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# Effective method for calculating modes of multilayer waveguide

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**Abstract**. A fast and efficient numerical method for finding the modes of a multilayered waveguide is proposed. Using the complex vector of the Riemann-Silberstein has resulted in a reduction of the order of the differential equations describing the passage of light through the different layers, as well as a double reduction of the searched variables. The approximation of the differential equations is made by the method of Galyorkin by a suitable choice of the base functions. The calculation of the effective indices and their corresponding wave configurations is realized by the inverse-shifting power method with Rayleigh's quantity. The method was successfully applied waveguide systems, generating values close in the effective indices.

#### 1. Introduction

Waveguides are essential building blocks of diverse photonic integrated circuits such as polarizers, switches, filters, rotators, and modulators. To accomplish the desired characteristics, these functional devices are mainly designed by altering the material characteristics by using electro-optic, magneto-optic, and thermo-optic modulations. The determination of eigenmodes is a fundamental problem for waveguide optics. Several techniques are commonly used for the computation of the electromagnetic modes of waveguides, including finite element methods, mode-matching techniques, method of lines, and finite difference methods. Most significant are finite-element frequency-domain (FEFD)-based eigenvalue mode solvers [2, 3], the finite-element beam propagation methods (FE-BPMs), the finite-difference beam propagation method (FD-BPM), and the finite-difference frequency-domain (FDFD)-based eigenvalue mode solvers [6,7].

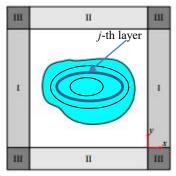
Many methods completely neglect the anisotropy of the constituent materials. The methods which take into consideration the material anisotropy require the diagonal permittivity tensor expressed in the coordinate system of the waveguide. For waveguide with layers of liquid crystals (LC) with arbitrary molecular orientations, the nine elements of the permittivity tensor are all non-zero.

In this paper we present an algorithm, based of Galjorkin's method of pseudoorthogonal functions for solving full-vector modes of optical waveguides with arbitrary permittivity tensor, i.e., with general three dimensional (3D) anisotropy. This can be observed in [6,7] as we incorporate perfectly matched layers (PML) as the absorbing boundary conditions at the outer boundaries of the computational domain. For the purpose of optimal numerical realization we have proposed the numerical scheme with only one complex array similar to the complex potential of Riemann- Silberstein [1], instead of four field components (two for transverse electric field components  $E_x$ ,  $E_y$  and two for transverse magnetic field components  $H_x$  and  $H_y$  - total four arrays). The eigenvectors and eigenvalues of the waveguide were calculated using a dynamic shifted inverse power method with the Rayleigh quantity.

#### 2. The model

Multi-layer waveguides are a system of layers with different refractive indices designed to limit the spread of the electromagnetic wave in a single (core) or in a small number of layers. If a material consists of an anisotropic layer (for example, represents a crystal, polymer, etc.) we have a 3D anisotropy. For modeling the properties and distribution of the electromagnetic (EM) waves we use the system of partial differential equations of Maxwell, under appropriate boundary conditions associated with the properties of media of layers through which they pass and reflect. We assume that the properties of the media are modeled by the non-diagonal and non-symmetrical complex permittivity tensor  $[\varepsilon]$  and by the diagonal tensor of magnetic permeability  $[\mu]$ .

For the analysis of the waveguide, the computational domain is normally used (figure 1), where the waveguide cross-section in the transverse (x, y) plane is truncated and surrounded by PML (perfect matched layers), in which the attenuation of the wave does not depend on its direction, but by artificially introducing appropriate electrical and magnetic losses. The incorporation of PML regions allows the analysis of leaky modes.



**Figure 1.** The cross-section of an arbitrary waveguide with the PML, placed at the edges of the computing domain.

A periodic dependence on a wave of time is assumed, i.e. the presence of the factor  $\exp(i\omega t)$  where  $\omega$  is the angular frequency and t the time. The direction of propagation of an electromagnetic wave is parallel to the axis 0z, i.e. the expression  $\exp(-i\beta z)$  describes the propagation, where  $\beta$  is the constant of propagation. It is also assumed, that the tensors of dielectric permittivity  $[\varepsilon]_j$  and magnetic permeability  $[\mu]_j$  in any "j-th" layer are independent of time t.

