Singular analysis to homogenize planar metamaterials as nonlocal effective media

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Homogenization of metamaterials based on the analysis of their reflection and transmission spectra often leads to nonphysical values of the effective permittivity and permeability. Here we address this challenge by analyzing the scattering spectra in terms of perfectly emitting and absorbing modes considering nonlocal constitutive relations. The decomposition of the scattering spectra into even and odd modes permits us to quantify the nonlocal contributions and provides explicit formulas for the effective permittivity and permeability which always satisfy the passivity and causality constraints.

I. INTRODUCTION

The engineering of photonic structures at a subwavelength scale offers a unique ability to tune the electric and magnetic resonances [1] and develop new applications [2–4]. The design of metamaterials raises an intricate question of how to retrieve the effective permittivity and permeability of inhomogeneous structures [5–7]. For planar metamaterials, the effective parameters can be retrieved by comparing their reflection and transmission spectra with the spectra of a homogeneous slab [8,9]. Despite its wide use, this approach bears intrinsic difficulties related to branch discontinuities [10] and inversion of the scattering problem [11]. It is also known that in some cases the retrieved effective parameters can violate the passivity and causality constraints [12,13]. Alternative approaches addressing these difficulties have been proposed using a field averaging inside the elementary cell [14,15] or analyzing the band structure [16,17]. However, these approaches are strictly numerical and cannot be applied directly to extract the effective parameters from experimental data.

Here, we develop a singular approach to homogenize metamaterials based on the analysis of the reflection and transmission spectra in terms of perfectly emitting and absorbing modes. As a key to derive physically relevant homogenized parameters, we take into account the effects of spatial dispersion through nonlocal constitutive relations. This general approach preserves the physical properties of the effective parameters at high frequencies and in the vicinity of resonances, where the nonlocal contributions cannot be neglected [18]. The decomposition of scattering spectra into even and odd modes also quantifies the nonlocal contribution and provides explicit formulas for the effective permittivity and permeability which always satisfy the passivity and causality constraints.

II. LOCAL AND NONLOCAL PARAMETERS

The effective medium theory for planar metamaterials can be reformulated as a question of whether a homogeneous slab exists which has the same set of parameters [19]. The ability to undertake such a comparison implies that the resonances caused by the geometry of the structure should be converted into the resonances of a homogeneous medium. This involves a certain form of constitutive relations for the effective medium, and in general they should be nonlocal. In the most common cases, the nonlocal contributions are weak, and the constitutive relations can be reduced to the following form [20]:

\[ D = \varepsilon E + \alpha \kappa \times H, \]
\[ B = \mu H - \alpha \kappa \times E, \]

where \( \varepsilon(\omega) \) is permittivity, \( \mu(\omega) \) is permeability, and the parameter \( \alpha(\omega) \) is responsible for the spatial dispersion of the first order which is proportional to \( \kappa = c \kappa / \omega \). It will be shown later that \( \alpha \sim \omega^2 \) so that the nonlocal effects disappear at low frequencies. Moreover, it can be shown that the constitutive relations Eqs. (1) allow the propagation of plane waves with the refractive index \( n = \sqrt{\varepsilon \mu} / (1 + \alpha) \) and impedance \( \eta = \sqrt{\mu / \varepsilon} \) (see Appendix A).

To retrieve the effective parameters, we analyze the scattering properties of the metamaterial by the \( S \) matrix relating the amplitudes of the ingoing \( (u_+, v_+) \) and outgoing \( (u_-, v_-) \) plane waves (Fig. 1). For structures with the mirror symmetry in the plane \( z = 0 \), the \( S \) matrix can be diagonalized via an eigenvalue and eigenvector decomposition where the diagonal components \( S_{\pm}(\omega) \) and \( S_{\pm}(\omega) \) correspond to the even and odd eigenvalues [23]. The reflection and transmission coefficient for plane-wave incidence are then determined as \( R = u_- / u_+ = (S_- S_0) / 2 \) and \( T = v_- / u_+ = (S_+ S_0) / 2 \) [23]. The modes of the photonic device can be divided into perfectly emitting \( (\omega_r^+ \text{ and perfectly absorbing}) \) and \( (\omega_r^- \text{ and perfectly absorbing}) \), corresponding to poles \( \text{det}(S(\omega_r^+)) = 0 \) and zeroes \( \text{det}(S(\omega_r^-)) = 0 \) of the \( S \) matrix. We have already shown that the knowledge of these singular complex frequencies leads to analytical formulas for any diagonal component \( n (=\varepsilon^- \text{ or } \varepsilon^+) \) of the \( S \) matrix [23]:

\[ S_n(\omega) = A_n \exp(i B_n \omega) \prod_{\omega \in \omega_r^+ \omega \in \omega_r^-} \frac{\omega - \omega_r^+}{\omega - \omega_r^-}. \]

