In this paper, based on a new treatment for local base transformation, a modified operator marching method is provided to accurately compute optical propagation in the inhomogeneous waveguide terminated by a perfectly matched layer. Compared with the adjoint operator method (AOM), high-precision results of the optical propagation can be obtained in numerical simulations, which demonstrate that the new treatment is much better than the AOM. This technique is helpful to optimize the designs of the optical waveguides and the integrated optics devices.© 2015 Optical Society of America

1. INTRODUCTION

High-precision computation of optical propagation is very important for optimizing the designs of optical waveguides and integrated optics devices [1,2]. For the bounded waveguides along the transverse direction (denoted by z in this paper), many researchers have studied the computation of the wave propagation in the inhomogeneous optical waveguides or in the acoustical waveguides with a varied wavenumber. There are some efficient computational methods for the wave propagation, such as the beam propagation method for gradient refractive-index media [3] or for complex systems [4], the operator formalism for paraxial propagation in homogeneous and inhomogeneous media [5], and the marching scheme based on the Dirichlet-to-Neumann (DtN) map for weakly range-dependent waveguides [6–8].

By using the perfectly matched layers (PMLs) for the unbounded waveguides along the transverse direction [9], the transverse plane can be truncated to a bounded and relatively small region. Therefore, the propagation problem is formulated in a domain with just one direction (i.e., x direction) having a particularly large length [10]. For this special geometric feature, the operator marching method (OMM) [6,11,12], namely a one-way reformulation based on the DtN map, can be used to reduce the boundary value problem to an initial value problem. Compared with direct Helmholtz solvers, such as the finite difference and the finite element methods, the OMM is much more practical.

In the OMM there is a local base transformation to be done in each marching step by searching a coordinate matrix related to the eigenvalue problem. For a bounded waveguide, the transverse operator is self-adjoint, and its system of linearly independent eigenfunctions forms an orthogonal basis [13]. Thus, in this case, the process of the local base transformation is easy. However, for an unbounded waveguide, a PML is applied to terminate it to a bounded region, and the original Helmholtz equation with real coefficients is transformed into a partial differential equation (PDE) with complex coefficients [14,15]. Thus, the resulting transverse operator of the PDE is not self-adjoint. It leads to the loss of the orthogonality for the eigenfunction system. This brings great difficulty in the numerical implementation of the local base transformation.

To solve this difficulty, the adjoint operator method (AOM) was constructed [7]. In the AOM, a bi-orthogonal set for the eigenfunctions of the transverse operator is formed. However, further research showed that the bi-orthogonality of the two sets (the eigenfunction set and the bi-orthogonal set) is not very good in numerical implementation [16]. This would destroy the computational accuracy of wave propagation seriously.

In this paper, an unacceptable error is shown, which is produced in computing the coordinate matrix by use of the AOM. This error may further affect the propagation results obtained by the OMM severely. We also give an interpretation of the bad bi-orthogonality of the AOM. Additionally, a new treatment for the local base transformation is provided. Numerical results show that the bi-orthogonality of the new treatment is much better than that of the AOM. We also investigate the relationship between the two methods through theoretical derivation. It is shown that the new treatment is equivalent to the AOM if the transverse operator is discretized on infinite grids. However, in terms of practical effect, the new treatment is more efficient.
than the AOM, and some high-precision results of optical propagation in inhomogeneous media are obtained.

This paper is organized as follows. Section 2 presents the mathematical model in the unbounded waveguide. In Section 3, we introduce the AOM and explain the difficulty of this method in local base transformation. A new treatment is given in this section; the relationship between the two methods is also investigated. In Section 4, we give the outline of the modified OMM. Then, some numerical examples are presented to illustrate the correctness of our statement and the efficiency of the new treatment. Finally, some conclusions are given in Section 5.

