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Detailed Comparison of Two Approximate Methods for the Solution of the Scalar Wave Equation for a Rectangular Optical Waveguide

Thomas Rasmussen, Jørn Hedegaard Povlsen, Anders Bjarklev, Ole Lumholdt, Bo Pedersen, and Karsten Rottwitt

Abstract—Two approximate methods for the determination of the fundamental mode of an optical waveguide with rectangular core cross section and step refractive-index profiles are presented and analyzed thoroughly. Both methods are based on Garlerkin's method. The first method uses Hermite–Gauss basis functions and the second uses the guided and nonguided slab waveguide solutions as basis functions. The results obtained by our methods are compared with results from an accurate circular harmonic analysis to determine the accuracy.

I. INTRODUCTION

RECENTLY, the interest in integrated optical waveguides in silica on silicon for telecommunication purposes has increased. These waveguides have rectangular core cross sections and step refractive-index profiles [1]. Normally, it is desirable that only the fundamental mode is guided. For accurate analysis and design it is important to have a simple and fast method for the determination of the eigenfields for such waveguides.

Many authors have presented methods for solving the wave equation for a single-mode rectangular waveguide. One method is the effective index method (EIM) [2] which is a very fast but inaccurate method. Goell has presented a circular harmonic analysis that is based on the solution of a nonlinear matrix-eigenvalue equation involving all six field components [3]. This method is very accurate but time consuming. Another accurate method is the finite element method [4], but this requires computations involving large matrices, which is also time consuming. Garlerkin’s method has been used with trigonometric [5] and Hermite–Gauss basis functions [6] to transform the scalar wave equation into a linear eigenvalue matrix equation. For a rectangular core the two latter methods require calculus with large matrices to be accurate.

In this paper we present two fast and simple methods for the determination of the electric field in a dielectric waveguide with rectangular core cross section. Both methods are based on Garlerkin’s method. In the first case we have used the Hermite–Gauss functions as basis but, in contrast to the method described in [6], we have optimized the spot-sizes of the Hermite–Gauss functions. In the second method we have used the guided and nonguided modes of two slab waveguides as basis functions. The nonguided modes are introduced by including an air-cladding boundary at a variable distance from the waveguide center. The core refractive indexes and the distances from the waveguide centers to the cladding boundaries for the two slab waveguides are optimized. The accuracies of our methods are determined by comparisons with results from the circular harmonic analysis [3].

II. THEORY

This section will briefly describe our methods in general, and introduce the two sets of basis functions mentioned in the introduction.

Fig. 1 shows the geometry for which the wave equation should be solved, as well as it defines the geometrical parameters, n1 and n2 are the core and cladding refractive indexes, respectively, a is the core width, and b is the core height.

The scalar wave equation for an electromagnetic wave propagating in the z direction $E(x, y, z) = E_0(x, y)\exp(i(\omega t - k_0 z))$ is written as

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + n^2(x, y)k^2 - \beta^2 E_0(x, y) = 0$$

where $n(x, y)$ is the refractive index, $k$ is the wave number of free space, $\omega$ is the angular frequency and $\beta$ is the propagation constant. $E_0(x, y)$ can always be expanded in a complete set of functions $F_i(x)$ and $G_j(y)$ as

$$E_0(x, y) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} c_{i,j} F_i(x) G_j(y).$$

We choose $F_i(x)$ and $G_j(y)$ to be orthonormal functions. In Garlerkin’s method the summations are truncated at some finite number $N$. This approximation is then inserted in
the wave equation. By multiplying with \( F_i(x) \cdot G_m(y) \) and integrating over the total \( x - y \) plane we achieve
\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_i(x) G_m(y) \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + n^2(x, y) k^2 \right] \sum_{i=0}^{N} \sum_{j=0}^{N} c_{i,j} F_i G_j dx dy
= \beta^2 c_i.
\]

Using this the partial differential wave equation may be transformed into a \( N^2 \times N^2 \) matrix eigenvalue equation
\[
A c = \beta^2 c
\]
with the matrix elements given by
\[
A_{i,m,j,k} = \left\langle F_i(x) G_m(y) \mid \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + n^2(x, y) k^2 \right| F_j G_k \rangle.
\]

The basis functions will in general include one or more free parameters. Thus, we write the basis functions as \( F_i(x) \) and \( G_m(y) \), with \( t_x \) and \( t_y \) being the free parameters. For a given number \( N \) the propagation constant \( \beta \) can be found as a function of \( t_x \) and \( t_y \) by solving the eigenvalue equation (2). This results in an underestimate of the correct value of the propagation constant therefore, by maximizing \( \beta(t_x, t_y) \) the most accurate solution to the scalar wave equation for a given \( N \) is obtained.

