Direct Realization of the Pseudospectral Method of Calculating Waveguide Mode

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Often in the applied problems of integrated optics we use regular open gradient (general) planar waveguides. Waveguides perform conversion, amplification and transmission of light signals, similar to how it occurs with electrical signals in integrated circuits, but the speed of information transfer through such devices is much higher. The mathematical model of light propagation in a waveguide is described by Maxwell’s equations and the corresponding boundary conditions. The Maxwell’s equations in Cartesian coordinates are separated into two independent sets for the TE and TM polarizations. Systems for the TE and TM polarizations can be transformed into ODEs of the second order. The boundary conditions for equations are reduced to two pairs of boundary conditions. The problem of finding modes in regular open gradient planar waveguide is described in terms of an eigenvalue problem (The generalized eigenvalue problem of two matrices). Numerical simulation of these waveguides requires modern numerical methods with high efficiency and accuracy.

This article describes the method for finding wave modes for a three-layer waveguide.

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1. Introduction

Optical waveguides are spatially inhomogeneous optical structures that serve to transmit light energy over sufficiently large distances [1–5]. The regular waveguide consists of a dielectric waveguide layer (or a few ones) of refractive index \( n_f \) (or \( n_{f1}, \ldots, n_{fN} \)) and the dielectric cladding with smaller refraction indices: \( n_s \) in the substrate layer and \( n_c \) in the cover layer as in Fig. 1.

There are exact and approximate analytical methods for simulation of waveguide modes in open gradient planar waveguides with selected refractive index in the guiding layer. In the case of an arbitrary piecewise continuous profile the approximate calculation of the electromagnetic field of guided modes is possible only by using numerical methods, implemented on a computer.

We will use Cartesian coordinates associated with the waveguide geometry as in Fig. 2.

The Maxwell equations can be split into two independent systems of equations. For each system, there are three types of waveguide modes: guided modes, substrate radiation modes, and cover radiation modes. Their solutions are, respectively,

\[ E_y(x, y, z, t) = E_y(x) \exp\{i\omega t - i\beta z\}, \]
Both equations for the modes can be written in the more customary form [11–14]

\[-p(x) \frac{d}{dx} \left( \frac{1}{p(x)} \frac{d\psi(k,x)}{dx} \right) + V(x)\psi(k,x) = k^2 \psi(k,x) \quad (1)\]

Here \( p(x) = \epsilon(x) \) for TE-modes, \( p(x) = \mu(x) \) for TN-modes, \( V(x) = -k_0^2 n^2(x) \), \( n^2(x) = \epsilon(x) \mu(x) \), \( V(x) \) is a piecewise continuous function (continuous in each of the layer), \( k^2 = -k_0^2 \beta^2 \) is the spectral parameter, and \( \psi_{TE}(x) = E_y(x), \psi_{TM}(x) = H_y(x) \).
2. Description of the Method

This article describes how to find waveguide modes in the case of potential discontinuity. The problem of describing a complete set of modes in an ordinary plane waveguide is formulated in terms of the eigenvalue problem for a second-order self-adjoint differential operator (1).

Solutions on the left and on the right are decreasing exponents in the case of real $\varepsilon_s, \varepsilon_c$ [7]:

\[
\psi_- (x) = C_- \exp \{\gamma_- (x + 1)\}, \\
\psi_+ (x) = C_+ \exp \{-\gamma_+ (x - 1)\}.
\]

Here $\gamma_{s,c} = k_0 \sqrt{\beta^2 - n_{s,c}^2} = (\frac{2\pi}{\lambda}) \sqrt{V_{s,c} - k^2}$.

In the waveguide layer, we seek the solution in the form of an expansion in the Chebyshev polynomials of the first kind [6,9]:

\[
\psi_f (k, x) = \sum_{j=0}^N C_j (k) T_j (x).
\] (2)

In this relation we substitute the $x_1, x_2, \ldots, x_{N-1}$. In points $x_0, x_N$ we require the following conditions:

\[
\psi_s (k, x_0) = \psi_f (k, x_0), \quad \varphi_s (k, x_0) = \varphi_f (k, x_0) \\
\psi_f (k, x_N) = \psi_c (k, x_N), \quad \varphi_f (k, x_N) = \varphi_c (k, x_N).
\]

Polynomial of degree $n$ is denoted $T_n (x)$, and is given by the trigonometric formula [8,9,14]:

\[
T_n (x) = \cos(n \arccos (x)).
\] (3)