For the boundary conditions of the considered anisotropic waveguide in the PML regions, the permittivity and permeability tensors are taken to be:

$$[\varepsilon_{PML}] = \varepsilon_0 \begin{cases} \frac{s_y s_z}{s_x} \varepsilon_{xx} & s_z \varepsilon_{xy} & s_y \varepsilon_{xz} \\ s_z \varepsilon_{yx} & \frac{s_x s_z}{s_y} \varepsilon_{yy} & s_x \varepsilon_{yz} \\ s_y \varepsilon_{zx} & s_x \varepsilon_{zy} & \frac{s_x s_y}{s_z} \varepsilon_{zz} \end{cases}, \quad [\mu_{PML}] = \mu_0 \begin{cases} \frac{s_y s_z}{s_x} \mu_{xx} & 0 & 0 \\ 0 & \frac{s_x s_z}{s_y} \mu_{yy} & 0 \\ 0 & 0 & \frac{s_x s_z}{s_z} \mu_{zz} \end{cases}. \quad (1)$$

Using ideas from papers [6, 7] we may determine the complex PML parameter s, which controls the field attenuation as follows:

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$$s = 1 - i\alpha = 1 - i\frac{\sigma_e}{\omega \varepsilon_0 n^2} = 1 - i\frac{\sigma_m}{\omega \mu_0}..$$
 (2)

Here  $\sigma_e$  and  $\sigma_m$  are the electric and magnetic conductivities of the PML,  $\varepsilon_0$  and  $\mu_0$  are permittivity and permeability of free space, and n is the refractive index of the adjacent computing domain. This relation means that the wave impedance of a PML medium exactly equals that of the adjacent medium in the computing window regardless of the angle of propagation.

2.1. Application of the modified vector of Riemann-Silberstein for reducing and simplifying the system of partial differential equations for calculating modes of an anisotropic waveguide.

Our new original proposal is to replace the six unknown calculated field components  $\vec{E} = (E_x, E_y, E_z)$ 

and  $\vec{H} = (H_x, H_y, H_z)$  with only three complex field components  $\vec{F} = (F_x, F_y, F_z)$  by analogy [1] with Riemann-Silberstein vector. For this purpose, we present the permittivity and permeability tensors as:

$$\mathcal{E}_{0}[\mathcal{E}] = \mathcal{E}_{0} \begin{cases}
\mathcal{E}_{xx} & \mathcal{E}_{xy} & \mathcal{E}_{xz} \\
\mathcal{E}_{yx} & \mathcal{E}_{yy} & \mathcal{E}_{yz} \\
\mathcal{E}_{zx} & \mathcal{E}_{zy} & \mathcal{E}_{zz}
\end{cases} = \mathcal{E}_{0} \begin{cases}
n_{xx} & n_{xy} & n_{xz} \\
n_{yx} & n_{yy} & n_{yz} \\
n_{zx} & n_{zy} & n_{zz}
\end{cases}^{2} = \mathcal{E}_{0}[n]^{2} ..$$
(3)

$$\mu_0[\mu] = \mu_0 \begin{cases} \mu_{xx} & 0 & 0 \\ 0 & \mu_{yy} & 0 \\ 0 & 0 & \mu_{zz} \end{cases} = \mu_0 \begin{cases} m_{xx} & 0 & 0 \\ 0 & m_{yy} & 0 \\ 0 & 0 & m_{zz} \end{cases}^2 = \mu_0[m]^2 .. \tag{4}$$

Let vector  $\vec{F}$  by analogy with Riemann-Silberstein vector be  $\vec{F} = \sqrt{\frac{\mathcal{E}_0}{2}}[n]\vec{E} + i\sqrt{\frac{\mu_0}{2}}[m]\vec{H}$ ,  $i = \sqrt{-1}$ .

Then for each of the layers the according to the assumptions  $\operatorname{div}(\vec{F}) = 0$  and  $\operatorname{rot}(\vec{F}) = -\frac{\omega}{c}[n][m]\vec{F} = -\frac{\omega}{c}[\alpha]\vec{F}$ , where  $c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$  is the velocity of light in free space.

