Analyzing Leaky Waveguide Modes by Pseudospectral Modal Method

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Abstract—Leaky modes are important when optical waveguides fail to confine light completely. Computing waveguide modes to high accuracy is challenging if the waveguide has high index-contrast and sharp corners. The propagation constant of a leaky mode is complex, its imaginary part is an important physical quantity (the decay rate along the waveguide axis). To find complex propagation constants with a small imaginary part, high-accuracy numerical solutions are necessary. The pseudospectral modal method (PSMM), originally developed for diffraction gratings, has recently been reformulated as a full-vectorial waveguide mode solver. In this work, the PSMM is extended to analyze two challenging waveguide benchmark problems involving leaky modes.

Index Terms—Optical waveguides, waveguide mode solver, pseudospectral modal method.

I. INTRODUCTION

Optical waveguides appeared in recent years, such as silicon waveguides, plasmonic or hybrid-plasmonic waveguides, and photonic crystal fibers, often have high index-contrast, sharp corners, metallic components, and complicated microstructures. Over the last several decades, many numerical methods have been developed for computing guided and leaky modes of optical waveguides, but accurate solutions are still difficult to get for waveguides with sharp corners, due to the field singularities at the corners. Numerical methods for optical waveguides can be classified as linear and nonlinear ones, depending on whether the approximate matrix eigenvalue problems they produce are linear or nonlinear. The finite difference method [1]–[3], the finite element method [4]– [7], and the multidomain pseudospectral method [8]-[10] are linear methods. The boundary integral equation method [11]-[15] and the mode matching method (MMM) (including its numerical variants) [16]-[24] are nonlinear methods. The MMM and its variants are only applicable to waveguides with vertical and horizontal interfaces, but they can produce accurate solutions, since the resulting nonlinear matrix eigenvalue problems involve relatively small matrices. In a recent work [25], we developed a new variant of the MMM based on the pseudospectral modal method (PSMM) for diffraction gratings

Copyright (c) 2015 IEEE. Personal use of this material is permitted. However, permission to use this material for any other purposes must be obtained from the IEEE by sending a request to pubs-permissions@ieee.org. [26]–[29]. As a mode solver, the PSMM is highly competitive, since it is easier to implement than the classical analytic MMM and it is more accurate than the numerical variants based on Fourier series and finite differences.

In this Letter, we extend the PSMM to compute leaky waveguide modes. The propagation constant of a typical leaky mode has a small imaginary part related to the rate of exponential decay along the waveguide axis. Computing leaky modes to high accuracy is necessary, since the decay rate can be very small and it must be determined accurately.

II. PSEUDOSPECTRAL MODAL METHOD

The PSMM was originally developed for in-plane [26]– [28] and conical [29] diffraction of gratings. The full-vectorial PSMM waveguide mode solver [25] follows Ref. [29], and it can be regarded as a new variant of the classical MMM for waveguide analysis [16]–[19]. Essentially, it only differs from earlier variants of MMM in how the one-dimensional (1-D) modes are solved and how the field components are matched. In this section, we present the necessary changes for computing leaky modes.

We consider z-invariant waveguides for which the cross sections (in the xy plane) have only material interfaces parallel to the x or y axis, where $\{x, y, z\}$ is a Cartesian coordinate system. For simplicity, we consider two waveguides with their cross sections shown in Fig. 1. For both waveguides, we have three horizontal interfaces at $y = y_1$, y_2 and y_3 , and two vertical interfaces at $x = x_1$ and x_2 . The MMM can use either vertical or horizontal segments. We use the vertical segments given by $x < x_1$, $x_1 < x < x_2$ and $x > x_2$. Since these two waveguides have a horizontal reflection symmetry, it is only necessary to match the wave field on one vertical interface at $x = x_2$.

The MMM expands the wave field in each segments using 1-D transverse electric (TE) and transverse magnetic (TM) modes. A TM mode in a vertical segment satisfies

$$\varepsilon \frac{d}{dy} \left(\frac{1}{\varepsilon} \frac{d\phi}{dy} \right) + k_0^2 \varepsilon \phi = \hat{\delta}^2 \phi \tag{1}$$

where ε is the relative permittivity and it depends only on y in the segment, ϕ is the mode profile (a function of y), and $\hat{\delta}$ is the propagation constant of the 1-D mode. Since y is unbounded, it is necessary to truncate y. We assume y is truncated to $y_0 < y < y_*$ and impose the zero boundary condition $\phi = 0$ at $y = y_0$ and y_* . To handle leaky modes, it is usually necessary to use perfectly matched layers (PMLs) [30]. A PML can be regarded as a complex coordinate stretching