In this formula, the constants \( A_n \) and \( B_n \) assure a correct asymptotic behavior, and the product is taken over all resonances matching the symmetry of \( S_n \).

It has been established that the effective parameters are related to the reflection and transmission

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to the absorption spectrum.

plotted as solid lines. (c) The contributions of the even and odd modes with the electric field polarized along the $y$ boundaries of the elementary cell are shown as a dashed contour.

results of the analytical formulas [22] with parameters in Table I are coefficients [8]:

$G$ constraints [12]. These difficulties can be lessened by rewriting

everywhere, and in general it does not have a unique solution because of the branch discontinuities [10]. Second, the extracted parameters often violate the passivity and causality constraints [12]. These difficulties can be lessened by rewriting the system of Eqs. (3) in terms of even and odd modes:

where $d$ is the thickness of the elementary cell. Using directly the system of Eqs. (3) to retrieve the homogenized parameters is notorious for several difficulties. First of all, it can be solved only numerically, and in general it does not have a unique solution because of the branch discontinuities [10]. Second, the extracted parameters often violate the passivity and causality constraints [12]. These difficulties can be lessened by rewriting the system of Eqs. (3) in terms of even and odd modes:

At low frequencies the correction $\alpha$ for nonlocal effects can be neglected so that $n_{\text{eff}}^2 = \varepsilon_{\text{eff}}/\mu_{\text{eff}}$. The system of Eqs. (4) can be solved explicitly and leads to the following formulas for the effective permittivity and permeability:

As expected, the even (odd) modes are responsible for the weak nonlocal effects, which is generally weak, it is sufficient to keep the first two terms in the continued fractions expansion: $\arctanh z \approx z/(1 - z^2/3)$. This leads to the following formula for the refractive index:

The refractive index has exactly the same form as prescribed by the constitutive relations Eqs. (1), and it turns out that all of the effective parameters can be found explicitly from the reflection and transmission spectra.

Strictly speaking, Eqs. (5) are valid not only for normal incidence but also for an oblique one provided that the reflection and transmission spectra in the right-hand side of the formulas are specified for the same angle of incidence and polarization. Notice however that if the unit cell of metamaterial is anisotropic the extracted parameters cannot be equal for all directions of incidence.

Moreover, the effective parameters should not necessarily coincide for a single layer of metamaterial and for a stack of identical layers along the $z$ axis [25]. This is because the equivalence between a homogeneous slab and a layer of metamaterial is not full. In fact, each layer of metamaterial is a subwavelength grating, and the scattering on them involves not only the reflected and transmitted waves but also evanescent waves of different diffraction orders. They can be ignored in the far field, but on the other hand their contribution can be significant when the stacking of metamaterials is considered.

