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An extended Fourier modal method for plane-wave scattering from finite structures

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ABSTRACT

This paper extends the area of application of the Fourier modal method from periodic structures to aperiodic ones, in particular for plane-wave illumination at arbitrary angles. This is achieved by placing perfectly matched layers at the lateral sides of the computational domain and reformulating the governing equations in terms of a contrast field which does not contain the incoming field.

Keywords: Fourier modal method, FMM, rigorous coupled-wave analysis, RCWA, aperiodic, finite, isolated, perfectly matched layer, PML, contrast-field formulation, CFF, aFMM-CFF

1. INTRODUCTION

The Fourier modal method (FMM), also referred to as Rigorous Coupled-Wave Analysis (RCWA), has a several decades long history in the field of rigorous diffraction modeling. It was first formulated by Moharam and Gaylord in 1981.¹ Being based on Fourier-mode expansions, the method is inherently built for periodic structures such as diffraction gratings. Over the years, the stability and convergence properties of the method have been improved by the introduction of a number of techniques, such as the enhanced transmittance matrix approach,^{2,3} adaptive spatial resolution,⁴ Li rules and normal vector fields for correct Fourier factorization.⁵⁻⁹

One important limitation of the FMM is given by the fact that it can only be used for computational problems defined for periodic structures (such as diffraction gratings). This is because the modes used to represent the field are themselves periodic. A straightforward workaround for this limitation is the *supercell approach*; the aperiodic structure is still assumed to be periodic but with a large enough period so that the interaction of neighboring structures is negligible.

Lalanne and his co-workers¹⁰⁻¹² have applied the FMM to waveguide problems. The aperiodicity of the waveguide was dealt with by placing *perfectly matched layers* (PMLs)¹³ on the lateral sides of the computational domain. PMLs are introduced in the domain by performing the mathematical operations of analytic continuation and coordinate transformation. Physically, PMLs can be seen as some fictitious absorbing and non-reflecting materials. In this way, artificial periodization is achieved, i.e. the structure of interest is repeated in space, but there is no electromagnetic coupling between neighboring cells.

The above approach, combining standard FMM with PMLs, is applicable only for the case of normal incidence of the incoming field, which is sufficient for waveguide problems. In this paper we show that for oblique incidence we need to reformulate the standard FMM such that the incident field is not part of the computed solution. We propose a decomposition of the total field into a *background field* (containing the incident field) and a *contrast field*. The problem is reformulated with the contrast field as the new unknown. The background field solves a corresponding *background problem* which has a simple analytical solution. The main effect of the reformulation is that the homogeneous system of second-order ordinary differential equations becomes non-homogeneous. The ideas conveyed in this paper are demonstrated on two model problems: diffraction of TE-polarized light from a binary one-dimensional grating (periodic model problem) and from a single line (aperiodic model problem).

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2. THE STANDARD FOURIER MODAL METHOD

The structure considered in the periodic model problem is an infinitely periodic binary grating with a period Λ illuminated by TE-polarized light. The permittivity profile $\epsilon(x, z)$ is invariant in the y direction and is shown in Figure 1. The field is assumed to be time-harmonic, $\tilde{E}_y(x, z, t) = E_y(x, z) \exp(i\omega t)$. The solution of the periodic model problem satisfies

$$\frac{\partial^2}{\partial x^2} E_y(x, z) + \frac{\partial^2}{\partial z^2} E_y(x, z) + k_0^2 \epsilon(x, z) E_y(x, z) = 0, \quad (1)$$

where E_y is the y component of the electric field and the wavenumber k_0 is defined by $k_0 = \omega \sqrt{\epsilon_0 \mu_0}$, with ϵ_0 and μ_0 respectively the electric permittivity and magnetic permeability of vacuum. The incoming field is given by a plane wave

$$E_y^{inc}(x, z) = \exp(-i(k_{x0}x + k_{z0}z)), \quad (2)$$

with $k_{x0} = k_0 n_1 \sin \theta$ and $k_{z0} = k_0 n_1 \cos \theta$. Here, n_1 is the refractive index of the superstrate and θ is the angle the wavevector $[k_{x0}, k_{z0}]^T$ makes with the z axis. The wavelength of the incoming wave is given by $\lambda = 2\pi/(n_1 k_0)$. Note that the incident field satisfies the following condition

$$E_y^{inc}(0, z) = E_y^{inc}(\Lambda, z) \exp(ik_{x0}\Lambda). \quad (3)$$

This condition is referred to as the *pseudo-periodicity condition* or the *Floquet condition*. It may be proven¹⁴ that for periodic structures also the resulting total field must be pseudo-periodic.