Consequently, for each layer it is necessary to solve the differential system:

$$\begin{pmatrix}
0 & i\beta & \frac{\partial}{\partial y} \\
-i\beta & 0 & -\frac{\partial}{\partial x} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0
\end{pmatrix}
\begin{pmatrix}
F_x \\
F_y \\
F_z
\end{pmatrix} = -\frac{\omega}{c} \begin{pmatrix}
n_{xx}m_{xx} & n_{xy}m_{yy} & n_{xz}m_{zz} \\
n_{yx}m_{xx} & n_{yy}m_{yy} & n_{yz}m_{zz} \\
n_{zx}m_{xx} & n_{zy}m_{yy} & n_{zz}m_{zz}
\end{pmatrix}
\begin{pmatrix}
F_x \\
F_y \\
F_z
\end{pmatrix}.$$
(5)

To form the eigenmode equations we need to eliminate  $\vec{F}_z$  from the third of equations (5), i.e.,

$$F_{z} = \left(\frac{c}{\omega n_{zz} m_{zz}} \frac{\partial}{\partial y} - \frac{n_{zx} m_{xx}}{n_{zz} m_{zz}}\right) F_{x} - \left(\frac{c}{\omega n_{zz} m_{zz}} \frac{\partial}{\partial x} - \frac{n_{zy} m_{yy}}{n_{zz} m_{zz}}\right) F_{y} ..$$
 (6)

And after some obvious algebraic simplification we have:

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$$\begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
\begin{pmatrix}
F_x \\
F_y
\end{pmatrix} = i\beta \begin{pmatrix}
F_x \\
F_y
\end{pmatrix}$$
(7)

$$A_{11} = -\frac{c}{\omega n_{zz} m_{zz}} \frac{\partial^2}{\partial x \partial y} + \frac{n_{zx} m_{xx}}{n_{zz} m_{zz}} \frac{\partial}{\partial x} + \frac{n_{yz}}{n_{zz}} \frac{\partial}{\partial y} + \frac{\omega}{c} \left( n_{yx} m_{xx} - \frac{n_{zx} n_{yz} m_{xx}}{n_{zz}} \right)$$
(8)

$$A_{12} = \frac{c}{\omega n_{zz} m_{zz}} \frac{\partial^2}{\partial x^2} + \left( \frac{n_{zy} m_{yy}}{n_{zz} m_{zz}} - \frac{n_{yz}}{n_{zz}} \right) \frac{\partial}{\partial x} + \frac{\omega}{c} \left( n_{yy} m_{yy} - \frac{n_{zy} n_{yz} m_{yy}}{n_{zz}} \right)$$
(9)

$$A_{21} = -\frac{c}{\omega n_{zz} m_{zz}} \frac{\partial^2}{\partial y^2} + \left( \frac{n_{zx} m_{xx}}{n_{zz} m_{zz}} - \frac{n_{xz}}{n_{zz}} \right) \frac{\partial}{\partial y} + \frac{\omega}{c} \left( \frac{n_{zx} n_{xz} m_{xx}}{n_{zz}} - n_{xx} m_{xx} \right)$$
(10)

$$A_{22} = \frac{c}{\omega n_{zz} m_{zz}} \frac{\partial^2}{\partial y \partial x} + \frac{n_{xz}}{n_{zz}} \frac{\partial}{\partial x} + \frac{n_{zy} m_{yy}}{n_{zz} m_{zz}} \frac{\partial}{\partial y} + \frac{\omega}{c} \left( \frac{n_{xz} n_{zy} m_{yy}}{n_{zz}} - n_{xy} m_{yy} \right)$$
(11)

When the waveguide media can be represented by diagonal permittivity tensor  $[\varepsilon]$  and with an identity permeability tensor  $[\mu]$ , (i.e. when [n] is related to the refractive index), which is fulfilled for most optical media, then a significant simplification is achieved:

$$A_{11} = -\frac{c}{\omega n_{zz}} \frac{\partial^2}{\partial x \partial y}, A_{12} = \frac{c}{\omega n_{zz}} \frac{\partial^2}{\partial x^2} + \frac{\omega n_{yy}}{c}, A_{21} = -\frac{c}{\omega n_{zz}} \frac{\partial^2}{\partial y^2} - \frac{\omega n_{xx}}{c}, A_{22} = \frac{c}{\omega n_{zz}} \frac{\partial^2}{\partial y \partial x}.$$
(12)

After successfully solving the eigenmode system (7) for each eigenvalue  $\beta$  and eigenvector  $\vec{F}$  we can easily find configurations of corresponding mode fields  $\vec{E}$ ,  $\vec{H}$  and the density of their electromagnetic energy W by using the expressions:

$$\vec{E} = \frac{1}{\sqrt{2\varepsilon_0}} [n]^{-1} (\vec{F} + \vec{F}^*), \ \vec{H} = \frac{-i}{\sqrt{2\mu_0}} [m]^{-1} (\vec{F} - \vec{F}^*), \ W = |\vec{F}| = \vec{F} \cdot \vec{F}^*,$$
(13)

where  $\vec{F}^*$  is the complex conjugate of  $\vec{F}$ .