2. BASIC PROBLEM

When the refractive index is independent of y, Maxwell’s equations can be reduced to scalar Helmholtz equations. The governing equation is

\[ \partial^2_u + \partial^2_z u + \kappa^2(x, z) u = 0 \]  \hspace{1cm} (1)

for the transverse electric (TE) polarization, where u is the y component of the electric field, \( \kappa \) is called the wavenumber, and \( \kappa^2(x, z) = \kappa_0^2 n^2(x, z) \); here \( \kappa_0 \) is the free space wavenumber, and \( n(x, z) \) is the refractive-index function.

For simplicity, we consider a two-layer waveguide with one side bounded by a perfect electric conductor [17,18] (shown in Fig. 1). The boundary condition is \( u(x, 0) = 0 \) at \( z = 0 \). Assume the refractive index is invariant for \( x > L \) and there is only the outgoing wave for \( x > L \). The medium is homogeneous for \( z > D \) and \( n(x, z) = n_1 \) in this domain. In \([0, D]\), \( n(x, z) = n_0(x, z) \) is a continuous function, and \( n_0(x, z) > n_1 \) is required. At \( x = 0 \), the incident wave \( u(0, z) \) is given as \( u_0(z) \).

The transverse variable \( z \) can be truncated by the PML technique [9,19]. In this case, the term \( \partial^2_z \) is replaced by \( s^{-1}(z) \partial_z^2 [s^{-1}(z) \partial_z^2] \), where \( s(z) = 1 + i \sigma(z) \) and \( \sigma(z) \neq 0 \) only in the PML region \([H, D]\). Therefore, Eq. (1) becomes

\[ \partial^2_u + s^{-1}(z) \partial_z^2 [s^{-1}(z) \partial_z^2] u + \kappa^2(x, z) u = 0. \]  \hspace{1cm} (2)

The boundary conditions for Eq. (2) are

\[
\begin{aligned}
    u(x, 0) &= 0, \\
    u(x, D_1) &= 0, \\
    u(0, z) &= u_0(z), \\
    u_x &= i \left( \frac{1}{i} \frac{d}{dz} \left( \frac{1}{d} \right) + \kappa^2(L, z) u_x, x = L, \right)
\end{aligned}
\]  \hspace{1cm} (3)

where \( i = \sqrt{-1} \) and the square root is defined in Section 3A.

The transverse plan can be truncated to a relatively small region. Therefore, the propagation problem is formulated in a domain with just one direction (i.e., \( x \)), having a particularly long length [10]. For this special geometric feature, the OMM, a one-way reformulation based on the Dirichlet-to-Neumann (DtN) map, can be used to reduce the boundary value problem in Eqs. (2) and (3) to an initial value problem.

3. TWO METHODS FOR THE LOCAL BASE TRANSFORMATION

In the numerical implementation of the resulting operator Riccati equation from the DtN map, a local base transformation needs to be done in each marching step by searching a coordinate matrix \( N \) satisfying \( V_1 = V_0 N \), where \( V_0 \) and \( V_1 \) are known eigenvector matrices of the transverse operator of Eq. (2) at different locations. \( N \) can be obtained by the orthogonality of the eigenfunctions when the operator is self-adjoint. However, for the unbounded problem terminated by PMLs, the transverse operator is not self-adjoint, and, hence, the eigenfunctions are not orthogonal. This results in a difficulty in the local base transformation. The most intuitive treatment is to find the inverse matrix of \( V_0 \), i.e., \( N = V_0^{-1} V_1 \), but it is time-consuming and unstable. However, with this connection, the AOM and a new treatment for the local base transformation are described in Section 3B.