Formula (3) can be replaced by recurrence expressions for $T_n (x)$:

\[
T_0 (x) = 1, \quad T_1 (x) = x, \quad T_{n+1} (x) = 2xT_n (x) - T_{n-1} (x) n \geq 1.
\]

The polynomial $T_n (x)$ has $n$ zeros in the interval $[-1,1]$, and they are located at the points [8]:

\[
x = \cos \left( \frac{\pi (k - \frac{1}{2})}{n} \right), \quad k = 1,2,\ldots,n.
\]

In this same interval there are $N+1$ extrema (maxima and minima) [8], located at

\[
x = \cos \left( \frac{\pi k}{n} \right), \quad k = 0,1,\ldots,n,
\]

we can also find the derivative of this function. $T_n' (x)$ derivatives of Chebyshev polynomials approximating the derivative of the function $f(x)$ are calculated using the following formula [10]:

\[
T_n' (x) = n \cdot \sin (n \cdot \arccos (x)), \quad x \in (-1,1), \\
T_n' (x) = n^2 x^{n+1}, \quad x = -1 \text{ or } x = 1.
\]
The second derivative is given by the following formulas:

\[ T_n''(x) = \frac{-n^2 \cos(nt)}{\sin^2(t)} + \frac{n \cos(t) \sin(nt)}{\sin^3(t)}, \quad x \in (-1, 1), \]

\[ T_n''(x) = \frac{n^3(n-1)x^{n+2}}{3}, \quad x = -1 \text{ or } x = 1. \]

We can get a new eigenvalues and eigenfunctions by expanding the interval \((a, b)\). If \(a \neq -1\) and \(b \neq 1\), it is necessary to use the following formula:

\[ \widetilde{T}_j''(x) = T_j''(x) \left( \frac{2}{b-a} \right)^2 = \frac{d^2T_j(x)}{dx^2} \left( \frac{2}{b-a} \right)^2, \]

\[ \widetilde{T}_j'(x) = \frac{2T_j'(x)}{b-a} = \frac{dT_j(x)}{dx} \frac{2}{b-a}. \]

We obtain SLAE for undetermined coefficients \(C_s, C_0, C_1, \ldots, C_N, C_c\).

Let us consider the case of TE modes. The substitution from (2) into (1) leads to the following relation:

\[ -\sum_{j=0}^{N} C_j(k) T_j''(x_l) + V(x_l) \sum_{j=0}^{N} C_j(k) T_j(x_l) = \sum_{j=0}^{N} k^2 C_j(k) T_j(x_l). \tag{4} \]

On the interval \((-\infty, x_0)\) the solution for equation (4) satisfies the following asymptotic condition \((x) x \to -\infty.\) On the interval \((x_N, \infty)\) the solution satisfies the asymptotic condition \((x) x \to \infty.\) We write down boundary conditions of the third kind with the help of Chebyshev polynomials:

\[ \sum_{j=0}^{N} C_j(k) T_j(x_0) = C_s \left( e^{\gamma_s(x_0-x_0)} = 1 \right), \quad \sum_{j=0}^{N} C_j(k) T_j'(x_0) = \gamma_s C_s, \]

\[ \sum_{j=0}^{N} C_j(k) T_j(x_N) = C_c \left( e^{-\gamma_c(x_N-x_N)} = 1 \right), \quad \sum_{j=0}^{N} C_j(k) T_j'(x_N) = -\gamma_c C_c. \]

Denote \(f_j^1 = T_j'(x_0) - \gamma_s T_j(x_0)\) and \(f_j^2 = T_j'(x_N) + \gamma_c T_j(x_N)\).

From the boundary conditions we obtain the following system:

\[ \begin{cases} 
 f_0^1 C_0(k) + f_N^1 C_N(k) = -\sum_{j=1}^{N-1} f_j^2 C_j(k), \\
 f_0^2 C_0(k) + f_N^2 C_N(k) = -\sum_{j=1}^{N-1} f_j^2 C_j(k). 
 \end{cases} \]

Solve this system by Cramer:

\[ \det = f_0^1 f_N^2 - f_N^1 f_0^2, \]
\[
C_0 (k) = \frac{-1}{\det} \sum_{j=1}^{N-1} (f_N^1 f_j^2 - f_N^2 f_j^1) C_j (k),
\]
\[
C_N (k) = \frac{1}{\det} \sum_{j=1}^{N-1} (f_0^1 f_j^2 - f_0^2 f_j^1) C_j (k).
\]