## 2.2. Application of Galjorkin's method with a new basis of pseudo-orthogonal functions for solving the differential eigen system.

We look for the solution similar to the method of collocation using Galjorkin's method assuming that solutions  $F_x(x, y)$ ,  $F_y(x, y)$  are presented by a linear combination of types:

$$F_{x}(x,y) = \sum_{i=1}^{N_{1}-1} \sum_{i=1}^{N_{2}-1} F_{xij} \varphi_{ij}(x,y) + F_{x}(x_{0}, x_{N_{1}}, y),$$
(14)

$$F_{y}(x,y) = \sum_{i=1}^{N_{1}-1} \sum_{j=1}^{N_{2}-1} F_{yij} \varphi_{ij}(x,y) + F_{y}(x,y_{0},y_{N_{2}}),$$
(15)

where  $F_{xij}$  and  $F_{yij}$  are the exact values of the solution  $(F_x, F_y)$  at the point of the irregular rectangular grid with coordinates  $(x_i, y_j)$ . Here  $N_1$  and  $N_2$  are the corresponding number of irregular grid divisions of variables x and y, i.e.  $x = \{x_0, x_1, \dots, x_i, \dots, x_{N_1}\}$  and  $y = \{y_0, y_1, \dots, y_j, \dots, y_{N_2}\}$ . Functions  $F_x(x_0, x_{N_1}, y) = F_x(x_0, y) + F_x(x_{N_1}, y)$ ,  $F_y(x, y_0, y_{N_2}) = F_y(x, y_0) + F_y(x, y_{N_2})$  are chosen to satisfy the boundary conditions.

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Unlike commonly used in finite element methods linear functions (having derivatives different from zero of only the first order) or spline functions (having derivatives different from zero to a maximum of second or third order) the proposed functions have derivatives of any order.

Pseudo-orthogonal functions  $\varphi_{ij}(x, y)$  as we presented in [2] are equal to 1 at grid point  $(x_i, y_j)$  or equal to 0 at any other point on the grid. They have non-zero derivatives of any row and are defined as:

$$\phi_{ij}(x,y) = \begin{cases}
0, & x \notin [x_{i-1}, x_{i+1}], y \notin [y_{j-1}, y_{j+1}] \\
\sin\left(\frac{\pi}{2} \cdot \frac{x - x_{i-1}}{x_i - x_{i-1}}\right) \sin\left(\frac{\pi}{2} \cdot \frac{y - y_{j-1}}{y_j - y_{j-1}}\right), & x \in [x_{i-1}, x_i], y \in [y_{j-1}, y_j] \\
\sin\left(\frac{\pi}{2} \cdot \frac{x_{i+1} - x}{x_{i+1} - x_i}\right) \sin\left(\frac{\pi}{2} \cdot \frac{y - y_{j-1}}{y_j - y_{j-1}}\right), & x \in [x_i, x_{i+1}], y \in [y_{j-1}, y_j] \\
\sin\left(\frac{\pi}{2} \cdot \frac{x - x_{i-1}}{x_i - x_{i-1}}\right) \sin\left(\frac{\pi}{2} \cdot \frac{y_{j+1} - y}{y_{j+1} - y_j}\right), & x \in [x_{i-1}, x_i], y \in [y_j, y_{j+1}] \\
\sin\left(\frac{\pi}{2} \cdot \frac{x - x_{i-1}}{x_i - x_{i-1}}\right) \sin\left(\frac{\pi}{2} \cdot \frac{y_{j+1} - y}{y_{j+1} - y_j}\right), & x \in [x_i, x_{i+1}], y \in [y_j, y_{j+1}]
\end{cases}$$
(16)

Therefore, we receive linear algebraic system for determining eigenvalues  $\beta$  and eigenvectors U.

$$\sum_{i=1}^{N_{1}-1}\sum_{j=1}^{N_{2}-1}U_{ij}\int_{x_{0}}^{x_{N_{1}}}\int_{y_{0}}^{y_{N_{2}}}\hat{A}\varphi_{ij}(x,y)\varphi_{km}(x,y)dxdy = i\beta\sum_{i=1}^{N_{1}-1}\sum_{j=1}^{N_{2}-1}U_{ij}\int_{x_{0}}^{x_{N_{1}}}\int_{y_{0}}^{y_{N_{2}}}\varphi_{ij}(x,y)\varphi_{km}(x,y)dxdy, \quad (17)$$
 where  $\hat{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad U = \begin{pmatrix} F_{x} \\ F_{y} \end{pmatrix}$  for each  $k = 1, 2, \dots, N_{1} - 1$  and  $m = 1, 2, \dots, N_{2} - 1$ .