The first step in the FMM is to divide the computational domain into layers such that the permittivity $\epsilon(x, z)$ is z -independent in each particular layer. For our periodic model problem this division generates three layers as shown in Figure 1.

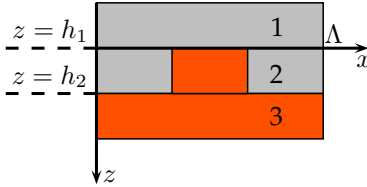


Figure 1. Geometry of the periodic model problem and division into layers.

Then the field in layer i ($i = 1, 2, 3$) satisfies

$$\frac{\partial^2}{\partial x^2} E_{y,i}(x, z) + \frac{\partial^2}{\partial z^2} E_{y,i}(x, z) + \epsilon_i(x) E_{y,i}(x, z) = 0. \quad (4)$$

Note that ϵ_i , ($i = 1, 3$) is constant in layers 1 and 3. In this case the solution of (4) may be written in terms of a Rayleigh expansion. However, when the PML is added later, the Rayleigh expansion is not applicable. Therefore, for generality, we treat these layers in the same way as the middle layer(s).

The second step in the FMM is to expand the x -dependent quantities into Fourier modes

$$E_{y,i}(x, z) = \sum_{n=-\infty}^{\infty} s_{n,i}(z) \exp(-ik_{xn}x), \quad (5a)$$

$$\epsilon_i(x) = \sum_{n=-\infty}^{\infty} \hat{\epsilon}_{n,i} \exp\left(i \frac{2\pi n}{\Lambda} x\right), \quad (5b)$$

where

$$k_{xn} = k_0 n_1 \sin \theta - n \frac{2\pi}{\Lambda}, \quad n \in \mathbb{Z}.$$

Note that the modes $\exp(-ik_{xn}x)$ satisfy the condition of pseudo-periodicity. Thus, the solution obtained by superposition will necessarily be pseudo-periodic. By substituting the expansions (5) in (4) and truncating the series to the harmonics $n = -N, \dots, N$ we get

$$-k_{xn}^2 s_{n,i}(z) + \frac{d^2}{dz^2} s_{n,i}(z) + \sum_{m=-N}^N \hat{\epsilon}_{n-m,i} s_{m,i}(z) = 0, \quad n = -N, \dots, N, \quad (6)$$

or in matrix form

$$\frac{d^2}{dz^2} \mathbf{s}_i(z) = k_0^2 \mathbf{A}_i \mathbf{s}_i(z), \quad \text{with } \mathbf{A}_i = \mathbf{K}_x^2 - \mathbf{E}_i, \quad (7)$$

where \mathbf{K}_x is a diagonal matrix with the values k_{xn}/k_0 on its diagonal and \mathbf{E}_i is a Toeplitz matrix with the (n, m) -entry equal to $\epsilon_{n-m,i}$ for $-N \leq n, m \leq N$.

Equation (7) is a homogeneous second-order ordinary differential equation whose general solution is given by

$$\mathbf{s}_i(z) = \mathbf{s}_i^+(z) + \mathbf{s}_i^-(z) = \mathbf{W}_i (\exp(-\mathbf{Q}_i(z - h_{i-1})) \mathbf{c}_i^+ + \exp(\mathbf{Q}_i(z - h_i)) \mathbf{c}_i^-), \quad (8)$$

where h_i is the position of the top interface of layer i (we take $h_0 = h_1$), \mathbf{W}_i is the matrix of eigenvectors of \mathbf{A}_i and \mathbf{Q}_i is a diagonal matrix with square roots of the corresponding eigenvalues on its diagonal.