III. HERMITE-GAUSS BASIS FUNCTIONS

The Hermite-Gauss functions form an orthonormal set of functions as
\[
I_i(x, \sigma_x) = \frac{x}{\sigma_x} \exp \left( -\frac{x^2}{2\sigma_x^2} \right) / \sqrt{2\sigma_x \sqrt{\pi}}
\]
\[
G_j(y, \sigma_y) = \frac{y}{\sigma_y} \exp \left( -\frac{y^2}{2\sigma_y^2} \right) / \sqrt{2\sigma_y \sqrt{\pi}}.
\]

\( H_i(w) \) is the Hermite polynomial of order \( i \) and argument \( w \), \( \sigma_x \) and \( \sigma_y \) are the spot-sizes of the Hermite-Gauss functions.

The integrals involved in the matrix elements (3) can all be calculated analytically for a rectangular waveguide, as outlined in Appendix A. We use \( \sigma_x \) and \( \sigma_y \) as variational parameters. In [6] these values are fixed at
\[
\sigma_x = \sqrt{\frac{a}{2k \sqrt{n_1^2 - n_2^2}}}; \quad \sigma_y = \sqrt{\frac{b}{2k \sqrt{n_1^2 - n_2^2}}}.
\]

These two values were used as starting guess in our maximization of \( \beta \). The method is referred to as the optimized Hermite-Gauss method (OHGM) when \( \sigma_x \) and \( \sigma_y \) are optimized and otherwise as the Hermite-Gauss method (HGM).

IV. SLAB WAVEGUIDE SOLUTIONS

Fig. 2 shows how the original waveguide structure is divided into two slab waveguides with core refractive indexes \( n_x \) and \( n_y \), respectively. We include a set of higher order nonguided modes by introducing a cladding-air boundary at the distances \( x_{max} \) and \( y_{max} \) from the waveguide center. The field is assumed to be zero at these boundaries. The guided solutions are given by
\[
F(x, (n_x, x_{max})) = \begin{cases} 
C_x \cos \left( \frac{\pi x}{a} \right) \sinh \left( \frac{\pi x}{a} (x_{max} - x) \right) / \sinh \left( \frac{\pi x}{a} (x_{max} + \frac{\pi}{2}) \right) & x > \frac{\pi}{2} \\
C_x \cos \left( \frac{\pi x}{a} \right) \sinh \left( \frac{\pi x}{a} (x_{max} + \frac{\pi}{2}) \right) / \sinh \left( \frac{\pi x}{a} (x_{max} + \frac{\pi}{2}) \right) & x < \frac{-\pi}{2}
\end{cases}
\]

with \( \phi = 0 \) for the even and \( \phi = \pi/2 \) for the odd modes. \( u_x \) and \( v_x \) are determined from the equations
\[
u_x \coth \left( \frac{\pi x}{a} (x_{max} - \frac{\pi}{2}) \right) = \tan \left( \frac{\pi x}{a} \right)
\]
\[
u_x^2 + \nu_x^2 = a^2 k^2 (n_x^2 - n_2^2) = V_x^2.
\]

For the nonguided modes the solutions are given by
\[
F(x, (n_y, y_{max})) = \begin{cases} 
C_y \cos \left( \frac{\pi y}{b} \right) \sinh \left( \frac{\pi y}{b} (x_{max} - x) \right) / \sinh \left( \frac{\pi y}{b} (x_{max} + \frac{\pi}{2}) \right) & x > \frac{\pi}{2} \\
C_y \cos \left( \frac{\pi y}{b} \right) \sinh \left( \frac{\pi y}{b} (x_{max} + \frac{\pi}{2}) \right) / \sinh \left( \frac{\pi y}{b} (x_{max} + \frac{\pi}{2}) \right) & x < \frac{-\pi}{2}
\end{cases}
\]

with \( u_x \) and \( v_x \) determined from
\[
u_x \coth \left( \frac{\pi x}{b} (x_{max} - \frac{\pi}{2}) \right) = \tan \left( \frac{\pi x}{b} \right)
\]
\[
u_x^2 + \nu_x^2 = b^2 k^2 (n_y^2 - n_2^2) = V_y^2.
\]

Similar expressions exist for the \( y \) dependency. The total set of the guided and nonguided modes form an orthonormal set of functions by proper choice of \( C_x \) and \( C_y \).

