Fourier-Domain Electromagnetic Wave Theory for Layered Metamaterials of Finite Extent

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Stratified media consisting of metal and dielectric layers have been presented on the premise that they are metamaterials with electromagnetic properties described by plane-wave parameters derived from homogenization. The validity of homogenization rests upon consistency between plane-wave parameters and complete wave solutions to Maxwell’s equations, a comparison most easily performed if the wave solution is expressed in the Fourier domain. Here, we analytically develop the general Fourier-domain electromagnetic wave solution in a lossy, layered medium of finite extent. An advantage of Fourier-domain analysis is that the wave solution can be condensed into a product of three matrix factors: one governed by reflections from the medium boundaries, a second associated with Floquet-Bloch modes due to layer periodicity, and a third dependent on layer composition. We demonstrate two benefits of an analytical, factorized, Fourier-domain wave solution: 1) electromagnetic fields and power flow in any finite, lossy, layered structure can be interpreted in terms of separable factors dependent on distinct physical features of the structure and 2) plane-wave solutions derived from homogenization methods (such as effective medium theory, scattering parameter retrieval, and Floquet-Bloch analysis) can be directly validated in the Fourier domain. The general theory developed here enables unified analysis of layered metamaterials, whose diverse descriptions in the literature (such as hyperbolic, anisotropic, and negative-index) stem from the use of different homogenization methods.

1. Introduction

Recent contributions to the long tradition of inquiry into the electromagnetic properties of planar layered structures [1–10] have been sparked by the novel conceptualization of these structures - particularly those composed of sub-wavelength-thick layers of metal - as metamaterials. The metamaterial concept is used to describe a structure with sub-wavelength scale heterogeneity in terms of plane-wave parameters such as refractive index and impedance. Planar layered structures, which possess heterogeneity along just a single direction, are the simplest metamaterial form and provide an experimentally feasible template for metamaterial devices operating at visible frequencies and beyond due to the availability of thin film deposition techniques with layer thickness control on sub-nanometer scales. Exciting applications for layered metamaterials include flat lens imaging [11–14] and analog computation [15].

Classification of a heterogeneous structure as a metamaterial begins by seeking an analog homogeneous structure possessing a plane-wave solution that mimics the more intricate wave solution corresponding the original structure. This process, known as homogenization, yields familiar plane-wave parameters to approximate wave behavior in the heterogeneous structure. Each homogenization technique invokes a unique set of assumptions, which are not always justified, to arrive at its plane-wave parameters. Effective medium theory can be used to define an effective permittivity tensor through volumetric averaging of the local permittivity values [2, 16, 17], which, for a layered structure, simplifies to a thickness-weighted average of the layer permittivity values. Although effective medium theory is intuitive, it relies upon the electrostatic approximation which neglects time-derivative terms in Maxwell’s equations. The scattering parameter method [18–21] is based on equating the reflection and transmission coefficients of a heterogeneous structure to those of an equivalent homogeneous structure. Drawbacks include non-uniqueness [22, 23] and the absence of correlation to the fields inside the structure. It is possible to derive effective constitutive parameters by averaging local permittivity values weighted by the fields [24] or energy densities [25] inside a structure, although this method also suffers from non-uniqueness. If a structure is periodic, a unique set of homogeneous parameters can be defined using the Floquet-Bloch theorem [26, 27]. The wave inside a structure is decomposed into a set of Floquet-Bloch modes $k_{FB}$ [28–31] and if one mode carries dominant power, it is assumed to approximate the entire wave and its plane-wave parameters are conferred to the structure [32–38]. The Floquet-Bloch modes of a periodic layered structure can be found by imposing translational invariance of the wave over a period within a multiplicative exponential factor [7], a procedure that implicitly assumes infinite extent and no loss. When the

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medium is lossy, the Floquet-Bloch modes are complex-valued \[39,41\], but no longer discrete [32]. When the medium is finite, translational invariance is altogether lost due to reflections from the end facets of the medium and a dependence on the excitation conditions in the external bounding media [29].

The validity of the metamaterial approximation depends upon consistency between plane-wave parameters derived by homogenization and complete wave solutions to Maxwell’s equations. Direct comparison between the two can be challenging because plane-wave parameters are most naturally interpreted in the spatial-frequency domain, whereas wave solutions from numerical solvers and analytical techniques (such as those based on matrix formalism [3,7,9,10,22]) are commonly communicated in the spatial domain. The obvious resolution is to obtain Fourier-domain wave solutions, but the most common solution techniques based on Fourier expansion of a single field component (known as the plane-wave expansion method [45] or Fourier expansion of the electric and magnetic field components into a series of plane waves [30,31,38] are limited to lossless, non-dispersive, and infinitely periodic media not applicable to finite-sized, metal-dielectric metamaterials. Recently, Fourier transformation of the numerically-computed wave solution in a finite-sized, lossless periodic layered medium has revealed a correlation between the spatial frequency content of the wave and the Floquet-Bloch modes corresponding to an unbounded version of the periodic medium [22]. This correlation, however, has not been made mathematically explicit and has yet to be established for the case of loss, a condition vital for analysis of metamaterials which frequently incorporate metals.

The goal of this work is to analytically derive the Fourier-domain electromagnetic wave solution for a general layered configuration that accommodates periodic or aperiodic layer arrangements under the realistic constraints of loss and finite extent. The wave solution is distilled into a compact, factorized form consisting of a term due to reflections from the medium boundaries, another associated with the complex-valued Floquet-Bloch modes of the unit cell, and a third that is dependent on the layer thickness and composition. In contrast to plane-wave parameters obtained by homogenization, the factorized, Fourier-domain wave solution is fully consistent with Maxwell’s equations and provides physical insight into the effects of loss, finite extent, and periodicity. We apply the wave solution to analyze the electromagnetic fields and power flow in several representative metal-dielectric layered metamaterials at optical frequencies and to validate plane-wave parameters obtained by homogenization techniques such as effective medium theory, scattering parameter retrieval, and Floquet-Bloch analysis. Of the three, Floquet-Bloch analysis provides the closest approximation to the complete wave solution, an observation that is consistent with previous reports [22] and can now be explained by the explicit appearance of Floquet-Bloch modes in the factorized, Fourier-domain wave solution.

