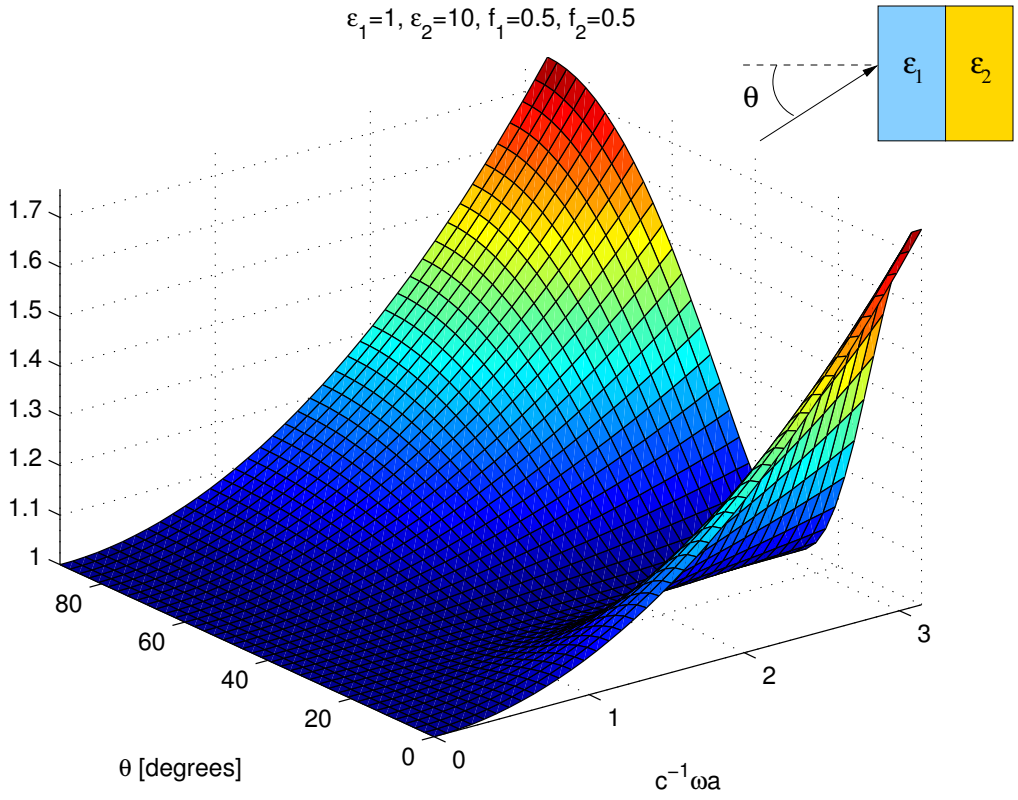

Figure 2: The factor in square brackets for the TM mode in (7.7). The corresponding factor for the TE mode given by (7.6) is independent of θ, and corresponds to the case $\theta = 0$ in this graph. The parameters are $\epsilon_1 = 1$, $\epsilon_2 = 10$, $f_1 = f_2 = 0.5$.

velocity of each mode. The group velocity, which is concerned with the propagation time through a slab of the medium, will still be the same in the effective medium if the dispersion is properly taken into account (say, through a stationary phase analysis). Thus, when interpreting material measurements, the material properties are more easily extracted from measurements involving relatively thin substrates, say shorter than a wavelength, since the interpretation would then have to be based on the phase velocity.

At the present level of understanding, we can only define temporally dispersive effective material parameters in very simple cases, typically for a fixed propagation direction. Thus, the spatial dispersion seems fundamentally inherent in the problem, and probably only vanishes in the extreme homogenization limit $\boldsymbol{k} \to \mathbf{0}$.

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