Fig. 3 shows a graphical solution to the characteristic equations (4) and (5). The filled circle indicates a guided solution.
and the open circles indicate the first 13 nonguided solutions. These depend on the value of $x_{\text{max}}$ (in Fig. 3 $x_{\text{max}} = 5 \cdot a$ is used as an example). The variational parameters for this method are $n_x$, $n_y$, $x_{\text{max}}$ and $y_{\text{max}}$. The matrix elements can be calculated analytically as outlined in Appendix B. We refer to this method as the slab waveguide method (SWM).

V. RESULTS

To compare the above described methods we have analyzed rectangular waveguides with aspect ratios $a/b$ equal to 1 and 2, respectively. For $a/b = 1$ the normalized propagation constant $P^2$ has been calculated for a normalized frequency $B$ of 1.0 that is in the single-mode region for this waveguide. $P^2$ and $B$ are defined as

$$P^2 = \frac{(\beta/k)^2 - n_0^2}{n_1^2 - n_0^2}; \quad B = \frac{bk}{\pi \sqrt{n_1^2 - n_0^2}}.$$  

A simple multidimensional newton-iteration method has been used to maximize $\beta$ as described earlier. The relative error of the calculated values of $P^2$ compared to the reference value obtained by the circular harmonic analysis [3] are shown in Fig. 4 for increasing number of basis functions. By calculating the propagation constant as a function of the number of circular harmonics we have found the accuracy of the reference value to about $10^{-4}$. As mentioned in the introduction the circular harmonic method gives a vector solution while the methods we compare are solutions to the scalar wave equation. We have calculated the vector correction to the normalized propagation constant from a perturbation method [7] to $1 \cdot 10^{-4}$.

As seen from Fig. 4 the optimized Hermite–Gauss method represents a clear improvement in accuracy compared to the Hermite–Gauss method for a given number $N$. For the OHGM about 8–10 Newton iterations was necessary to reach the optimum values of $\sigma_x$ and $\sigma_y$ with a relative error less than $10^{-6}$. The calculation time for the HGM is approximately proportional to $N^6$, while the calculation time for the OHGM is around 50 times larger since the latter method requires around 50 times as many eigenvalue solutions as the HGM. Still, calculations for up to $N = 14$ with the HGM show relative errors above 10%. Thus, the HGM is not a practical method for the solution of the wave equation for a single mode rectangular waveguide. Further, Fig. 4 shows that the slab waveguide method requires fewer basis functions than the OHGM for the same accuracy. Since the calculation time as a function of $N$ is approximately the same for the SWM as for the OHGM, the former method is the fastest for a specified accuracy.

The error in $P^2$ calculated at $B = 1.0$ with the simple effective index method is 3%. The SWM with $N = 1$ may be thought of as an optimized effective index method and, as seen from Fig. 4, the error is less than 1%. Furthermore, for $N = 1$ $P^2$ is calculated directly without the solution of an eigenvalue equation, and only $n_x$ and $n_y$ should be optimized. Therefore, this is a very fast and simple method.

Fig. 5(a) and (b) shows plots of the normalized propagation constant $P^2$ as a function of normalized frequency calculated by the circular harmonic method, the optimized Hermite–Gauss method (with $N = 8$), the slab waveguide method (with $N = 1$), and the effective index method for $a/b = 1$ (Fig. 5(a)) and $a/b = 2$ (Fig. 5(b)).