A factorized Fourier-domain wave solution contributes to the resolution of the following research questions pertinent to layered implementations of metamaterials: How accurately do plane-wave solutions derived by homogenization approximate the complete wave solution? How do the conditions of material loss and finite extent, both of which are important in the analysis of any practical layered metamaterial device, affect the validity of the metamaterial concept? Is there a systematic method to understand the relationship between the internal electromagnetic fields and power flow in a layered structure and the physical parameters of the structure? Finally, are there better ways to describe the electromagnetic properties of layered metamaterials than through approximate plane-wave solutions provided by homogenization?

2. Generalized Description of a Layered Medium

We consider a generalized one-dimensionally periodic medium (Figure 1) immersed in free space and composed of \( M \) repeated unit cells, each consisting of \( J \) layers, yielding a total of \( MJ \) layers. The unit cells are referenced by the integer \( m = 0, \ldots, M - 1 \) and the layers within any unit cell are referenced by the integer \( j = 1, \ldots, J \). Each layer in the medium is uniquely labeled by the integer \( \ell = mJ + j = 1, \ldots, MJ \) and, for sequential consistency, the free-space half-spaces to the left and right of the medium are labeled \( \ell = 0 \) and \( \ell = MJ + 1 \), respectively. Layer \( \ell \) has a thickness of \( d_{\ell} \) and its linear electromagnetic properties are generally specified by a complex-valued relative permittivity \( \epsilon_{\ell} \) (the underline denotes a complex variable) and a complex-valued relative permeability \( \mu_{\ell} \), resulting in a complex-valued refractive index \( n_{\ell} \)

\[
n_{\ell} = \text{sgn}(\Re[\epsilon_{\ell}]|\mu_{\ell}| + \Re[\mu_{\ell}]|\epsilon_{\ell}|)\sqrt{\frac{\epsilon_{\ell}}{\mu_{\ell}}}, \tag{1}
\]

which is permitted to have a real part that is positive (right-handed) or negative (left-handed). The total thickness of the layered medium is \( L = \sum_{\ell=1}^{MJ} d_{\ell} \). Due to periodic repetition of the unit cell, the quantities \( d_{\ell}, \epsilon_{\ell}, \mu_{\ell} \), and \( n_{\ell} \) corresponding to layer \( j \) of an arbitrary unit cell \( m \), can be equivalently denoted \( d_j, \epsilon_j, \mu_j, \) and \( n_j \) corresponding to layer \( j \) of unit cell \( m = 0 \). The plane of the layers is aligned parallel to the \( xy \) plane and we denote the location of the plane between layer \( \ell \) and \( \ell + 1 \) as \( z_\ell \), setting the position of the plane of the first interface \( z_0 = 0 \) without loss of generality.

An electromagnetic plane wave is incident onto the medium from the half-space \( z < 0 \) inclined at an angle \( \theta \) in the \( xz \) plane. Due to the independence of this configuration with respect to the \( y \) coordinate, any solution can be expressed as a linear combination of solutions obtained by assuming either transverse-electric (TE) polarization (electric field \( \vec{E} \) aligned to the \( y \) axis) or transverse-magnetic (TM) polarization (magnetic field \( \vec{H} \) aligned to the \( y \) axis). Here, we treat the case of TM...
polarization, noting that the transformations \( \mathbf{E} \to -\mathbf{E}, \) \( \mathbf{H} \to -\mathbf{H} \), and \( \epsilon \to \mu \) yield complimentary equations for TE polarization [9].

### 3. Wave Solution in the Spatial Domain

We derive a representation of the electromagnetic wave solution in the finite one-dimensional periodic layered structure for the case in which one of the end facets is subject to plane-wave illumination. An incident TM-polarized electromagnetic wave is given by

\[
\mathbf{H}(x,z) = H_0 e^{i(k_x0x + k_z0z)} \mathbf{\hat{y}},
\]

where \( H_0 \) is the amplitude, \( k_x0 \) and \( k_z0 \) are the real-valued wave-vector components along the \( x- \) and \( z- \) axes, respectively, and \( k_0 = \sqrt{k_x0^2 + k_z0^2} \) is the free-space wave vector. The wave is time-harmonic where an \( e^{-i\omega t} \) dependence is assumed but suppressed. Invoking field continuity across the interfaces, the magnetic field in an arbitrary layer \( \ell \) can be written as a sum of two counter-propagating waves using matrix formalism

\[
\mathbf{H}(x,z) = \mathbf{H}_\ell(x,z) \mathbf{\hat{y}} = e^{ik_{x,\ell}x} \left( e^{ik_{z,\ell}(z-z_\ell)} - e^{-ik_{z,\ell}(z-z_\ell)} \right)^T \left( \begin{array}{c} A_{\ell} \\ B_{\ell} \end{array} \right) \mathbf{\hat{y}},
\]

where \( T \) denotes the transpose operator, \( A_\ell \) and \( B_\ell \) are the wave coefficients, and \( k_{z,\ell} \) is the wave-vector component in layer \( \ell \) along the \( z- \) axis (note that \( k_{z,\ell} \) corresponding to layer \( j \) of an arbitrary unit cell \( m \) can be equivalently denoted \( k_{z,j} \) corresponding to layer \( j \) of unit cell \( m = 0 \)). The wave-vector component \( k_{z,\ell} \) is related to the layer refractive index by

\[
k_{z,\ell} = n_\ell \sqrt{k_0^2 - \left( \frac{k_{z,0}}{n_\ell} \right)^2},
\]

where, according to [1], \( n_\ell \) can have a real part that is either positive or negative, describing a right- or left-handed medium, respectively.