#### 3. Numerical examples

As a first example we solve a 19 layer  $Ga_xAl_{1-x}As$ -AlAs waveguide structure for which the nine TE mode effective indices are nearly degenerated [4]. The index profile consists of six thin layers of  $Ga_{0.8}Al_{0.2}As$  separated by AlAs layers and the three layers of  $Ga_{0.6}Al_{0.4}As$  that are also separated by AlAs layers.

**Table 1.** Calculated TEn mode normalized propagation constants by our method, compared with the results presented in [4].

Mode	Our results at 4096 divisions	Results in[4]
TE0	3.0130388 + 0.000000009i	3.013039
TE1	3.0130253 + 0.000000003i	3.013025
TE2	3.0130091 + 0.000000011i	3.013008
TE3	3.0129832 + 0.000000037i	3.012984
TE4	3.0129566 + 0.000000145i	3.012957
TE5	3.0129342 + 0.000000101i	3.012933
TE6	3.0129119 + 0.000000048i	3.012915
TE7	3.0128931 + 0.000000993i	3.012891
TE8	3.0127597 + 0.000003457i	3.012753

As a second example, we applied our method to the analysis of 3D anisotropy of a nematic LC channel optical waveguide, calculated through the pseudospectral method in [5].

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**Table 2.** Calculated effective indices at various values of angle  $\varphi$  for the first seven modes, compared with results in [5].

Mode	Results for twist angle φ					Results for twist angle $\varphi$ in [5]				
	$0_{0}$	$30^{0}$	$45^{0}$	$60^{0}$	$90^{0}$	$0_{0}$	$30^{0}$	$45^{0}$	$60^{0}$	$90^{0}$
1	1.674	1.674	1.675	1.675	1.674	1.674	1.674	1.674	1.674	1.673
2	1.630	1.629	1.628	1.629	1.630	1.629	1.627	1.627	1.629	1.631
3	1.620	1.623	1.619	1.617	1.614	1.620	1.622	1.620	1.617	1.613
4	1.575	1.576	1.576	1.572	1.570	1.574	1.574	1.574	1.572	1.570
5	1.553	1.544	1.546	1.554	1.561	1.553	1.543	1.546	1.553	1.560
6	1.533	1.538	1.533	1.525	1.513	1.534	1.540	1.534	1.524	1.514
7	1.501	1.502	1.501	1.502	1.501	1.502	1.502	1.502	1.502	1.502

#### 4. Conclusions

This study has developed an efficient modesolver for solving anisotropic multilayer waveguides with full 3D anisotropy.

Using the method of Galjorkin with our new proposed system of pseudo-orthogonal functions leads to a sparse eigen algebraic system with band structure. The advantage of these functions is that they are sufficiently smooth and have derivatives of any order.

We generalized the idea of Silberstein when permittivity  $\varepsilon$  and permeability  $\mu$  of the layer's media are tensors  $[\varepsilon]$  and  $[\mu]$ . This is achieved by presenting them as the product of two identical tensors [n] and [m]. So for each layer, it is sufficient enough to solve only a single equation  $\vec{F} = -\frac{\omega}{n}[n][m]\vec{F}$ .

Instead of using the standard eigenvalue matrix equation for the constant of propagation  $\beta$  involving four transverse field components, we involve only two (as in the complex vector of Riemann-Silberstein) which halves the required computer memory and necessary calculation time.

Numerical results have shown that the proposed scheme is more efficient and still accurate for investigating all mode problems compared to the finite element methods or finite-difference methods that are generally used.

Algorithm has been successfully used to solve guided modes on a liquid-crystal optical waveguide with arbitrary molecular director orientation and for solving of 19-layered waveguide structure, in which case the nine TE mode effective indices are nearly degenerated.

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