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Fig. 1. Two optical waveguides: (a) a silicon wire; (b) a rib waveguide.

that replaces y in Eq. (1) by a complex \hat{y} . For $s_p(y) = d\hat{y}/dy$, Eq. (1) is replaced by

$$\frac{\varepsilon}{s_p} \frac{d}{dy} \left(\frac{1}{\varepsilon s_p} \frac{d\phi}{dy} \right) + k_0^2 \varepsilon \phi = \hat{\delta}^2 \phi, \quad y_0 < y < y_*.$$
 (2)

The above gives rise to a discrete sequence of TM modes $\{\phi_j, \hat{\delta}_j\}$ for j = 1, 2, 3, ... Similarly, we have a discrete sequence of TE modes $\{\psi_j, \hat{\nu}_j\}$ for j = 1, 2, 3, ...

Assuming the time dependence is $e^{-i\omega t}$ (ω is the angular frequency), a waveguide mode depending on z as $e^{i\beta z}$ (β is the propagation constant) propagates towards $z = +\infty$. In each vertical segment, assuming β is given, the electromagnetic field can be expanded using the 1-D TE and TM modes. For example, in the segment $x > x_2$,

$$E_y = \frac{1}{\varepsilon} \sum_{j=1}^{\infty} a_j \hat{\delta}_j^2 \phi_j(y) e^{\mathbf{i}[\delta_j(x-x_2)+\beta z]}, \quad x > x_2, \quad (3)$$

where a_j (for j = 1, 2, ...) are unknown coefficients and

$$\delta_j = \sqrt{\hat{\delta}_j^2 - \beta^2}.$$
(4)

For computing leaky modes, the above complex square root must be carefully defined. A leaky mode propagating towards $z = +\infty$ should attenuate as z is increased, therefore, the imaginary part of β should be positive. If $\hat{\delta}_j$ is real and Re[$\hat{\delta}_j^2 - \beta^2$] > 0, the standard complex square root gives a δ_j in the lower half plane, since the negative real axis is the branch cut. This is incorrect, since δ_j should change continuously with Im(β). A simple solution to this problem is to redefine the complex square root by rotating the branch cut to the negative imaginary axis. That is,

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For the TE modes $\{\psi_j, \hat{\nu}_j\}$, we similarly define $\nu_j = \sqrt{\hat{\nu}_j^2 - \beta^2}$. Consequently, we can expand the four field components E_y , H_y , E_z and H_z using the 1-D modes.

In the PSMM [25], the 1-D modes are solved by the Chebyshev collocation method. If we discretize Eq. (2) directly, we can choose the number of points in each interval of y, but cannot change how these points are distributed. To gain more flexibility, we introduce a real coordinate transform $y = g(\xi)$, then Eq. (2) becomes

$$\frac{\varepsilon}{s_p s_g} \frac{d}{d\xi} \left(\frac{1}{\varepsilon s_p s_g} \frac{d\phi}{d\xi} \right) + k_0^2 \varepsilon \phi = \hat{\delta}^2 \phi, \quad \xi_0 < \xi < \xi_*, \quad (5)$$

where $s_g(\xi) = dg/d\xi$, $g(\xi_0) = y_0$ and $g(\xi_*) = y_*$. Using the Chebyshev collocation method, if ξ (also y) is discretized by N points, we solve Eq. (5) with the boundary conditions $\phi = 0$ at ξ_0 and ξ_* , and find N numerical TM modes. Similarly, we find N numerical TE modes. With the four components E_y , H_y , E_z and H_z expanded in the numerical 1-D modes in each vertical segments, we can set up a homogeneous linear system

$$\mathbf{F}(\beta)\boldsymbol{x} = \boldsymbol{0},\tag{6}$$

by matching these components at all discretization points on vertical interfaces, where x is a vector for the unknown coefficients. For the two waveguides shown in Fig. 1, assuming proper symmetry of the waveguide mode, it is only necessary to match the components on one vertical interface at $x = x_2$. In that case, **F** is a $(4N) \times (4N)$ matrix. The propagation constant β can be solved iteratively from the condition that **F** is a singular matrix. We use the condition $\sigma_1(\mathbf{F}) = 0$, where σ_1 is the smallest singular value of the matrix. A more efficient but less robust method is to solve β from

$$f(\beta) = \frac{1}{\boldsymbol{a}^{\mathsf{T}}\boldsymbol{w}} = 0, \tag{7}$$

where w is the solution of Fw = b, and a, b are two randomly chosen column vectors [13]. Typically, using the secant method or Müller's method, only a small number of iterations are needed. The required number of operations in each iteration is $O(N^3)$.