The wave solution can be solved by relating the wave coefficients \( A_\ell \) and \( B_\ell \) across the \( M \times J + 1 \) boundaries. The wave coefficients in an arbitrary layer \( \ell \) can be related to the coefficients in an adjacent layer \( \ell + 1 \) by

\[
\left( \begin{array}{c} A_{\ell+1} \\ B_{\ell+1} \end{array} \right) = \mathbf{T}_\ell \mathbf{P}_\ell \left( \begin{array}{c} A_\ell \\ B_\ell \end{array} \right),
\]

where the propagation matrix \( \mathbf{P}_\ell \) corresponding to layer \( \ell \) is given by

\[
\mathbf{P}_\ell = \left( \begin{array}{cc} e^{ik_{z,\ell}d_\ell} & 0 \\ 0 & e^{-ik_{z,\ell}d_\ell} \end{array} \right),
\]

and the transmission matrix \( \mathbf{T}_\ell \) corresponding to the interface between layer \( \ell \) and \( \ell + 1 \) is given by

\[
\mathbf{T}_\ell = \frac{1}{2} \left( 1 + \frac{\mathbf{P}_\ell}{\mathbf{P}_\ell} \right) \left( 1 - \frac{\mathbf{P}_\ell}{\mathbf{P}_\ell} \right),
\]

with \( \mathbf{P}_\ell = \left( k_{z,\ell+1}/k_{z,\ell} \right) \). Assuming unidirectional wave excitation from the left half-space, the wave coefficients in layer 1 are related to the coefficients in the left half-space by

\[
\left( \begin{array}{c} A_1 \\ B_1 \end{array} \right) = \mathbf{T}_0 \left( \begin{array}{c} A_0 \\ B_0 \end{array} \right) = \mathbf{T}_0 \left( \begin{array}{c} 1 \\ \ell \end{array} \right),
\]

where \( \mathbf{T}_0 \) is the transmission matrix from the left half-space into the first layer, \( \ell \) is the complex-valued reflection coefficient of the entire layered system, and the incident wave amplitude has been assumed to be unity. The wave coefficients in layer \( MJ \) are related to the coefficients in the right half-space by

\[
\left( \begin{array}{c} A_{MJ+1} \\ B_{MJ+1} \end{array} \right) = \left( \begin{array}{c} \ell \\ 0 \end{array} \right) = \mathbf{T}_{MJ} \left( \begin{array}{c} A_{MJ} \\ B_{MJ} \end{array} \right),
\]

where \( \mathbf{T}_{MJ} \) is the transmission matrix from layer \( MJ \) into the right half space, \( \ell \) is the complex-valued transmission coefficient. Relation of the wave across the \( MJ+1 \) boundaries yields \( 2MJ+2 \) linear equations, which is sufficient to solve for the \( 2MJ+2 \) unknowns \( \ell \) and \( \ell \), in addition to the \( 2MJ \) wave coefficients in the \( MJ \) layers.

Upon solving for the unknown quantities, \( \mathbf{H}_\ell \) in each layer \( \ell \) is completely specified and we can succinctly express the total field distribution in the spatial domain as

\[
\mathbf{H}(x,z) = \mathbf{H}(x,z) \mathbf{\hat{y}} = \sum_{\ell=1}^{MJ} \text{rect} \left( \frac{z - z_{c,\ell}}{d_\ell} \right) \mathbf{H}_\ell(x,z) \mathbf{\hat{y}},
\]

where \( z_{c,\ell} \) is the location of the center of layer \( \ell \) and the rect function is defined as

\[
\text{rect} \left( \frac{z - z_{c,\ell}}{d_\ell} \right) = \begin{cases} 1 & z_{c,\ell} - d_\ell/2 \leq z \leq z_{c,\ell} + d_\ell/2 \\ 0 & \text{otherwise} \end{cases}
\]

Equation [9] offers a valid representation of the field as a piece-wise function subdivided into spatial intervals corresponding to the layer regions. Although this form is amenable to numerical routines for solving sets of linear equations, there are at least two disadvantages. First, compartmentalization of the wave solution into the individual layers does not afford physical insight into the collective behavior of the solution across repeated sets of layers. Second, representation of the solution in the spatial domain does not produce immediate connections to homogenization parameters, which are generally represented in the spatial-frequency domain. In the next section, we apply Fourier transformation to the piece-wise wave solution and demonstrate the utility of this strategy for decomposing the wave solution into physically meaningful terms and for enabling comparisons with plane-wave parameters obtained by homogenization.
4. Factorized Fourier-Domain Wave Solution

We re-express the general wave solution given by (9) in the spatial-frequency domain by

\[
H(\kappa_x, \kappa_z) = \int_0^{2\pi J} \int_{-\infty}^{\infty} H(x, z) e^{-i\kappa_x x} e^{-i\kappa_z z} dx \, dz,
\]

where \( \kappa_x \) and \( \kappa_z \) are the spatial frequency variables along the respective \( x \) and \( z \) directions. Substitution of (9) into (10) and development of the integrand using well-known Fourier relations and theorems yields

\[
H(\kappa_x, \kappa_z) = (2\pi)^2 \delta(\kappa_x - k_{x,0}) \sum_{\ell=1}^{M J} d_{\ell} \text{sinc} \left( \frac{\kappa_z d_{\ell}}{2\pi} \right) e^{-i\kappa_z z_{c,\ell}} \ast \left( e^{-i\kappa_z z_{c,\ell}} \sum_{j=1}^{\infty} \frac{d_j}{2\pi} \right) T
\]

\[
\left( \frac{A_{mJ+j}}{B_{mJ+j}} \right).
\]

where \( \delta \) is the Dirac delta function.

In this section, we outline a series of mathematical manipulations that can be applied to (11) to produce a physically insightful factorized Fourier-domain wave solution. First, we re-write the single summation in (11) as a nested double summation over the number of layers in a unit cell and the number of unit cells by making the variable substitutions \( d_{\ell} = d_j \) and \( k_{z,\ell} = k_{z,j} \) and the

Index substitution \( \ell = mJ + j \), resulting in

\[
H(\kappa_x, \kappa_z) = (2\pi)^2 \delta(\kappa_x - k_{x,0}) \sum_{m=0}^{M-1} \sum_{j=1}^{J} d_j \text{sinc} \left( \frac{\kappa_z d_j}{2\pi} \right) e^{-i\kappa_z z_{c,mJ+j}} \ast \left( e^{-i\kappa_z z_{c,mJ+j}} \sum_{j=1}^{\infty} \frac{d_j}{2\pi} \right) T
\]

\[
\left( \frac{A_{mJ+j}}{B_{mJ+j}} \right).
\]

Carrying out the convolution operation in (12) and using the relation \( z_{c,mJ+j} - z_{mJ+j-1} = d_j/2 \) yields

\[
H(\kappa_x, \kappa_z) = (2\pi)^2 \delta(\kappa_x - k_{x,0}) \sum_{m=0}^{M-1} \sum_{j=1}^{J} d_j e^{-i\kappa_z z_{c,mJ+j}} \text{sinc} \left[ \left( \frac{\kappa_z - k_{z,j}}{2\pi} \right) d_j/2 \right] T
\]

\[
\left( \frac{A_{mJ+j}}{B_{mJ+j}} \right).
\]