A. AOM and Its Limitation

The eigenvalue problem of Eq. (2) is very important. It is defined as

\[ L(x) \phi(z) = \lambda \phi(z), \]  \hspace{1cm} (4)

with the boundary conditions

\[ \phi(0) = 0, \quad \phi(D_1) = 0, \]  \hspace{1cm} (5)

where the transverse operator is

\[ L(x) = \frac{1}{i} \frac{d}{dz} \left( \frac{1}{i} \frac{d}{dz} \right) + \kappa^2(x, z). \]  \hspace{1cm} (6)

The square root operator,

\[ L^{1/2}(x) = \sqrt{\frac{1}{i} \frac{d}{dz} \left( \frac{1}{i} \frac{d}{dz} \right) + \kappa^2(x, z)}, \]  \hspace{1cm} (7)

is defined to satisfy

\[ L^{1/2}(x) \phi(z) = \sqrt{\lambda} \phi(z), \quad 0 < z < D_1, \]  \hspace{1cm} (8)

where \( \phi(z) \) and \( \lambda \) are the same as Eq. (4). The branch of the square root is chosen as \((\pi/2, -\pi/2]\).

Denote the adjoint operator of \( L(x) \) as \( L^*(x) \); let \( \phi_i(z) \) and \( \phi_j(z) \) be the normalized eigenfunctions of \( L(x) \) and \( L^*(x) \) separately, and their corresponding eigenvalues \( \lambda_i \) and \( \lambda_j \) satisfying \( \lambda_i = \lambda_j \), where \( i \neq j \), the overline represents taking the conjugation. The definition of adjoint operator as well as the proof of Eq. (11) can be found in Appendix A.

It is easy to prove:

\[ \int_0^{D_1} \delta_{ij} \phi_i(z) \phi_j(z) dz = \delta_{ij}. \]  \hspace{1cm} (9)
where
\[
\delta_{ij} = \begin{cases} 
1, & \text{if } i = j; \\
0, & \text{if } i \neq j.
\end{cases}
\] (10)

The eigenfunctions \( \{ \phi_i(z) \} \) of \( L^* \) can be obtained from \( \phi_i(z) \); that is,
\[
\overline{\phi}_i(z) = s(z)\phi_j(z).
\] (11)

By Eqs. (9) and (11), we have
\[
\int_0^{D_1} s(z)\phi_i(z)\phi_j(z)dz = \delta_{ij}.
\] (12)

In practical calculation, \( L \) is discretized as a matrix \( D \). The eigenvector decomposition for \( D \) is first calculated as
\[
DV_0 = V_0\Lambda_0.
\] (13)

Then, by Eq. (12), we have
\[
V_0^T SWV_0 = I,
\] (14)

where the superscript \( T \) means transpose, \( W \) is a weight matrix determined by a numerical quadrature formula, and \( S \) is a diagonal matrix whose diagonal elements are values of \( s(z) \) at the corresponding nodes. Thus,
\[
N = V_0^TSWV_1, \quad \text{if } V_1 = V_0N.
\] (15)

However, this method can hardly be used in the numerical implementation of local base transformation. The reason is that the bi-orthogonality is not very good in numerical implementation \( \text{(i.e., } V_0^TSWV_0 \text{ is far away from } I) \). It is not that the eigenvalues or eigenfunctions are calculated inaccurately, but that the numerical integrals for the PML modes are difficult, since the eigenfunctions change rapidly in the PML layer \( \text{(shown in Example 1). This difficulty may bring an unacceptable error when we use Eq. (15) to calculate the coordinate matrix } N \). In addition, this error further affects the solution solved by the OMM severely \( \text{(shown in Example 2).} \)

**B. New Treatment for Local Base Transformation**

A new treatment for local base transformation is introduced in this section. Let us denote the discretization matrix of \( L \) as \( D \), and \( D^H \) is the conjugate transpose of \( D \). Suppose \( \phi_i \) and \( \xi_j \) are the normalized eigenvectors of \( D \) and \( D^H \), respectively, and assume their corresponding eigenvalues are \( \lambda_j \) and \( \bar{\lambda}_j \). Then
\[
(\phi_i, \xi_j) = \delta_{ij}.
\] (16)

where \( (\cdot, \cdot) \) is the ordinary inner product in Euclidean space.