The radiation condition in layers 1 and 3 implies that only the term corresponding to outgoing waves is kept in (8), thus $\mathbf{c}_1^+ = \mathbf{d}_0$ and $\mathbf{c}_3^- = 0$. The vector $\mathbf{d}_0 \in \mathbb{R}^{(2N+1)}$ is an all-zero vector except for entry $N+1$ which is equal to 1 and corresponds to the incoming field. The other constant vectors \mathbf{c}_i^\pm are unknown, and can be determined from the interface conditions between the layers.¹

3. ARTIFICIAL PERIODIZATION WITH PERFECTLY MATCHED LAYERS

PMLs were first suggested by Berenger¹³ as a method of imposing the radiation condition¹⁵ on the boundary of the computational domain in FDTD. PMLs can be obtained by an analytic continuation of the solution of (1) (defined in real coordinates) to a complex contour

$$\tilde{x} = x + i\beta(x), \quad x \in \mathbb{R}, \quad (9)$$

where $\beta(x)$ is a function which has a non-zero value only inside the PMLs. The analytic continuation (9) transforms propagating waves into evanescent waves.

The procedure of obtaining a PML requires an analytic continuation from \mathbb{R} to \mathbb{C} followed by a coordinate transformation back to \mathbb{R} . The operations can be represented formally as

$$E(x) \xrightarrow{\{1\}} \tilde{E}(\tilde{x}) \xrightarrow{\{2\}} \tilde{E}(x), \quad \text{with } x \in \mathbb{R}, \tilde{x} \in \mathbb{C}. \quad (10)$$

Operation $\{1\}$ does not formally change the equation but changes its solution by modifying the domain of the space variable x . Operation $\{2\}$ is required in order to avoid working in complex coordinates. It is defined as a coordinate transformation

$$\tilde{x} = f(x) = x + i\beta(x), \quad (11)$$

applied to the equation in \tilde{x} . This coordinate transformation eliminates the derivatives with respect to complex variables

$$\frac{\partial}{\partial \tilde{x}} = \frac{\partial x}{\partial \tilde{x}} \frac{\partial}{\partial x} = \left(\frac{\partial \tilde{x}}{\partial x} \right)^{-1} \frac{\partial}{\partial x} = \frac{1}{f'(x)} \frac{\partial}{\partial x}. \quad (12)$$

The aperiodic model problem with normal incidence can be solved by decoupling the neighboring cells with the help of PMLs placed at the lateral sides of the domain. The inclusion of PMLs in the domain modifies Equation (4) to

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_{y,i}(x, z) \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_{y,i}(x, z) + k_0^2 \epsilon_i(x) \tilde{E}_{y,i}(x, z) = 0. \quad (13)$$

The quantities $\tilde{E}_{y,i}(x, z)$ and $\epsilon_i(x)$ are expanded as in (5). Additionally, $1/f'(x)$ has to be decomposed in Fourier modes

$$\frac{1}{f'(x)} = \sum_{n=-\infty}^{\infty} \hat{f}_n \exp\left(i\frac{2\pi n}{\Lambda}x\right), \quad (14)$$

Truncation of the infinite sums yields

$$\frac{d^2}{dz^2}\mathbf{s}_i(z) = k_0^2 \mathbf{A}_i \mathbf{s}_i(z), \quad \mathbf{A}_i = (\mathbf{F}\mathbf{K}_x)^2 - \mathbf{E}_i, \quad (15)$$

where \mathbf{F} is the Toeplitz matrix associated with the Fourier coefficients \hat{f}_n . Compared to (7), the modification introduced by the PML is minor: a "stretching matrix" \mathbf{F} appears in the computations.

Since the FMM uses an expansion in pseudo-periodic modes the resulting solution has to be pseudo-periodic. We show that the pseudo-periodicity requirement is only satisfied for normal incidence. We write the total field as a sum of the incident and the scattered field

$$\tilde{E}_y = \tilde{E}_y^{inc} + \tilde{E}_y^s.$$

The scattered field (it is an outgoing field) is damped exponentially to "almost zero" at $x = 0$ and $x = \Lambda$. The original incoming field is given by

$$E_y^{inc}(x, z) = \exp(-i(k_{x0}x + k_{z0}z)). \quad (16)$$

For normal incidence $k_{x0} = 0$, so it is independent of the stretched coordinate x and is not affected by the PML. Thus, the total field is pseudo-periodic.