The unit cell summation in (13) can be simplified using the relationship

\[
z_{c,mJ+j} = mD + z_{j-1} + d_j/2,
\]

where \( D = \sum_{j=1}^{J} d_j \) is the thickness of the unit cell and \( z_{j-1} \) is the position of the interface between layer \( j-1 \) and \( j \) within unit cell \( m = 0 \). Substitution of (14) into
\( H(\kappa_x, \kappa_z) = (2\pi)^2 \delta(\kappa_x - k_{x,0}) \sum_{j=1}^{J} d_j e^{-i\kappa_x z_j-1} \)

\[
\begin{pmatrix}
  e^{-i(\kappa_z - k_{z,0})d_j/2} \sin[(\kappa_z - k_{z,0})d_j/2]\pi
  e^{-i(\kappa_z + k_{z,0})d_j/2} \sin[(\kappa_z + k_{z,0})d_j/2]\pi
\end{pmatrix}^T
\]

\[
\sum_{m=0}^{M-1} e^{-i\kappa_m D} m D \left( \begin{array}{c}
  A_{m,J+j}
  B_{m,J+j}
\end{array} \right).
\]

(15)

Equation (15) expresses the wave solution in terms of wave coefficients \( A_{m,J+j} \) and \( B_{m,J+j} \) distributed throughout the medium, which provides little additional insight over the spatial-domain representation of the wave solution in (9). We can further simplify the solution in terms of the wave coefficients in just the first unit cell by using the matrix relationship between wave coefficients in different layers. The wave coefficients in layer \( \ell \) are related to the coefficients in an arbitrary layer \( \ell + s \) (where the integer \( s \leq MJ - \ell \)) within the layered medium by

\[
\begin{pmatrix}
  A_{\ell+s}
  B_{\ell+s}
\end{pmatrix} = \mathbf{W}_{\ell+s,\ell} \begin{pmatrix}
  A_{\ell}
  B_{\ell}
\end{pmatrix},
\]

(16)

where the transfer matrix \( \mathbf{W}_{\ell+s,\ell} \) is determined from the transmission and propagation matrices by

\[
\mathbf{W}_{\ell+s,\ell} = \prod_{q=\ell}^{\ell+s-1} \mathbf{T}_q \mathbf{P}_q.
\]

(17)

The coefficients \( A_{m,J+j} \) and \( B_{m,J+j} \) corresponding to layer \( j \) within an arbitrary unit cell \( m \) can be related to the coefficients \( A_j \) and \( B_j \) corresponding to layer \( j \) within unit cell \( m = 0 \) by

\[
\begin{pmatrix}
  A_{m,J+j}
  B_{m,J+j}
\end{pmatrix} = \mathbf{U}_j^m \begin{pmatrix}
  A_j
  B_j
\end{pmatrix},
\]

(18)

where \( \mathbf{U}_j^m \) is the unit cell transfer matrix from layer \( j \) to \( j + J \) and can be expressed as

\[
\mathbf{U}_j = \mathbf{W}_{j+J,j}.
\]

We can now simplify (15) in terms of wave coefficients \( A_j \) and \( B_j \) distributed throughout a unit cell referenced from layer \( j \)

\[
\begin{pmatrix}
  e^{-i(\kappa_z - k_{z,0})d_j/2} \sin[(\kappa_z - k_{z,0})d_j/2]\pi
  e^{-i(\kappa_z + k_{z,0})d_j/2} \sin[(\kappa_z + k_{z,0})d_j/2]\pi
\end{pmatrix}^T
\]

\[
\sum_{m=0}^{M-1} (e^{-i\kappa_m D} \mathbf{U}_j)^m \left( \begin{array}{c}
  A_j
  B_j
\end{array} \right).
\]

(20)

The unit cell transfer matrix referenced from layer \( j \), \( \mathbf{U}_j \), can be related to the unit cell transfer matrix referenced from layer 1, \( \mathbf{U}_1 \), using the relation

\[
\mathbf{U}_j^m = \mathbf{W}_{j,1} \mathbf{U}_1^m \mathbf{W}_{j,1}^{-1}.
\]

(21)

Eigenvalue decomposition of \( \mathbf{U}_1 \) yields

\[
\begin{pmatrix}
  \mathbf{Q} \ \mathbf{\Lambda} \ \mathbf{Q}^{-1}
\end{pmatrix}
\]

(22)

where \( \mathbf{Q} \) is the eigenvector of \( \mathbf{U}_j \) and \( \mathbf{\Lambda} \) is the eigenvalue of \( \mathbf{U}_1 \) whose diagonal elements are the corresponding eigenvalues \( \mathbf{\Lambda}^+ \) and \( \mathbf{\Lambda}^- \). Because the determinant of \( \mathbf{U}_1 \) is unity, the eigenvalues are inverses of each other, \( \mathbf{\Lambda}^- = 1/\mathbf{\Lambda}^+ \). As a result, the eigenvalues can be related to the Floquet-Bloch mode, \( k_{FB} \), by

\[
\mathbf{\Lambda}^\pm = e^{\pm i k_{FB} D}.
\]

(23)

To arrive at the final form of the magnetic field solution from (15), we apply eigenvalue decomposition of the unit cell transfer matrix and relate the wave coefficients in layer \( j \) to the wave coefficients in the left half space, resulting in

\[
\begin{pmatrix}
  e^{-i\kappa_m D} \mathbf{\Lambda}^m
\end{pmatrix} \mathbf{Q}^{-1} \mathbf{T}_0 \left( \begin{array}{c}
  1
  \ell
\end{array} \right),
\]

(24)

where we have highlighted three distinctive matrix factors - a layer matrix \( \mathbf{L}_j \) dependent on the thickness and wave vector in the \( j \)th layer of the unit cell, a Floquet-Bloch matrix \( \mathbf{FB} \) dependent on the eigenvalues of the
unit cell, and a weighting matrix $\mathbf{C}$ dependent on the reflection coefficient. The magnetic field solution can be succinctly written as

$$H(\kappa_x, \kappa_z) = (2\pi)^2 \delta(\kappa_x - k_x, 0) \sum_{j=1}^{J} L_j \mathbf{FB} \mathbf{C}, \quad (25)$$

where the three matrix factors have the following general form

$$L_j = \begin{pmatrix} L_j^+ & L_j^- \end{pmatrix}, \quad \mathbf{FB} = \begin{pmatrix} \mathbf{FB}^+ & 0 \\ 0 & \mathbf{FB}^- \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} \mathbf{C}^+ & \mathbf{C}^- \end{pmatrix}. \quad (26)$$