In fact, since
\[
(D\phi_i, \xi_j) = \lambda_i(\phi_i, \xi_j),
\] (17)

\[
(\phi_i, D^H\xi_j) = \bar{\lambda}_j(\phi_i, \xi_j),
\] (18)

and
\[
(D\phi_i, \xi_j) = (\phi_i, D^H\xi_j),
\] (19)

we have
\[
(\lambda_i - \bar{\lambda}_j)(\phi_i, \xi_j) = 0.
\] (20)

Thus, if the eigenvalues of \( D \) are different from each other, we have

\[
(\phi_i, \xi_j) = \delta_{ij}.
\] (21)

In practical calculation, the eigenvector decompositions for \( D \) and \( D^H \) are first calculated as
\[
DV_0 = V_0\Lambda, \quad D^H\tilde{V}_0 = \tilde{V}_0\Lambda^H,
\] (22)

where \( V_0 \) and \( \tilde{V}_0 \) are the eigenvector matrices, and \( \Lambda \), \( \Lambda^H \) are the diagonal eigenvalue matrices. Then, by Eq. (16), we have
\[
\tilde{V}_0^H V_0 = I.
\] (23)

Thus,
\[
N = \tilde{V}_0^H V_1, \quad \text{if } V_1 = V_0N.
\] (24)

There is an inconspicuous relationship between the new treatment and the AOM. The details are described in Appendix A, but we give the conclusion here.

Suppose \( \phi(z) \) and \( \varphi(z) \) are the eigenfunctions of \( L \) and \( L^* \), respectively, and the eigenvalue corresponding to \( \varphi(z) \) is \( \lambda \).

Denote \( \hat{\phi} \) \( \text{(an approximation of } \phi(z) \text{ at discrete nodes)} \) as an eigenvector of \( D \) and \( \hat{\lambda} \) as an eigenvector of \( D^H \). We immediately have
\[
\int_0^{D_1} \varphi(z)\hat{\phi}(z)dz \approx (\phi, \xi).
\] (25)

Form Eq. (25), we have a statement that the new treatment is equivalent to the AOM if the transverse operator is discretized as an infinite matrix. However, discretizing an operator on infinite grids is impossible, in practice, for the limitation of computer memory. For the finite grids, the new treatment is much more efficient than the AOM. \( \text{(The details are shown in Example 2.)} \)

**4. NUMERICAL METHOD AND EXAMPLES**

In this section, we give the outline of the OMM. Then, some examples are given to show our method and statements. Example 1 is used to illustrate the difficulty encountered in the AOM. Example 2 illustrates that the bi-orthogonality computed by Eq. (16) is much better than the one computed by Eq. (12); further, this example also demonstrates that the new treatment is equivalent to the AOM in some sense. Example 3 compares the wave propagation computed by the OMM, in which the local base transformation is implemented in two different ways. The results show that implementing the local base transformation by the new treatment is much better than the one by the AOM. In Example 4, we compute a general waveguide with the refractive index varying in both transverse and range directions.

**A. Modified OMM**

By the forward preparations, the new formulas can be obtained by a small, but important, modification of the OMM in [11]. We also take the segment, \( x_0 \), \( x_1 \), for example. The marching formulas indicate the relation of operators from \( x_1 \) to \( x_0 \). Suppose \( L(x_{1/2}) \) and \( L(x_{3/2}) \) are approximated by the matrices \( D_0 \) and \( D_1 \), respectively. Their truncated local eigenvector decompositions are
\[
D_0V_{0m} = V_{0m}\Lambda_{0m}, \quad D_1V_{1m} = V_{1m}\Lambda_{1m},
\] (26)
where $V_{jm}(i = 0, 1)$ are the $n \times m$ eigenvector matrices, and $\Lambda_{jm}$ are the $m \times m$ diagonal eigenvalue matrices.