III. BENCHMARK PROBLEMS

In this section, we consider two waveguide benchmark problems. The first waveguide is a silicon wire as shown in Fig. 1(a). The silicon core has a $0.5 \,\mu m \times 0.22 \,\mu m$ rectangular cross section. It is placed on a $1 \,\mu m$ thick SiO₂ buffer layer below which is the infinite silicon substrate. The waveguide is considered for free space wavelength $\lambda = 1.55 \,\mu m$, assuming the refractive indices of silicon, SiO₂ and air cladding are $n_b = 3.5$, $n_c = 1.45$ and $n_t = 1$, respectively. Since the SiO₂ layer is finite, power can leak to the substrate, thus the waveguide has no guided modes. Our objective is to calculate the fundamental leaky mode with a complex propagation constant β . Since Im(β) is an important physical quantity and it is very small, numerical solutions with high accuracy are necessary.

Assuming the interface between the silicon substrate and the SiO₂ buffer layer is $y = y_1 = 0$, we have $y_2 = 1 \,\mu\text{m}$ and $y_3 = 1.22 \,\mu\text{m}$. We truncate the y variable to $y_0 < y < y_*$, where $y_0 = -1.5 \,\mu\text{m}$ and $y_* = 5.22 \,\mu\text{m}$. The bottom substrate layer $y_0 < y < y_1$ is turned to a PML with function

$$s_p(y) = 1 + \mathbf{i}\alpha \left(\frac{y - y_1}{y_0 - y_1}\right)^3, \quad y < y_1,$$

where $\alpha = 80$. The top layer $y_3 < y < y_*$ is further divided into an air layer $y_3 < y < y_4 = 3.72 \,\mu\text{m}$ and a PML $y_4 < y < y_*$ with

$$s_p(y) = 1 + \mathbf{i}\alpha \left(\frac{y - y_4}{y_* - y_4}\right)^3, \quad y > y_4,$$

for the same α . The entire y-interval (y_0, y_*) is discretized following the Chebyshev points on five subintervals, with a total of N points (excluding the end points of the subintervals). The eigenvalue problems for the TE and TM modes are then approximated by matrix eigenvalue problems involving $N \times N$ matrices.

In Table I, we list the propagation constant β calculated

TABLE I PROPAGATION CONSTANT β of the fundamental leaky mode of the silicon wire calculated by the PSMM mode solver for different number of discretization points N.

N	$\operatorname{Re}(\beta/k_0)$	$\operatorname{Im}(\beta/k_0)$		
220	2.4123719902	2.47635×10^{-8}		
240	2.4123719882	2.79235×10^{-8}		
260	2.4123719863	2.88768×10^{-8}		
280	2.4123719850	2.91019×10^{-8}		
300	2.4123719842	2.91414×10^{-8}		
320	2.4123719836	2.91378×10^{-8}		
340	2.4123719831	2.91365×10^{-8}		
360	2.4123719828	2.91365×10^{-8}		
380	2.4123719825	2.91355×10^{-8}		
400	2.4123719823	2.91346×10^{-8}		
420	2.4123719821	2.91331×10^{-8}		
440	2.4123719819	2.91345×10^{-8}		
460	2.4123719818	2.91347×10^{-8}		
480	2.4123719817	2.91348×10^{-8}		
500	2.4123719816	2.91347×10^{-8}		

using PSMM for different values of N. Keeping 10 and 5 significant digits for the real and imaginary parts, respectively, we obtain $\text{Re}(\beta/k_0) = 2.412371982$ and $\text{Im}(\beta/k_0) = 2.9135 \times$ 10^{-8} . This result agrees perfectly with two previous calculations [31] based on the classical MMM [20] and the aperiodic Fourier modal method (FMM) [22] (a numerical variant of MMM based on Fourier series). These authors reported the real part with 7 significant digits: $\operatorname{Re}(\beta/k_0) = 2.412372$. For the imaginary part, they reported 5 or 6 digits, that is $\text{Im}(\beta/k_0) =$ 2.9135×10^{-8} or $\text{Im}(\beta/k_0) = 2.91348 \times 10^{-8}$. Other methods have been used to analyze this waveguide [31], but the results appear to be less accurate. Wang et al. [10] studied this waveguide by a multidomain pseudospectral method. Their result is $\operatorname{Re}(\beta/k_0) = 2.412374$ and $\operatorname{Im}(\beta/k_0) = 2.9198 \times 10^{-8}$. For N = 500, it takes about 5s on a current iMac to find the singular values of the complex $(4N) \times (4N)$ matrix F. The solution converges in a few iterations, and the total required time is less than half a minute.