In [26], we have distinguished “forward” and “backward” elements of each matrix factor using the superscript “$+$” and “$-$”, respectively. Developing the matrix factors in [25] yields

$$H(\kappa_x, \kappa_z) = (2\pi)^2 \delta(\kappa_x - k_x, 0) \sum_{j=1}^{J} \left( L_j^+ \right)^T \left( \mathbf{FB}^+ \mathbf{C}^+ \right), \quad (27)$$

which, in contrast to the spatial-domain solution in [9], requires summation of only $J$ terms corresponding to the layers of the unit cell and describes collective wave behavior across repeated sets of unit cells through the elements of the Floquet-Bloch matrix, whose behavior will be examined in the next section.

Given the vector spectral magnetic field $\vec{H}(\kappa_x, \kappa_z) = H(\kappa_x, \kappa_z) \hat{y}$ and the vector spectral electric field $\vec{E}(\kappa_x, \kappa_z) = E_x(\kappa_x, \kappa_z) \hat{x} + E_z(\kappa_x, \kappa_z) \hat{z}$. It is possible to define the spectral time-averaged Poynting vector

$$\langle \vec{S}(\kappa_x, \kappa_z) \rangle = \frac{1}{2} \Re \left[ \vec{E}(\kappa_x, \kappa_z) \times \vec{H}^*(\kappa_x, \kappa_z) \right]. \quad (28)$$

This is similar to the spectral Poynting vector proposed in Ref. [34, 91] and used in Ref. [35] to analyze energy propagation of discrete Floquet-Bloch modes in infinite, lossless dielectric photonic crystals, except now extended to accommodate a continuous range of Fourier field components in a finite, lossy periodic system. It should also be noted that the spectral time-averaged Poynting vector defined in [26] is not equivalent to the Fourier transform of the spatial time-averaged Poynting vector, which would involve the convolution of the spectral electric and magnetic fields. It does, however, enable the spatial frequency $\kappa_z$ present in the electric and magnetic fields to be envisioned as an electromagnetic plane wave having a well-defined time-averaged direction of power flow, which is useful, for instance, for the characterization of the wave in terms of forward- and backward-propagating wave components.

5. Understanding the Roles of Finite Extent and Loss

The elements of the Floquet-Bloch matrix are given by

$$\mathbf{FB}^\pm = e^{-i(\kappa_x \pm \hat{k}_{FB}) M^{1/2} D M \Delta_{FB} [\kappa_z \pm \Re(\hat{k}_{FB})]*} \sin \left( \dfrac{M[k_z \pm i\Im (\hat{k}_{FB})]/D/2}{2\pi} \right), \quad (29)$$

where the Dirac comb $\Delta_{FB} [\kappa_z \pm \Re(\hat{k}_{FB})]$ is

$$\Delta_{FB} [\kappa_z \pm \Re(\hat{k}_{FB})] = \sum_{N=-\infty}^{\infty} \delta[k_z - 2\pi N/D \pm \Re(\hat{k}_{FB})], \quad (30)$$

describing an infinite comb of discrete spatial-frequency harmonics spaced by $2\pi/D$. Because the Dirac comb is convolved with the sinc function in [29], the elements $\mathbf{FB}^\pm$ contain harmonics widened through the combined effects of finite extent ($M < \infty$) and material loss ($\Im(\hat{k}_{FB}) \neq 0$). The forward element $\mathbf{FB}^+$ has a principal harmonic centered at $\Re(\hat{k}_{FB})$ and the backward element $\mathbf{FB}^-$ has a principal harmonic centered at $-\Re(\hat{k}_{FB})$.

For a medium of infinite extent ($M \to \infty$), the elements of the Floquet-Bloch matrix approach

$$\lim_{M \to \infty} \mathbf{FB}^\pm = \begin{cases} M \Delta_{FB} [\kappa_z \pm \hat{k}_{FB}] & \Im(\hat{k}_{FB}) = 0 \\ \Delta_{FB} [\kappa_z \pm \Re(\hat{k}_{FB})]* & D/\sqrt{\kappa_z^2 + \Im(\hat{k}_{FB})^2} \neq 0. \end{cases} \quad (31)$$

In the absence of loss, $\mathbf{FB}^\pm$ are discrete spectra with peaks at harmonics of $\pm \Re(\hat{k}_{FB})$. The resulting magnetic field solution consists of discrete forward and backward Floquet Bloch modes (equivalent to the classical Floquet-Bloch solution) with amplitudes that can be explicitly determined by $(2\pi)^2 \sum_j L_j^+ \mathbf{C}^+$ and $(2\pi)^2 \sum_j L_j^- \mathbf{C}^-$, respectively. In the presence of loss, $\mathbf{FB}^\pm$ are continuous spectra with peaks that are centered about harmonics of $\pm \Re(\hat{k}_{FB})$ and broadened due to the effect of $\Im(\hat{k}_{FB})$.

6. Analysis of Metal-Dielectric Layered Metamaterials

We consider the configuration in which a metal-dielectric layered system is subjected to normal-incidence, TM-polarized illumination ($k_x, 0 = 0$). If the system consists of a bi-layer unit cell, the factorized, Fourier-domain magnetic field solution takes the form

$$\mathbf{H}(\kappa_z) = 2\pi \begin{pmatrix} L_1^+ + L_2^+ \\ L_1^- + L_2^- \end{pmatrix}^T \begin{pmatrix} \mathbf{FB}^+ \mathbf{C}^+ \\ \mathbf{FB}^- \mathbf{C}^- \end{pmatrix}, \quad (32)$$

where $L_1^\pm$ and $L_2^\pm$ are the forward and backward elements of layer matrices respectively associated with layers 1 and 2 of the unit cell. Let’s take the case bi-layer
Fig. 2. Decomposition of the wave solution in a metal-dielectric bi-layer system consisting of alternating layers of 30-nm-thick Ag and 30-nm-thick TiO$_2$, assuming a normally incident TM-polarized wave with a free-space wavelength of $\lambda_0 = 365$ nm. a) The forward and backward components of the layer matrix $|L_1|^2$ corresponding to the 30-nm-thick Ag layer. b) The forward and backward components of the layer matrix $|L_2|^2$ corresponding to the 30-nm-thick TiO$_2$ layer. c), d), and e) depict the forward and backward components of $|\text{FB C}|^2$, the magnetic field spectrum $|H|^2$, and the $z$-component of the time-averaged spectral Poynting vector, respectively, for the case of 2 unit cells; f), g), and h) depict the same set of information for the case of 10 unit cells. The horizontal gray lines in e) and h) correspond to zero values of the spectral Poynting vector.