For making use of Eq. (16), we need to find the two decompositions of $D_0^H$ and $D_1^H$. Suppose

$$D_0^H \tilde{V}_{0m} = \tilde{V}_{0m} \Lambda_{0m}^H \quad D_1^H \tilde{V}_{1m} = \tilde{V}_{1m} \Lambda_{1m}^H$$

(27)

We have

$$\tilde{V}_{im}^H \tilde{V}_{jm} = I, \quad (i = 0, 1)$$

(28)

The local base transformation can be done by

$$N = \tilde{V}_{im}^H \tilde{V}_{jm}$$

(29)

Alternatively, from Eq. (12), the local base transformation can also be done by

$$N = V_{0m}^T S W V_{1m}$$

(30)

where $W$ is the weight matrix determined by the numerical quadrature formula, and $S$ is a diagonal matrix whose diagonal elements are values of $s(z)$ at the discrete nodes. Then the marching formulas from $x_1$ to $x_0$ in matrix form [7,11] are

$$Q = N Q_1 N^{-1},$$

(31)

$$P_1 = (i \sqrt{\Lambda_{0m}} + Q)^{-1} (i \sqrt{\Lambda_{0m}} - Q),$$

(32)

$$P_0 = 1^{h} \sqrt{\Lambda_{0m}} P_1 1^{h} \sqrt{\Lambda_{0m}},$$

(33)

$$U = (I - P_0)(I + P_0)^{-1},$$

(34)

$$Q_0 = i \sqrt{\Lambda_{0m}} U,$$

(35)

$$Z_0 = N Z_1 N^{-1}(I + P_0) 1^{h} \sqrt{\Lambda_{0m}} (I + P_0)^{-1},$$

(36)

where $Q_1$ and $Z_1$ are known at $x_1$, and $b = x_1 - x_0$. By the marching formulas, $Q_0$ and $Z_0$ at $x_0$ are obtained. The same process from $x = L$ to $x = 0$ can be done step by step. $Q_1$ and $Z_1$ at $x = L$ act as the initial values, where $Z_1 = I$ and $Q_1 = \Lambda_{1m}$. The wave field at $x = L$ can be solved by

$$u = V_{0m} Z_0 V_{0m}^H \tilde{V}_{0m} u_0,$$

(37)

or

$$u = V_{0m} Z_0 V_{0m}^H S W u_0,$$

(38)

for $N$ computed by Eqs. (29) or (30), respectively.

**B. Numerical Examples**

Example 1

To illustrate the difficulty encountered in the AOM, consider the eigenvalue problem of a one-layer and half-open waveguide terminated by a PML:

$$H = 3 \, (\mu m), \quad D_1 = 4 \, (\mu m), \quad \sigma(z) = \frac{100 r^3}{1 + r^2},$$

where

$$\tau(z) = \begin{cases} 0, & 0 \leq z \leq H; \\ \frac{\pi}{D_1}, & H < z \leq D_1. \end{cases}$$

(40)

In Fig. 2, we plot $E_n$ for a different $n$, where $E_n$ is a measurement for the bi-orthogonality and defined as

$$E_n = \max_{1 \leq j \leq n} \left( \int_0^{D_1} \phi_j(z) \phi_k(z) dz \right), \quad j \neq k,$$

(41)

where $\phi_j(z)$ and $\phi_k(z)$ are solutions corresponding to the eigenvalues $\lambda_j$ and $\lambda_k$ for Eq. (39), satisfying

$$\int_0^{D_1} \phi_j(z) \phi_k(z) dz = 1.$$

(42)

All the integrals are computed numerically by the Clenshaw–Curtis quadrature [20] with 400 points, where the eigenfunction values are taken from the analytical solutions. By Eq. (12), $E_n$ should be zero; however, the numerical result is far away from it. This indicates that the integrals can hardly be computed with high accuracy by numerical quadrature, even if the exact eigenfunctions are used. Of course, using more points can improve the accuracy; however, that is not practical, since it reduces the computational efficiency.