It is important to stress that the above discussion is valid only for normal incidence. For oblique incidence $k_{x0} \neq 0$ and the incoming field will be affected by the analytic continuation. We look at what happens to the incident field on the complex contour \tilde{x} ,

$$\tilde{E}_y^{inc}(\tilde{x}, z) = e^{-i(k_{x0}\tilde{x} + k_{z0}z)} = e^{-i(k_{x0}x + k_{z0}z)} e^{k_{x0}\beta(x)}. \quad (17)$$

Thus, although the scattered field is still damped exponentially to zero at $x = 0$ and $x = \Lambda$ and satisfies the pseudo-periodic BC, the incoming field on the complex contour violates the pseudo-periodicity

$$\tilde{E}_y^{inc}(f(0), z) \neq \tilde{E}_y^{inc}(f(\Lambda), z) \exp(ik_{x0}\Lambda). \quad (18)$$

Consequently, also the total field violates this condition and cannot be represented by a superposition of the modes in (5a). Therefore, in the next section we remove the problematic part (which includes the incoming field) from the unknown and reformulate the problem such that its solution can have the representation (5a).

4. THE CONTRAST-FIELD FORMULATION OF THE FMM

As shown in the previous section, the presence of PMLs determines the following form of the governing equation

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y + k_0^2 \epsilon(x, z) \tilde{E}_y = 0. \quad (19)$$

The total field is decomposed into a *contrast field* and a *background field* (this can also be viewed as a decomposition into a periodic part and a non-periodic part)

$$\tilde{E} = \tilde{E}^c + \tilde{E}^b, \quad (20)$$

where \tilde{E}^b is chosen to be the field formed in materials defined by $\epsilon^b(x, z)$

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y^b \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y^b + k_0^2 \epsilon^b(x, z) \tilde{E}_y^b = 0. \quad (21)$$

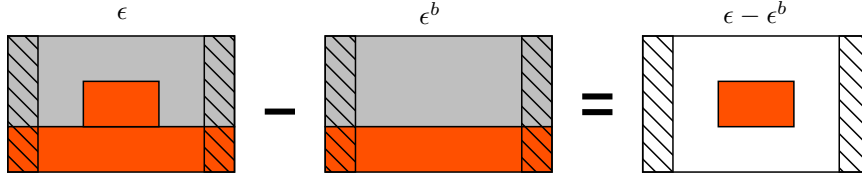


Figure 2. Permittivities involved in the source term of (22).

Subtracting (21) from (19) yields

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial \tilde{E}_y^c}{\partial x} \right) + \frac{\partial^2 \tilde{E}_y^c}{\partial z^2} + k_0^2 \epsilon(x, z) \tilde{E}_y^c = -k_0^2 (\epsilon(x, z) - \epsilon^b(x, z)) \tilde{E}_y^b. \quad (22)$$

We can still choose ϵ^b . However, it should be chosen in such a way that the solution of (21) can be computed analytically. Moreover, we want to choose ϵ^b so that the right-hand side of (22) vanishes in the PML. This is required in order to avoid dealing with a non-periodic source in the PML. If ϵ^b is chosen such that it represents the background of ϵ , i.e. ϵ without the scatterer (rectangular line), then the above mentioned requirements are satisfied; the RHS vanishes in the PML, and the background field \tilde{E}^b can be expressed analytically inside the scatterer.

Figure 2 shows the permittivities ϵ , ϵ^b , $\epsilon - \epsilon^b$, corresponding to the equations for total field (19), background field (21) and contrast field (22).

In order to solve (22), the background field of the aperiodic model problem is needed. It is difficult to find the analytical solution of (21). However, we note that for a perfect PML, the background fields of the aperiodic and periodic model problems coincide, i.e.

$$\tilde{E}_y^b(x, z) = E_y^b(x, z), \quad (x, z) \in \Omega_0$$

where Ω_0 the physical domain, in other words the computational domain without the PML region. Since $\epsilon(x, z) - \epsilon^b(x, z)$ is non-zero only in the scatterer (rectangular line), we may replace the source term of (22) by $-k_0^2 (\epsilon(x, z) - \epsilon^b(x, z)) E_{y,2}^b$. Thus, we only need the background field in layer 2. It is easily derived to be

$$E_{y,2}^b = E_{y,2}^{inc} + E_{y,2}^r = \exp(-q_2 z) \exp(-ik_{x0} x) + r \exp(q_2 z) \exp(-ik_{x0} x), \quad (23)$$

where

$$r = \frac{q_2 - q_3}{q_2 + q_3} b^2,$$

with $q_i = \sqrt{k_{x0}^2 - \epsilon_i^b}$, $i = 2, 3$, and $b = \exp(-q_2 h)$. The derivation is provided in Appendix A.