The second benchmark problem is the classical rib waveguide studied by many authors [22], [24], [30], [32]–[34]. A schematic of the waveguide is shown in Fig. 1(b). The width and the height of the rib are $w = 3 \,\mu\text{m}$ and $h_1 = 1 \,\mu\text{m}$, respectively. The thickness of the slab is h_2 and it varies from $0.1 \mu m$ to $0.9 \mu m$. The waveguide is considered for free space wavenumber $\lambda = 1.15 \,\mu\text{m}$. The refractive indices of the guiding layer, the substrate and the air cladding are $n_c = 3.44$, $n_b = 3.4$ and $n_t = 1$, respectively.

Using the PSMM, we calculate the fundamental quasi-TE and quasi-TM modes of the rib waveguide for a few values of h_2 , and list the normalized propagation constant B defined as

$$B = \frac{(\beta/k_0)^2 - n_b^2}{n_c^2 - n_b^2}$$

in Table II. For comparison, we also list the results obtained

TABLE II Normalized propagation constants B of the fundamental quasi-TE and quasi-TM modes of the rib waveguide.

h_2	PSMM: TE	MMM: TE	PSMM: TM	MMM: TM
0.1	0.30190788	0.30191	0.26745459	0.26745
0.3	0.31104338	0.31105	0.27514225	0.27513
0.5	0.32701401	0.32702	0.28899995	0.28899
0.7	0.35117264	0.35118	0.31070288	0.31070
0.9	0.38830976	-	0.34549570	-

by Selleri *et al.* [33] using the classical MMM. Although these authors only show five significant digits, the difference with our result is less than 10^{-5} for all cases. We have confidence that our results are accurate to the 7th digit after the decimal point. The results of many other numerical methods are summarized in [34].

As pointed by Vassallo [32], the fundamental quasi-TM mode is leaky when $h_2 = 0.9 \,\mu\text{m}$. Therefore, the number in Table II for this particular case is actually the real part of B. Many authors have studied this case, but failed to calculate the imaginary part. Using the aperiodic FMM, Hugonin *et al.* [22] obtained $\text{Im}(\beta/k_0) = 6.71 \times 10^{-7}$. We consider this case by truncating the y variable to (y_0, y_*) where $y_0 = -8 \,\mu\text{m}$ and $y_* = 2.1 \,\mu\text{m}$. The horizontal interfaces are located at $y_1 = 0, y_2 = h_2 = 0.9 \,\mu\text{m}$, and $y_3 = h_1 = 1 \,\mu\text{m}$. Although the quasi-TM mode in this case is leaky, it only leaks in the horizontal directions (as $x \to \pm \infty$). Therefore, it is not necessary to use PMLs in the y direction. In Table III, we show

TABLE III PROPAGATION CONSTANT β of the quasi-TM leaky mode of the RIB WAVEGUIDE WITH $h_2 = 0.9 \, \mu m$, calculated using the PSMM mode solver for different number of discretization points N.

N	$\operatorname{Re}(\beta/k_0)$	$\operatorname{Im}(\beta/k_0)$
100	3.4138744414	3.2856×10^{-7}
140	3.4138713456	8.5942×10^{-7}
184	3.4138693667	8.6521×10^{-7}
220	3.4138728239	6.7188×10^{-7}
260	3.4138728220	6.7186×10^{-7}
300	3.4138728210	6.7184×10^{-7}
340	3.4138728204	6.7184×10^{-7}
380	3.4138728199	6.7180×10^{-7}
420	3.4138728196	6.7181×10^{-7}
460	3.4138728194	6.7182×10^{-7}
500	3.4138728192	6.7178×10^{-7}
540	3.4138728191	6.7178×10^{-7}

the complex propagation constant β computed by the PSMM

with different values of N. If we keep 10 and 4 significant digits for the real and imaginary parts, then our result is $\text{Re}(\beta/k_0) = 3.413872819$ and $\text{Im}(\beta/k_0) = 6.718 \times 10^{-7}$. It agrees well with the result of Hugonin *et al.* [22].

IV. CONCLUSION

For optical waveguides with horizontal and vertical material interfaces only, the MMM and its numerical variants are popular. Compared with the classical MMM that calculates the 1-D modes analytically, the numerical variants are easier to implement and can still achieve high accuracy. The PSMM and the FMM are originally developed for diffraction grating problems, but they are in fact numerical variants of the MMM when used as full-vectorial waveguide mode solvers [22], [25]. The PSMM has outperformed the FMM for grating problems [28], [29], and delivers high-accuracy results for guided modes of optical waveguides. In this Letter, we use two benchmark problems to show that PSMM is capable of computing leaky modes to high accuracy. For leaky modes, the imaginary part of the propagation constant is an important physical quantity and it is often very small. Therefore, highly accurate numerical solutions are really needed.

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