Example 2

We now consider the eigenvalue problem of a one-layer and half-open waveguide terminated by a PML:

$$\begin{cases} \frac{1}{\pi z} \frac{d\phi(z)}{dz} + \kappa^2 \phi(z) = \lambda \phi(z), \\ \phi(0) = 0, \quad \phi(D_1) = 0, \end{cases}$$

(43)

where $\kappa = 3 \, (1/(\mu m))$, $H = \pi \, (\mu m)$, $D_1 = 1.5 \pi \, (\mu m)$, and the PML parameter is given by

$$\sigma(z) = \begin{cases} 0, & 0 \leq z \leq \pi; \\ 10 \cdot \exp \left(1 - \frac{z}{\pi} \right), & \pi < z \leq 1.5 \pi. \end{cases}$$

(44)

We discretize the operator in Eq. (43) by the Chebyshev pseudo-spectral method [21]; 102 points are used to approximate the operator. The differential matrix is denoted by $D$. The eigenvector of $D$ is an approximation of the eigenfunction $\phi_j(z)$ at the Chebyshev nodes, which is denoted as $\hat{\phi}_j$.

Now we investigate the eigenfunctions of $L^*$. By Eq. (11),

$$\phi_j(z) = \hat{s}(z) \hat{\phi}_j(z),$$

(45)
Thus, $\overline{S \hat{\phi}_j}$ is an approximation of $\hat{\phi}_j(z)$ at the Chebyshev nodes, where $S$ is a diagonal matrix whose diagonal elements are the value of $s(x)$ at the corresponding Chebyshev nodes. We denote this approximation as $\hat{\phi}_j^{(1)}$. Meanwhile, there is a relation as the following form:

$$\xi \approx W^H \phi,$$

where $\xi$ is the eigenvector of $D^H$, and $W$ is the weight matrix determined by some numerical quadrature formula. A detailed derivation is listed in Appendix A.

Then $\phi_j(z)$ can be approximated by $(W^H)^{-1} \xi$, where $\xi_j$ is the eigenvector of $D^H$, and $W$ is the weight matrix. We denote this approximation as $\hat{\phi}_j^{(2)}$.

In Fig. 3, the relative and absolute errors of the two approximations are displayed, where $n$ represents the index of eigenfunction. All the eigenvectors are normalized by the infinity norm. Relative ($E_R$) and absolute errors ($E_M$) for eigenfunctions between the two approximations are defined as follows:

$$E_M = \|\phi_n^{(1)} - \phi_n^{(2)}\|_\infty,$$

$$E_R = \sqrt{\left( \frac{W(\phi_n^{(1)} - \phi_n^{(2)}), (\phi_n^{(1)} - \phi_n^{(2)})}{W\phi_n^{(1)}, \phi_n^{(1)}} \right)}.$$

Numerical results in Fig. 3 show that the eigenfunctions obtained by the two methods coincide with each other very well, especially for small $n$. This implies that Eqs. (12) and (16) are equivalent.

In Fig. 4, we plot $\hat{E}_n$ for the two methods. $\hat{E}_n$ is the measurement for the bi-orthogonality and is defined as

$$\hat{E}_n = \max_{1 \leq j, k \leq n} (|\phi_j^T S W \phi_k|), \quad j \neq k$$

for the AOM, or

$$\hat{E}_n = \max_{1 \leq j, k \leq n} (|\xi_j^H \phi_k|), \quad j \neq k$$

for the new treatment, where they satisfy

$$\phi_j^T S W \phi_j = 1, \quad \text{and} \quad \xi_j^H \phi_j = 1,$$

respectively.

In fact, by Eqs. (12) and (25), $\hat{E}_n$ for the two methods is just a different way to approximate $E_n$ defined in Eq. (41). Numerical results show that $\hat{E}_n$ for the new treatment is much smaller than that of the OMM, which implies the new treatment is much better for local base transformation.

There is one interpretation for the dramatically different performance of the two methods. For the AOM, the bi-orthogonality is related to the inner product for $L^2$ space. To use this property, some numerical quadrature is needed. However, the PML modes change very rapidly and concentrate in the PML region for large $n$. This causes some difficulties in numerical implementation. Further, $\int_0^D s(x) \phi_j(x) \phi_k(x) dx$ is really smaller than $\int_0^D \phi_j(x) \phi_k(x) dx$. This property may enlarge the errors of the integration when we “unitize” the eigenfunctions. All of these features above result in AOM producing an unacceptable error in local base transformation, and this error further influences the solution solved by the OMM (shown in Example 3).