Once the right-hand side is given, Equation (22) may be solved with the FMM. For this purpose, the source term must also be expanded into Fourier modes. After truncation a non-homogeneous system of ordinary differential equations is obtained for each layer. The field is found by matching the general solutions at the layer interfaces.

5. NUMERICAL EXPERIMENTS

We consider the aperiodic model problem of scattering from an isolated resist line in air with a width of $100nm$ and a height of $20nm$ illuminated by a plane wave with a wavelength $\lambda = 628nm$ incident at an angle $\theta = \pi/6$. The computational domain has a width $\Lambda = 500nm$ and the lateral PMLs have a width of $100nm$. The geometry of the problem can be seen in Figure 3. Note that the distance unit in this and the following figures is equal to $100nm$. The refractive index of air and resist are given by $n_1 = 1$, $n_3 = 1.5$.

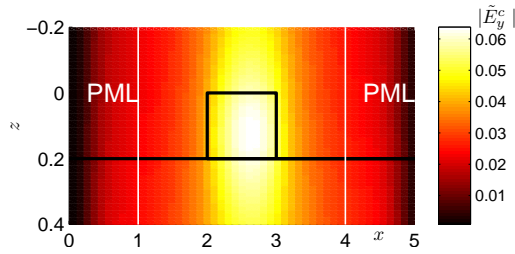


Figure 3. The contrast field computed with aFMM-CFF. One distance unit in the plot corresponds to $100nm$.

The contrast-field formulation of the FMM with PMLs is used to solve the problem. We refer to this method as the aperiodic Fourier modal method in contrast-field formulation (aFMM-CFF). For the implementation of the PMLs we need to define the coordinate transformation function which is chosen to be a polynomial of degree n ,

$$\tilde{x} = f(x) = \begin{cases} x + i\sigma_0 \frac{|x-x_l|^{(n+1)}}{n+1}, & 0 \leq x \leq x_l, \\ x, & x_l < x < x_r, \\ x - i\sigma_0 \frac{|x-x_r|^{(n+1)}}{n+1}, & x_r \leq x \leq \Lambda, \end{cases} \quad (24)$$

where x_l is the endpoint of the left PML, x_r is the start-point of right PML, σ_0 is the damping strength. We chose a quadratic PML ($n = 2$) with a damping strength $\sigma_0 = 10$. In the computations also the derivative of the stretching function is required.

$$\frac{d}{dx} f(x) = \begin{cases} 1 - i\sigma_0 |x - x_l|^n, & 0 \leq x \leq x_l, \\ 1, & x_l < x < x_r, \\ 1 - i\sigma_0 |x - x_r|^n, & x_r \leq x \leq \Lambda. \end{cases} \quad (25)$$

We will first confirm that the PML enforces the radiation condition. Figure 3 shows the contrast field computed with aFMM-CFF. We observe a decay of the field in the PML to 'almost zero' at the lateral boundaries, which implies that the PML acts as an absorbing layer. The solution in the PML is not physically relevant. In order to obtain the solution outside the physical domain, a Green's functions approach may be taken.¹⁶