III. FISHNET STRUCTURE

As a typical metamaterial to test our procedure, we consider a fishnet structure (Fig. 1) [26–28]. The elementary cell has the periods $a_x = a_y = 600$ nm. The rectangular hole inside the cell has the dimensions $b_x = 500$ nm and $b_y = 284$ nm. The thicknesses of metal and dielectric layers are $h_m = 45$ nm and $h_d = 30$ nm. The permittivity of silver is described by the Drude model $\varepsilon_m(\omega) = 1 - \omega_p^2/(\omega^2 + i \Gamma \omega)$ with the parameters $\hbar \omega_p = 9.02$ eV and $\Gamma = 0.0062 \omega_p$. The refractive index of the dielectric is $n_d = 1.38$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{(Color online) (a) Sketch of the fishnet structure; the boundaries of the elementary cell are shown as a dashed contour. (b) Reflection (blue), transmission (green), and absorption (shaded) spectra of the fishnet structure. The normal incidence is considered, with the electric field polarized along the $y$ axis. The results of the finite element method [21] are shown by filled circles, while the results of the analytical formulas [22] with parameters in Table I are plotted as solid lines. (c) The contributions of the even and odd modes to the absorption spectrum.}
\end{figure}
TABLE I. The parameters of even and odd modes for the spectra in Fig. 1. All frequencies are normalized to $\omega_0 = 2\pi c/\lambda_0$, which corresponds to the wavelength $\lambda_0 = 1 \mu m$.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Even modes</th>
<th>Odd modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$-0.990$</td>
<td>$0.996$</td>
</tr>
<tr>
<td>$B$</td>
<td>$0.486$</td>
<td>$0.463$</td>
</tr>
<tr>
<td>$\omega_1^+$</td>
<td>$0.849 + 0.275i$</td>
<td>$0.696 + 0.001i$</td>
</tr>
<tr>
<td>$\omega_1^-$</td>
<td>$0.855 - 0.283i$</td>
<td>$0.696 - 0.019i$</td>
</tr>
<tr>
<td>$\omega_2^+$</td>
<td>$0.991 - 0.008i$</td>
<td>$0.991 - 0.012i$</td>
</tr>
</tbody>
</table>

Notice that it is not possible to replace the fishnet structure by a slab at all frequencies. The homogenization can be performed only if there is one reflected or transmitted signal. Otherwise, the fishnet structure should be treated like a diffraction grating, and it is not possible to describe its properties by an averaged value of permittivity and permeability. Therefore, the diffraction channels of higher orders should be suppressed, which is always true if the incident wavelength is larger than the period of the structure ($\lambda/\lambda_0 > 0.6$ or $\omega/\omega_0 < 1.67$ for the structure in Fig. 1). This puts a natural limitation on any effective medium theory.

The validity range of the decomposition Eq. (2) into perfectly emitting and absorbing modes depends on the number of resonances taken into account, but it turns out that even a small number of resonances provides a remarkably good accuracy over a broad range of frequencies. For the fishnet structure, it is sufficient to use only one pair of even modes and two pairs of odd modes to reproduce the reflection and transmission spectra computed with the finite element method [Fig. 1(b)]. The resonant frequencies of these modes are summarized in Table I. They can be found as the solutions of the eigenvalue problems with the outgoing (for $\omega_+^r$) and ingoing ($\omega_+^i$) boundary conditions [23]. For simpler geometries such as multilayered structures, the resonant frequencies can be expressed in analytical form [19].

The spectral distributions of the effective parameters for the fishnet structure according to Eqs. (5) and (7) are shown in Fig. 2. The magnetic resonance at $0.7 \omega_0$ is particularly strong, and it can be noticed that it is accompanied by a peak in the nonlocal response. This peak is often associated not with the spatial dispersion but with the so-called antiresonant behavior [26,29,30], which leads to the negative imaginary part of permittivity and thus violates the passivity constraints [12]. The advantage of using Eqs. (5)–(8) is that they help to separate various effects and to preserve the physical meaning of the effective parameters. These formulas clearly show that the even and odd modes are responsible for the resonances of permittivity and permeability, respectively, while the nonlocal contributions can appear due to any of those resonances.

As a check of consistency, the extracted parameters can be used to compute the reflection and transmission spectra of a homogeneous slab which has the same thickness as the fishnet structure. The resulting spectra are shown in Fig. 3 together with the spectra of the fishnet structure, which were computed with the finite element method. Notice that the nonlocal effects cannot be neglected at high frequencies and in the vicinity of resonances. From the mathematical point of view, the difference between the spectra in Figs. 3(a) and 3(b) can be attributed to a more accurate representation of the hyperbolic arctangent. However, the important point of this work is to show that the higher-order terms in the expansion of arctangent can be linked to the different orders of spatial dispersion.

The effective permittivity and permeability derived according to Eqs. (5) always satisfy the causality and passivity constraints of excitations.
constraints. This can be demonstrated as follows. The energy conservation requires that for passive structures $|S_o| \leq 1$. The unit disk is mapped then onto the right half plane $\text{Re}(1 - S_o)/(1 + S_o)] \geq 0$ according to the properties of the Möbius transformation [31]. Since the prefactor $G$ is purely imaginary, the half plane is further rotated by $90^\circ$ so that $\text{Im}(\varepsilon^{\text{eff}}) \geq 0$ and $\text{Im}(\mu^{\text{eff}}) \geq 0$ for all real frequencies, and the structure always remains passive.