unit cell comprising a 30-nm-thick Ag layer and a 30-nm-thick TiO$_2$ layer. We will consider a system composed of two unit cells ($M = 2$) and another composed of ten unit cells ($M = 10$). The systems are bounded by free space and excited by a wave with a free-space wavelength $\lambda_0 = 365$ nm. We assume that Ag has a complex refractive index of $0.076 + 1.605i$ (interpolated from experimental data [46]) and that TiO$_2$ has a real refractive index of 2.80.

Figure 2 highlights, for the $M = 2$ and $M = 10$ cases, the modulus squared of the magnetic field solution and the elements of its matrix factors, in addition to the $z$-component of the time-averaged spectral Poynting vector. The magnetic field spectrum results from the confluence of broad spectral envelopes defined by $L_1^\pm$ (Ag layer) and $L_2^\pm$ (TiO$_2$ layer) and finer spectral combs defined by $FB^+ C^+$ and $FB^- C^-$. The Floquet-Bloch mode of the unit cell is $k_{\text{FB}} = 32.5 + 0.41 \mu\text{m}^{-1}$, corresponding to a Floquet-Bloch refractive index $n_{\text{FB}} = 1.89 + 0.02i$. The combs defined by $FB^+ C^+$ and $FB^- C^-$ are offset; the former with a principal peak located at $\Re(k_{\text{FB}})$ and the latter with a principal peak located at $-\Re(k_{\text{FB}})$. Increasing $M$ from 2 to 10 narrows the peaks of the combs, which in turn narrows the peaks in the magnetic field spectrum. Due to the losses in the metallic layer, the spectral peaks defined by $FB^+ C^+$ and $FB^- C^-$ have finite width even in the limit of an infinite system, underscoring the limitation of the classical Floquet-Bloch solution for describing the spectral composition of the wave in lossy periodic systems. For both the $M = 2$ and $M = 10$ cases, the magnitude of $|C^+|^2$ is larger than that of $|C^-|^2$.

As shown in Fig. 3, $|C^+|^2$ generally exceeds $|C^-|^2$, with the latter gradually approaching zero as the number of repetitions increases. It is noteworthy that the negative spatial frequency components of the wave solution are characterized by a time-averaged spectral Poynting vector that is negative, suggesting that these wave components are actually forward-propagating waves (having parallel phase and energy velocities) that have been reflected in the system. This is counter to the widely held belief that the negative spatial frequency components of a Floquet-Bloch field decomposition are backward-propagating waves [28].

The Floquet-Bloch refractive index can take on values with negative real parts, particularly for TM-polarized
and Floquet-Bloch analysis to describe layered systems. A more complete discussion on the application of effective medium theory to describe the layered structure as a homogeneous medium is provided in the Appendix.

There are two uncertainties associated with homogenization that have been recognized in the literature: 1) it is unknown how accurate a plane-wave solution approximates the true wave solution in the medium and, 2) for homogenization methods that produce an infinite number of plane-wave solutions, such as scattering parameter retrieval and Floquet-Bloch analysis, it is unclear which plane-wave solution best describes the true wave solution. The analytical Fourier-domain wave solution provides a useful tool to overcome these challenges. Concatenation of the field solutions obtained by systematic variation of \( \kappa_x \) over the range \(|\kappa_x| < k_0\) yields a two-dimensional Fourier-domain field distribution mapped as a function of spatial-frequency coordinates \( \kappa_x \) and \( \kappa_z \). The relative field amplitude at a particular \( (\kappa_x, \kappa_z) \) describes the relative contribution to the total wave solution made by a plane wave with spatial frequencies \( \kappa_x \) and \( \kappa_z \) along the respective \( x \) and \( z \) directions. Thus, the Fourier-domain field distribution can be overlaid on the wave vector diagrams to determine 1) if the plane-wave solutions produced by homogenization methods are present in the wave solution and 2) if present, the relative contributions of each plane-wave solution to the wave solution.

As a test case, we examine a finite periodic layered system immersed in free space and consisting of two bi-layer unit cells, each composed of a 30-nm-thick Ag layer and a 30-nm-thick TiO\(_2\) layer (again for TM polarization at a free-space wavelength \( \lambda_0 = 365 \) nm). The Fourier-domain wave solution is presented as the magnetic field amplitude spectrum mapped as a function of \( \kappa_z \) and \( |\kappa_x| < k_0 \), and the wave-vector diagrams are presented as complex-valued \( \kappa_z \) mapped over \(|\kappa_x| < k_0\).

As shown in Fig. 4, homogenization yields plane-wave solutions described by wave-vector diagrams consisting of either a single discrete branch (effective medium theory) or a family of discrete branches (scattering parameter retrieval and Floquet-Bloch analysis), whereas the magnetic field spectrum consists of a series of broad bands. Effective medium theory and scattering parameter retrieval are particularly poor at describing the spatial-frequency features of the wave solution; the former yields too few solutions and the latter yields too many solutions. Floquet-Bloch analysis gives the closest approximation of the wave solution, with the two most prominent bands of the wave solution fairly well aligned to two branches in the wave vector diagram. This is not surprising given the explicit appearance of Floquet-Bloch modes in one of the terms of the factorized Fourier-domain wave solution. However, the more complex features of the wave solution - variations of the magnetic field amplitude both within a band and between the bands and the presence of narrower subsidiary bands with weaker amplitudes - are beyond the descriptive capabilities of wave-vector diagrams obtained by Floquet-Bloch analysis. It should be noted that scattering parameter retrieval applied to a single unit cell