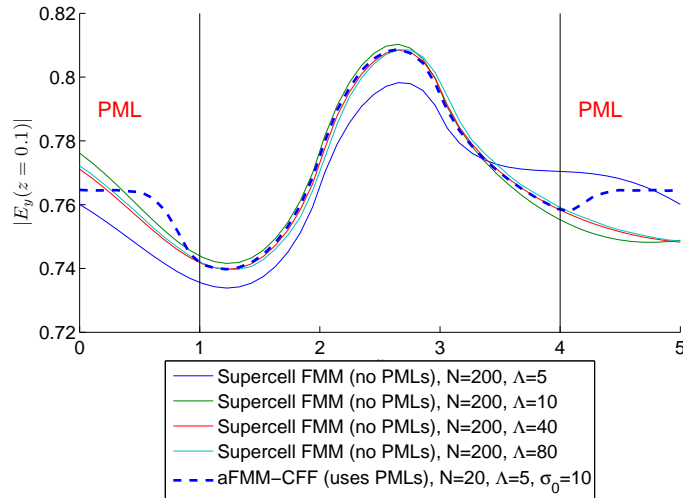


Figure 4. The total field for the isolated resist line problem (oblique incidence, TE-polarization) at $z = 0.1$ ($z = 10nm$) computed with aFMM-CFF and with supercell FMM. One distance unit in the plot corresponds to $100nm$.

Figure 4 shows the total field computed with aFMM-CFF. Solutions computed with supercell FMM are used as a reference. Clearly, in the limiting case $\Lambda \rightarrow \infty$, the solution of the periodic problem tends to the solution

computed with aFMM-CFF. This enables us to state the following: (1) the PML implementation is correct - it acts as a reflectionless absorbing layer, and (2) the amount of harmonics required to obtain a 'good' solution is much lower for aFMM-CFF than for supercell FMM. In our example the aFMM-CFF requires ten times less harmonics than the supercell FMM.

6. CONCLUSIONS

We have presented an extension of the FMM which enables simulation of scattering from finite structures illuminated by plane waves at arbitrary angles. The formulation in terms of a contrast field presented in this paper resembles the scattered field formulations used in FEM and FDTD. This reformulation however is less trivial for the FMM, since it requires solutions which can be written in analytical form.

As shown by the numerical computations, for the aperiodic model problem aFMM-CFF needed ten times less harmonics than the supercell FMM. In the view of the fact that the number of operations performed by the eigenvalue solver (which is the most demanding step in the method) scales cubically with the amount of harmonics, this results in a reduction by a factor of 10^3 in computational time.

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APPENDIX A. THE BACKGROUND FIELD

Here we derive the background field for the periodic background problem. The incident field is given by (2) and the resulting background field satisfies

$$\frac{\partial^2}{\partial x^2} E_y^b + \frac{\partial^2}{\partial z^2} E_y^b + k_0^2 \epsilon^b(x, z) E_y^b = 0. \quad (26)$$

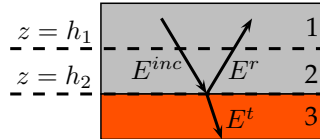


Figure 5. The background problem.

To solve (26), we use knowledge about angles of reflection and refraction. Figure 5 shows the representation of the solution in terms of plane waves. We assume $h_1 = 0$ and $h_2 = h$. In layer 2 ($0 < z < h$, see Figure 5) the field is written as

$$E_{y,2}^b = E_y^{inc} + E_y^r = \exp(-q_2 z) \exp(-ik_{x0} x) + r \exp(q_2 z) \exp(-ik_{x0} x). \quad (27)$$

In layer 3 ($z > h$)

$$E_{y,3}^b = E_y^t = t \exp(-q_3(z - h)) \exp(-ik_{x0} x), \quad (28)$$

where $q_i = \sqrt{k_{x0}^2 - \epsilon_i^b}$, $i = 2, 3$. The amplitudes r and t are unknown. They can be computed by matching the fields and their normal derivatives at the interface $z = h$.

$$E_y^{inc}(x, h) + E_y^r(x, h) = E_y^t(x, h), \quad (29)$$

$$\frac{\partial}{\partial z} E_y^{inc}(x, h) + \frac{\partial}{\partial z} E_y^r(x, h) = \frac{\partial}{\partial z} E_y^t(x, h). \quad (30)$$

Using the relations (27), (28) and setting $b = \exp(-q_2 h)$, we get a linear system of equations for r and t

$$rb^{-1} + b = t, \quad (31)$$

$$rq_2 b^{-1} - q_2 b = -tq_3. \quad (32)$$

This system has the solution

$$r = \frac{q_2 - q_3}{q_2 + q_3} b^2, \quad t = \frac{2q_2}{q_2 + q_3} b. \quad (33)$$

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