Equations (5) indicate that the effective permittivity and permeability can have only simple poles ($\omega_r^\text{L}$) and zeros ($\omega_i^\text{L}$) (with $r \in \varepsilon$ or $r \in \mu$). This follows from the fact that the diagonal components $S_\varepsilon$ and $S_\mu$ in Eq. (2) have only simple poles and zeros [23], and the application of the Möbius transformation in Eqs. (5) does not change the order of the singularities. The effective permittivity and permeability can thus be factorized as

$$\varepsilon^{\text{eff}}(\omega) = \varepsilon^{\text{eff}}(\infty) \prod_{r \in \varepsilon} \frac{\omega - \omega_r^\text{L}}{\omega - \omega_r^\text{T}},$$  

(9a)

$$\mu^{\text{eff}}(\omega) = \mu^{\text{eff}}(\infty) \prod_{r \in \mu} \frac{\omega - \omega_r^\text{L}}{\omega - \omega_r^\text{T}},$$  

(9b)

The comparison of Eqs. (9a) and (5a) shows that the transverse and longitudinal resonances of the effective permittivity satisfy the conditions $S_\varepsilon(\omega_r^\text{L}) = 1$ and $S_\mu(\omega_i^\text{L}) = -1$, respectively. The latter formulas can also be converted to the standard Drude-Lorentz formula by making the expansion into partial fractions [22,32]:

$$\varepsilon^{\text{eff}}(\omega) = \varepsilon^{\text{eff}}(\infty) \left[ 1 + \sum_{r \in \varepsilon} \frac{\sigma_r}{\omega - \omega_r^\text{T}} \right],$$  

(10a)

$$\mu^{\text{eff}}(\omega) = \mu^{\text{eff}}(\infty) \left[ 1 + \sum_{r \in \mu} \frac{\sigma_r}{\omega - \omega_r^\text{T}} \right],$$  

(10b)

where the residues $\sigma_r$ can be interpreted as the strength of the resonances at $\omega_r^\text{T}$. The precise values of the resonant frequencies for the fishnet structure example are given in Table II.

### IV. CONCLUSIONS

In conclusion, we derived a method able to retrieve the effective parameters of planar metamaterials from the reflection and transmission spectra uniquely. It was shown that the decomposition of the spectra into even and odd modes leads to the explicit analytical formulas for the effective permittivity and permeability that always satisfy the passivity and causality constraints. The nonlocal contributions can be quantified separately and we evidenced their significant influence on the calculation of the reflection and transmission spectra around the resonances.

### ACKNOWLEDGMENTS

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### APPENDIX A: SPATIAL DISPERSION OF THE FIRST ORDER

The solutions of Maxwell’s equations can be searched in the form of plane waves by assuming that the spatial and temporal dependence is described as $\exp(\mathbf{i} \cdot \mathbf{k} - \omega t)$. This leads to the following system of equations:

$$\mathbf{k} \times \mathbf{E} = \mathbf{B},$$  

(A1a)

$$\mathbf{k} \times \mathbf{H} = -\mathbf{D},$$  

(A1b)

where $\mathbf{k} = c \mathbf{k}/\omega$ is a normalized wave vector. The nonzero solutions can be obtained only when a certain form of the dispersion relation $\mathbf{k}(\omega)$ is satisfied. The specific form of the dispersion relation is determined by the constitutive relations $\mathbf{D}(\mathbf{E}, \mathbf{H})$ and $\mathbf{B}(\mathbf{E}, \mathbf{H})$. In the simplest case of isotropic media,

$$\mathbf{D} = \varepsilon \mathbf{E},$$  

(A2a)

$$\mathbf{B} = \mu \mathbf{H},$$  

(A2b)

where the permittivity $\varepsilon$ and permeability $\mu$ are some constants.