![Diagram](image)

**Fig. 3.** Forward and backward components of the weighting matrix \( \mathbf{C} \) corresponding to a metal-dielectric bi-layer system consisting of alternating layers of 30-nm-thick Ag and 30-nm-thick TiO\(_2\), assuming a normally incident TM-polarized wave with a free-space wavelength of \( \lambda_0 = 365 \) nm.
Fig. 4. Comparison of wave-vector diagrams describing electromagnetic wave behavior in a periodic layered structure consisting of two bi-layer unit cells, each consisting of a 30-nm-thick layer of Ag and a 30-nm-thick layer of TiO$_2$ for TM-polarization at a free-space wavelength $\lambda_0 = 365$ nm. Diagrams of the real (solid line) and imaginary (dashed line) parts of the wave-vector derived from a) effective medium theory (green), b) scattering parameter retrieval (red), and c) Floquet-Bloch analysis (blue) are compared against d) the magnetic field spectrum obtained from the Fourier-domain wave solution.

of a symmetric layered system with identical bounding spaces produces the same solutions as those obtained by Floquet-Bloch analysis due to the equivalence of the two procedures under these conditions [20].

8. Discussion

Plane-wave illumination of a layered structure is an archetypal configuration that can be solved analytically or by numerical electromagnetic solvers such as those based on finite-difference techniques. Although these solutions are typically expressed in the spatial domain, it is straightforward to apply numerical Fourier transformation to re-express them in the Fourier-domain [22].

In response, we must acknowledge that the value of a solution depends on both its consistency with fundamental laws (in this case, Maxwell’s equations) and its ability to communicate physical meaning in a compact and efficient manner. In recent years, the metamaterial concept has been used to provide a succinct and intuitive way to describe the electromagnetic properties of layered structures in terms of familiar plane-wave parameters. Although plane-wave solutions are easily communicated and understood, they generally sacrifice consistency with Maxwell’s equations. On the other hand, analytical spatial-domain wave solutions in terms of wave coefficients dispersed throughout the layered medium are consistent with Maxwell’s equations, but offer no insight into the collective behavior of the wave solution. Numerical wave solutions are also consistent with Maxwell’s equations, but comprise data arrays that are valid only for a particular geometry and difficult to succinctly communicate.

Thus, despite the availability of homogenization methods and analytical and numerical wave solutions for the layered geometry, the factorized, Fourier-domain wave solution developed here is important because it addresses a deficiency in methods to communicate the electromagnetic properties of layered metamaterials in a manner that is complete, consistent, and physically insightful.

9. Conclusion

Diverse classifications of layered metamaterials in the literature (using terms such as hyperbolic, anisotropic, and
negative-index) stem from the use of different homogenization methods. Continued advancement of layered metamaterials will rely upon improved methods for communicating their electromagnetic properties. We have explored a new method to express the analytical wave solution for a lossy layered media of finite extent in a factorized form by analysis in the Fourier domain. Some interesting outcomes of this work include:

1. Fourier-domain representation allows the wave solution to be condensed into a product of three, physically-intuitive matrix factors.

2. Floquet-Bloch modes can be made to explicitly appear in the Fourier-domain solution, without a priori invoking the Floquet-Bloch theorem.

3. In the limit of no loss and infinite extent, the Floquet-Bloch matrix factor asymptotically approaches a discrete set of Floquet-Bloch modes. The amplitude of the Floquet-Bloch modes can be explicitly determined from other matrix factors of the factorized, Fourier-domain solution.

4. The wave solution in periodic layered media of finite extent contains both forward (decay along $+z$) and backward (grow along $+z$) Floquet-Bloch modes.

5. For plane-wave illumination of layered structures composed exclusively of positive-index media, the positive and negative spatial-frequency components of the wave solution carry time-averaged power in the forward and backward directions, respectively. Thus, the negative spatial-frequency components are not backward-propagating waves with anti-parallel phase and energy velocities, but rather reflected forward-propagating waves with parallel phase and energy velocities.

6. Homogenization methods indicate the possibility of plane-wave solutions. A spatial-frequency representation of the wave solution is required to indicate if these plane-wave solutions are present and if so, their relative weights.

The theory developed here will help advance the science and technology of layered implementations of metamaterials by providing: 1) complete solutions to Maxwell’s equations for these systems in a physically insightful and intuitive way and 2) a means to rigorously and directly validate current applications of plane-wave solutions critical to the very definition of a metamaterial.

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can be expressed as

\( \varepsilon_{\perp} = \frac{\varepsilon_1 + \varepsilon_2}{f_1 \varepsilon_1 + f_2 \varepsilon_2}, \)

(A.1)

where \( f_1 = d_1/(d_1 + d_2) \) and \( f_2 = d_2/(d_1 + d_2) \) are the fractions of total volume occupied by the layers. For plane-wave propagation parallel to the plane of the layers, continuity of the displacement field and volumetric averaging of the displacement field over the bi-layer yields an effective permittivity component

\( \varepsilon_{\parallel} = f_1 \varepsilon_1 + f_2 \varepsilon_2. \)

(A.2)

Thus, the bi-layer system acts like a uniaxial crystal with an optical axis perpendicular to the plane of the layer.

10.B. Scattering Parameter Retrieval Applied to a Finite Layered Structure

Scattering parameter retrieval is a general technique based on the conceptual replacement of a finite heterogeneous system with a hypothetical, finite homogeneous system, where the parameters of the homogeneous medium have been retrieved assuming reflection and transmission coefficients identical to that of the heterogeneous medium. Here, we detail its application to describe the electromagnetic properties of the finite, lossy, periodic layered system generally depicted in Fig. 1. The reflection and transmission coefficients of the medium can be related to each other using transfer matrix formalism by

\[
\begin{pmatrix}
    t \\ s
\end{pmatrix} = W
\begin{pmatrix}
    1 \\ s
\end{pmatrix},
\]

(A.3)

where the total transfer matrix \( W \) can be expressed as

\[
W = W_{MJ+1,0} = T_{MJ+1}^{-1} U_L^M \eta^M T_0
\]

(A.4)

\[
= \begin{pmatrix}
    W_{1,1} & W_{1,2} \\ W_{2,1} & W_{2,2}
\end{pmatrix}.
\]

The reflection and transmission coefficients of the medium can be subsequently written as

\[
T = \frac{W_{2,1}}{W_{2,2}}
\]

(A.5)

and

\[
L = W_{1,1} - \frac{W_{1,2}W_{2,1}}{W_{2,2}},
\]

(A.6)

respectively.