If we substitute the coefficients (5) into (4), then we will obtain the following system of equations for the coefficients \(C_j (k)\), \(j = 1, N - 1\) in the form of an eigenvalue problem:
\[
M_{ij} = V (x_i) T_j (x_i) - T''_j (x_i), \quad B_{ij} = T_j (x_i),
\]
\[
M^0_{ij} = [V (x_i) T_0 (x_i) - T''_0 (x_i)] \frac{-1}{\det} (f_N^1 f_j^2 - f_N^2 f_j^1),
\]
\[
M^N_{ij} = [V (x_i) T_N (x_i) - T''_N (x_i)] \frac{1}{\det} (f_0^1 f_j^2 - f_0^2 f_j^1),
\]
\[
B^0_{ij} = T_0 (x_i) \frac{-1}{\det} (f_N^1 f_j^2 - f_N^2 f_j^1),
\]
\[
B^N_{ij} = T_N (x_i) \frac{1}{\det} (f_0^1 f_j^2 - f_0^2 f_j^1),
\]
\[
M (k)_{ij} = M_{ij} + M^0_{ij} + M^N_{ij},
\]
\[
B (k)_{ij} = B_{ij} + B^0_{ij} + B^N_{ij}.
\]

We compute the eigenvectors \(\vec{C}(k)\) and eigenvalues \(k^2\) for the system:
\[
M (k) \vec{C}(k) = k^2 B (k) \vec{C}(k).
\]

Figure 3. The graph of the first eigenfunction of the system (6)
3. The Initial Approximation

Since the problem has the capacity gap, it is necessary to choose the initial approximation. As an initial approximation we take the solution of the problem with the boundary condition independent of the spectral parameter $V_{s,c}$. To do this, we let the height of the potential well to infinity, ie, $V_{s,c} \rightarrow \infty$. In this case the spectral parameter $\gamma_{s,c}$, too, tend to infinity, which gives new relations:

$$\sum_{j=0}^{N} T_j (x_0) C_j (k) = 0, \quad \sum_{j=0}^{N} T_j (x_N) C_j (k) = 0.$$ 

As a result, $f_j^1 \wedge f_j^2$ take the form

$$\tilde{f}_j^1 = -T_j (x_0) \wedge \tilde{f}_j^2 = T_j (x_N).$$

We get the following value:

$$M_{ij} = V (x_i) T_j (x_i) - T_j'' (x_i), \quad B_{ij} = T_j (x_i).$$

$$M_{ij}^0 = -\left( V (x_i) T_0 (x_i) - T_0'' (x_i) \right) \left( -T_N (x_0) T_j (x_N) + T_N (x_N) T_j (x_0) \right) \left( -T_N (x_0) T_0 (x_0) + T_N (x_N) T_0 (x_0) \right),$$

$$M_{ij}^N = \left( V (x_i) T_N (x_i) - T_N'' (x_i) \right) \left( -T_0 (x_0) T_j (x_N) + T_0 (x_N) T_j (x_0) \right) \left( -T_0 (x_0) T_0 (x_0) + T_0 (x_N) T_0 (x_0) \right),$$

$$B_{ij}^0 = T_0 (x_i) \left( -T_N (x_0) T_j (x_N) + T_N (x_N) T_j (x_0) \right) \left( -T_N (x_0) T_0 (x_0) + T_N (x_N) T_0 (x_0) \right),$$

$$B_{ij}^N = T_N (x_i) \left( -T_0 (x_0) T_j (x_N) + T_0 (x_N) T_j (x_0) \right) \left( -T_0 (x_0) T_0 (x_0) + T_0 (x_N) T_0 (x_0) \right).$$

Figure 4. Graph of initial approximation

The new expressions no longer contain a dependence on the spectral parameter and correspond to the problem for a closed waveguide with boundary conditions of the first kind at the potential discontinuity points.

The expressions obtained give approximate values for eigenvalues and eigenvectors.
4. Conclusion

The solution of many problems of integrated optics includes a spectral analysis and spectral synthesis on the basis of a complete system of solutions of differential equations of second order operator that regulates the guided modes in an open waveguide. In the simplest case, a regular operator waveguide is essentially self-adjoint and has a continuous mixed range.

The method described in this paper allows one to find numerical solutions for a three-layer waveguide. This method can be modified for other types of tasks.

References