If the response of the medium is not instantaneous [33], this leads to the frequency dispersion, and the values of the permittivity $\varepsilon(\omega)$ and permeability $\mu(\omega)$ should be a function of frequency $\omega$. If the response of the medium is nonlocal [1], this leads to the spatial dispersion, and the effective parameters should also depend on the wave vector $\mathbf{k}$. If the nonlocal effects are weak, the following form of the constitutive relations can be considered [20]:

$$\mathbf{D} = \varepsilon \mathbf{E} + \alpha \mathbf{k} \times \mathbf{H},$$  

(A3a)

$$\mathbf{B} = \mu \mathbf{H} - \alpha \times \mathbf{E},$$  

(A3b)

where the parameter $\alpha(\omega)$ is responsible for the spatial dispersion of the first order.

The substitution of Eqs. (A3) into Eqs. (A1) gives

$$(1 + \alpha)\mathbf{k} \times \mathbf{E} = \mu \mathbf{H},$$  

(A4a)

$$(1 + \alpha)\mathbf{k} \times \mathbf{H} = -\varepsilon \mathbf{E}.$$  

(A4b)

This system can be simplified by eliminating $\mathbf{H}$,

$$(1 + \alpha)^2 \mathbf{k} \times \mathbf{k} \times \mathbf{E} = -\varepsilon \mu \mathbf{E},$$  

(A5)

and by taking into account that $\mathbf{k} \cdot \mathbf{E} = 0$:

$$[(1 + \alpha)^2 \mathbf{k} \times \varepsilon \mu] \mathbf{E} = 0.$$  

(A6)
The nonzero solutions exist when
\[ (1 + \alpha)\kappa = \sqrt{\varepsilon\mu}. \] (A7)
Notice that the magnitude of the vector \( \kappa \) coincides with the definition of the refractive index \( n \) in isotropic media because \( n = ck/\omega \). Therefore, the refractive index for the constitutive relations Eqs. (A3) can be defined as
\[ n = \frac{\sqrt{\varepsilon\mu}}{1 + \alpha}. \] (A8)
When the spatial dispersion is weak \( \alpha = 0 \), Eq. (A8) reduces to the standard expression \( n = \sqrt{\varepsilon\mu} \).

**APPENDIX B: THE LINK BETWEEN SINGULARITIES OF S AND T MATRICES**

According to the definitions of the \( S \) and \( T \) matrices, the amplitudes of plane waves on the opposite sides of the structure are related as
\[
\begin{align*}
\begin{pmatrix} u_- \\ v_- \end{pmatrix} &= S \begin{pmatrix} u_+ \\ v_+ \end{pmatrix}, \\
\begin{pmatrix} u_- \\ v_- \end{pmatrix} &= T \begin{pmatrix} u_+ \\ u_- \end{pmatrix}.
\end{align*}
\] (B1) (B2)

The even modes correspond to the following solution of the eigenvalue equation:
\[
S \begin{pmatrix} 1 \\ 1 \end{pmatrix} = S_e \begin{pmatrix} 1 \\ 1 \end{pmatrix},
\] (B3)
which is equivalent to
\[
\begin{pmatrix} S_e \\ 1 \end{pmatrix} = T \begin{pmatrix} 1 \\ S_e \end{pmatrix},
\] (B4)
as can be checked by direct comparison of the \( u_\pm \) and \( v_\pm \) components in Eqs. (B1) and (B2).

The \( T \) matrix of a slab can be decomposed in the following way:
\[
T = YT_DY^{-1},
\] (B5)
where \( T_D \) is a diagonal matrix,
\[
T_D = \begin{bmatrix} \Lambda_B & 0 \\ 0 & 1/\Lambda_B \end{bmatrix},
\] (B6)
and \( Y \) is an interface matching matrix \([34]\):
\[
Y \pm 1 = \frac{1}{1 \mp R_B} \begin{bmatrix} 1 & \mp R_B \\ \mp R_B & 1 \end{bmatrix}.
\] (B7)
The eigenvalues of the \( T \) matrix are related to the forward and backward propagating Bloch modes with \( \Lambda_B \mp 1 = \exp(\pm ikd) \), where \( k_B = n_{\text{eff}}\omega/c \) is the Bloch wave number, and \( d \) is the thickness of the slab. The parameter \( R_B \) has the meaning of the reflection coefficient for the Bloch waves at the interface with the ambient medium.