The figure demonstrates that the SWM gives a clear improvement in accuracy compared to the EIM. For a very weakly guided mode (small normalized frequency) the SWM depicts a cut-off at $B = 0.43$, while the OHGM depicts a cut-off at $B = 0.55$ when $a/b = 1$. For $a/b = 2$ the cut-off's are at $B = 0.37$ and $B = 0.42$ for the SWM and the OHGM, respectively. Calculations for larger numbers of basis functions show the same results. On the other hand, for the single mode waveguides reported in the literature $B$ is in the range from 1.0 to 1.4, where our methods have very good accuracy.

To investigate the accuracy of the propagation constant for higher order modes we have calculated the results shown on Fig. 6. The waveguide has $a/b = 1$, and we use the same notation as in [3] for the modes. As the slab waveguide method is both faster and more accurate than the optimized Hermite–Gauss method, results are shown for the former method only. Fig. 6 shows that the SWM gives a clear improvement in accuracy compared to the effective index method. The cut-off for the $E_{21}$ and the $E_{22}$ mode is calculated with a relative error of less than 3 and 1%, respectively.

VI. CONCLUSION

Two variance methods for the solution of the scalar wave equation for single-mode dielectric waveguides with rectangu-
Fig. 5. Normalized propagation constant for the fundamental mode as a function of normalized frequency calculated by the optimized Hermite-Gauss method (OHGM), the slab waveguide method (SWM), the effective index method (EIM), and the circular harmonic method (CHM). a) $a/b = 1$ b) $a/b = 2$.

Fig. 6. Normalized propagation constant for the first two higher order modes of a rectangular waveguide with $a/b = 1$ as a function of normalized frequency calculated by the slab waveguide method (SWM), the effective index method (EIM), and the circular harmonic method (CHM).

The matrix elements for the Hermite–Gauss methods are written as

$$A_{l,m,i,j} = I_{l_1}^{m_1} I_{l_2}^{m_2} + n_{l_1}^{2} \frac{k^2}{2} I_{l_2}^{m_1} I_{l_2}^{m_2} + (n_{l_1}^{2} - n_{l_2}^{2}) k^2 I_{l_2}^{m_1} I_{l_2}^{m_2}$$

with

$$I_{l_1}^{m_1} = \int_{-\infty}^{\infty} F_{l} \left( \frac{x}{\sigma_x} \right) \frac{\partial^2}{\partial x^2} F_{l} \left( \frac{x}{\sigma_x} \right) \, dx$$

$$I_{l_2}^{m_2} = \int_{-\infty}^{\infty} F_{l} \left( \frac{x}{\sigma_x} \right) \frac{\partial^2}{\partial x^2} F_{l} \left( \frac{x}{\sigma_x} \right) \, dx$$

$$I_{l_3}^{m_3} = \int_{-\infty}^{\infty} F_{l} \left( \frac{x}{\sigma_x} \right) \frac{\partial^2}{\partial x^2} F_{l} \left( \frac{x}{\sigma_x} \right) \, dx$$

Similar expressions are found for $I_{l_1}^{m_1}, I_{l_2}^{m_2},$ and $I_{l_3}^{m_3}$.

APPENDIX B

For the slab waveguide method the matrix elements are written as

$$A_{l,m,i,j} = I_{l} + I_{2} + I_{3} + I_{4}$$

For $l$ and $i$ both even or $l$ and $i$ both odd (and similarly for $m$ and $j$) $I_{1}, I_{2}, I_{3}$ and $I_{4}$ are given by

$$I_{l} = 4 \left[ \left( \frac{n_{l}^{2}}{a} \right)^{2} + \left( \frac{n_{l}^{2}}{b} \right)^{2} + n_{l}^{2} k^{2} \right] \cdot \int_{a/2}^{\infty} F_{l} F_{i} \, dx \int_{b/2}^{\infty} G_{m} G_{j} \, dy$$

The optical core and step refractive-index profile are investigated. The first method uses Hermite–Gauss functions as basis, and the second uses slab waveguide solutions as basis. Both methods provide values of the normalized propagation constant with errors less than 0.1% for practical rectangular single-mode waveguides. This is an order of magnitude better than the effective index method. The slab waveguide method is the fastest method, and even when only one slab waveguide mode is used the propagation constant for the fundamental mode can be calculated with an error of less than 1%. Finally we have shown that the slab waveguide method gives very accurate results for the propagation constants for higher order modes.
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