We next conceptually replace the medium with a fictitious, homogeneous, effective medium with an identical length \( L \) and immersed in free space. The homogeneous medium is characterized by an effective permittivity \( \varepsilon_e \), an effective permeability \( \mu_e \), an effective refractive index \( n_e \), and an effective impedance \( z_e \). The reflection coefficient, \( r_e \), and transmission coefficient, \( t_e \), of the effective medium are related to each other by

\[
\begin{pmatrix}
    t_e \\ s
\end{pmatrix} = W_e \begin{pmatrix}
    1 \\ s
\end{pmatrix},
\]

(A.7)

where the total transfer matrix of the effective medium can be expressed as

\[
W_e = \frac{(1 + p_e)}{4 p_e} \times
\]

\[
\begin{pmatrix}
    e^{-ik_{\perp,e}L} & i2\frac{1-p_e}{1+p_e} \sin(k_{\parallel,e}L) \\ e^{ik_{\perp,e}L} & -i2\frac{1+p_e}{1-p_e} \sin(k_{\parallel,e}L)
\end{pmatrix}
\]

(A.8)
where $k_{z,e}$ is the z-component of the wave-vector in the effective medium and $p_e = k_{z,e}/(r_e k_{z,0})$. The transmission coefficient of the effective medium can be written as

$$L_e = \frac{4p_e}{(1 + p_e^2)e^{-i k_{z,e}L} - (1 - p_e^2)e^{i k_{z,e}L}}$$

$$= \frac{1}{\cos(k_{z,e}L) - i(1 + p_e^2)\sin(k_{z,e}L)/(2p_e)}.$$  \hfill (A.9)

Similarly, the reflection coefficient $r_e$ can be written as

$$L_e = \frac{(1 - p_e^2)\left(e^{i k_{z,e}L} - e^{-i k_{z,e}L}\right)}{(1 + p_e^2)e^{-i k_{z,e}L} - (1 - p_e^2)e^{i k_{z,e}L}}$$

$$= \frac{i(1 - p_e^2)\sin(k_{z,e}L)}{2p_e \cos(k_{z,e}L) - i(1 + p_e^2)\sin(k_{z,e}L)}.$$  \hfill (A.10)

Equating $r_e = r$ and $L_e = t$, the parameters of the effective medium yielding reflection and transmission coefficients identical to that of the layered medium are given by

$$n_e = \pm \cos^{-1}\left[1 - \left(1 - \frac{\lambda^2}{2}\right)\pm 2\pi N\right] / k_0 L$$

$$p_e = \pm \sqrt{\frac{\lambda^2 - 1 + \frac{\lambda^2}{2}}{2\lambda^2}}.$$  \hfill (A.11)

where $N$ is an integer. There are two notable limitations associated with these parameters. First, there are an infinite number of possible solutions for the effective refractive index. Second, there exist two sets of solutions for $p_e$ and $n_e$, each having opposite sign (although for a system with loss only one set satisfies the physical constraints that $\Re(n_e) \geq 0$ and $\Re(p_e) \geq 0$). From the effective parameters given in (A.11), the remaining effective parameters can be obtained using the relations

$$\xi_e = \frac{p_e n_e}{n_e^2},$$

$$\mu_e = \frac{n_e^2}{\xi_e},$$  \hfill (A.12)

for which there again exists two sets of solutions, each having opposite sign. Care must be taken if solutions for $\xi_e$ and $\mu_e$ are then used to calculate $n_e$ using (1) in the main text, as only one set of solutions for $\xi_e$ and $\mu_e$ yield the correct value of $n_e$. It should also be pointed out that if the bounding half-spaces are not identical or if the unit cell is not symmetric, scattering parameter retrieval yields different effective parameters in the forward and backward direction.

10.C. Floquet-Bloch Analysis Applied to an Infinite Periodic Layered Structure

Floquet-Bloch analysis is commonly used to describe the properties of periodic layered media. Rigorously applicable to only infinite periodic medium, it is based on the conceptual replacement of the heterogeneous unit cell of a periodic system with a hypothetical homogeneous unit cell, where the refractive index of the homogeneous unit cell has been selected to have a transfer matrix trace identical to that of the heterogeneous unit cell. To describe its salient features, we first assume an infinitely periodic layered medium having a unit cell with thickness $D$, where the fields at the boundaries of the unit cell are related by the unit cell transfer matrix $U$. We next replace the unit cell with a fictitious, homogeneous effective unit cell with an identical length $D$. The fields at the boundaries of the effective unit cell are related by the effective unit cell transfer matrix

$$U_e = \begin{pmatrix} \cos(k_{z,e}D) & 0 \\ 0 & e^{-i k_{z,e}D} \end{pmatrix}.$$  \hfill (A.13)

Equating the traces of the transfer matrices for the unit cell and effective unit cell yields

$$\text{tr}(U_e) = \text{tr}(U)$$

$$2 \cos(k_{z,e}D) = U_{1,1} + U_{2,2}. \hfill (A.14)$$

Isolating the effective wave-vector to one side of (A.14) yields

$$k_{z,e}D = \pm \cos^{-1}\left(\frac{U_{1,1} + U_{2,2}}{2}\right) \pm 2\pi N,$$  \hfill (A.15)

where, notably, the effective wave-vector is non-unique. Equation (A.15) can be further simplified by re-writing the trace of the unit cell matrix in terms of the Floquet-Bloch mode

$$\text{tr}(U) = \lambda^+ + \lambda^- = e^{i k_{FB}D} + e^{-i k_{FB}D}.$$  \hfill (A.16)

Substituting (A.16) into (A.15) yields the compact relation

$$k_{z,e}D = k_{FB} \pm 2\pi N/D,$$  \hfill (A.17)

which describes a infinitely large family of discrete Floquet-Bloch modes. It is interesting to note that in contrast to scattering parameter retrieval, which generates two effective parameters based on two distinct equations (one for the transmission coefficient given by (A.9) and another for the reflection coefficient given by (A.10)), Floquet-Bloch mode analysis generates just one effective parameter based on one equation (equating the traces of the transfer matrices given in (A.14)).