The decomposition Eq. (B5) allows one to rewrite Eq. (B4) as
\[
Y^{-1} \begin{pmatrix} S_e \\ 1 \end{pmatrix} = T_DY^{-1} \begin{pmatrix} 1 \\ S_e \end{pmatrix},
\] (B8)
which gives in explicit form
\[
\begin{bmatrix} 1 \\ R_B \\ 1 \end{bmatrix} \begin{pmatrix} S_e \\ 1 \end{pmatrix} = \begin{bmatrix} \Lambda_B & 0 \\ 0 & \Lambda_B^{-1} \end{bmatrix} \begin{bmatrix} 1 \\ R_B \\ 1 \end{bmatrix} \begin{pmatrix} 1 \\ S_e \end{pmatrix}.
\]
This can be simplified to the equation
\[
S_e + R_B = \Lambda_B(1 + R_B S_e)
\] (B9)
and solved with respect to \( S_e \):
\[
S_e = \frac{\Lambda_B - R_B}{1 - \Lambda_B R_B}.
\] (B10)

However, it is more convenient to rewrite Eq. (B10) in a symmetric form:
\[
\frac{1 - S_e}{1 + S_e} = \frac{1 - \Lambda_B}{1 + \Lambda_B} \times \frac{1 + R_B}{1 - R_B}.
\] (B11)

The odd modes correspond to the following solution of the eigenvalue equation:
\[
S \begin{pmatrix} 1 \\ -1 \end{pmatrix} = -S_o \begin{pmatrix} 1 \\ -1 \end{pmatrix},
\] (B12)
which is equivalent to
\[
\begin{pmatrix} S_o \\ -1 \end{pmatrix} = T \begin{pmatrix} 1 \\ -S_o \end{pmatrix}.
\] (B13)
As in the case of even modes, similar derivations lead to the equation
\[
S_o = \frac{\Lambda_B + R_B}{1 + \Lambda_B R_B},
\] (B14)
which can be rewritten as
\[
\frac{1 - S_o}{1 + S_o} = \frac{1 - \Lambda_B}{1 + \Lambda_B} \times \frac{1 - R_B}{1 + R_B}.
\] (B15)

The system of Eqs. (B11) and (B15) allows one to switch from the basis of Bloch modes \( \{\Lambda_B, R_B\} \) to the basis of even and odd modes \( \{S_e, S_o\} \). The reverse conversion is also possible:
\[
\begin{align*}
\left( \frac{1 - \Lambda_B}{1 + \Lambda_B} \right)^2 &= \frac{1 - S_e}{1 + S_e} \times \frac{1 - S_o}{1 + S_o}, \\
\left( \frac{1 - R_B}{1 + R_B} \right)^2 &= \frac{1 + S_e}{1 - S_e} \times \frac{1 - S_o}{1 + S_o}.
\end{align*}
\] (B16a) (B16b)
as can be checked by direct substitution of Eqs. (B11) and (B15) to the right-hand side.

Instead of the quantities \( \Lambda_B \) and \( R_B \), one can also choose to work with the refractive index \( n_{\text{eff}} \) and impedance \( \eta_{\text{eff}} \). In this case, the system takes the following form:
\[
\tanh^2(n_{\text{eff}}/G) = \frac{1 - S_e}{1 + S_e} \times \frac{1 - S_o}{1 + S_o},
\] (B17a)
\[
\eta_{\text{eff}}^2 = \frac{1 + S_e}{1 - S_e} \times \frac{1 - S_o}{1 + S_o}.
\] (B17b)

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where $G = 2ic/(\omega d)$. The transformation is based on the following relations:

$$
\tanh \frac{x}{2i} = \frac{1 - \exp(ix)}{1 + \exp(ix)}, \quad (B18)
$$

$$
\eta_{\text{eff}} = \frac{1 - R_B}{1 + R_B}, \quad (B19)
$$

The main limitation of the system of Eqs. (B17), or alternatively the system of Eqs. (B16), is that it takes into account only two Bloch modes which propagate in the forward and backward directions. This is appropriate for homogeneous slabs, but in general the dimensions of the $T$ matrix should be increased to take into account the excitation of higher-order Bloch modes [35] as this is more relevant for gratinglike structures [36].