Fortunately, the new treatment based on Eq. (16) does not have this drawback. The eigenvectors of $D^H$ and $D$ are bi-orthogonal to each other in the discrete form. Look closely at Eq. (25); perhaps the new treatment can be assumed as implementing the AOM with the “optimal” numerical quadrature.

**Example 3**

In this example, we consider the problem Eq. (1). To facilitate the analysis, the medium is homogeneous, that is $n(x, z) = 3.3$ for $0 < z < 2.5$ ($\mu$m) and $n(x, z) = 3.17$ for $z > 2.5$ ($\mu$m). The PML profile terminating the waveguide is given by

$$\sigma(z) = \begin{cases} 0, & 0 \leq z \leq \mu; \\ 10 \cdot \exp \left(1 - \frac{4 - z}{(z - \mu)}\right), & \mu < z \leq 4. \end{cases}$$

The propagation distance $L$ is 10 ($\mu$m), and the free space wavelength is 1.55 ($\mu$m). To further simplify, the first eigenfunction
$\phi_1(z)$ is chosen as the incident wave. Thus, the solution at $x = L$ is $u(L, z) = e^{\sqrt{\lambda_1}L} \phi_1(z)$, where $\lambda_1 \approx 1.78 \times 10^2$ is the first eigenvalue. In Figs. 5–7, $\text{real}(u(L, z))$ and $\text{imag}(u(L, z))$ are represented as the real and imaginary parts of $u(L, z)$, respectively.

In this example, the coordinate matrix $N$ is an identity matrix in theory, but not in practice. Thus, implementing the local base transformation in different ways may affect the solution severely. Since the error in every step is accumulated, the total error increases as the range step size $h$ turns small.

In Fig. 5, we plot the solution obtained by the OMM method with different ranges of step sizes in the focused domain $[0, H]$ (without the PML). We use the “exact” solution $u(L, z) = e^{\sqrt{\lambda_1}L} \phi_1(z)$ as the reference, where $\phi_1(z)$ is obtained through solving the eigenvalue problem by the finite difference method. The transverse operator is discretized with 200 equidistant nodes, and 20 eigenfunctions are retained in the local eigenfunction expansion. In the figure, the “AOM” or “New” represent implementing the local base transformation by the AOM or the new treatment. Table 1 gives the relative errors (in $L^2$ norm) for different range step sizes.

It is very clear that the new treatment is much better than the AOM. For a general waveguide with the refractive-index profile varying in the range direction, the step size should be kept small for high accuracy. In this case, the AOM will completely fail since its performance is bad. However, the new treatment will still be available.

Example 4

In this example, we will compute a wave propagation problem in an inhomogeneous waveguide. The refractive index varies in both transverse and range directions. Similar to [22], we assume the refractive-index profile is given by

$$n^2(x, z) = \begin{cases} 
3.3^2 \left[ 1 - 0.04 e^{\pi/L} \left( \frac{z - 0.5}{2} \right)^2 \right], & 0 \leq z \leq 2.5 \text{ (\mu m)}; \\
3.17^2, & z > 2.5 \text{ (\mu m)}.
\end{cases}$$

The propagation distance $L$ is 10 (\mu m), and the free space wavelength is 1.55 (\mu m). The PML profile is the same as Example 3. We choose $u_0(z) = \sin(z) e^{-z}$ as the incident wave.

We first use a small-range step size, $h = 1/128$ (\mu m), to calculate a very accurate solution as the “exact” solution. After that, we calculate the solution with much larger-range steps, and then compare them with the more accurate “exact” solution. To verify the correctness of the new treatment, we also truncate the open waveguide to a very large domain, $[0, L] \times [0, G]$, where $G = 15$ (\mu m). Then a Dirichlet boundary condition is imposed at $z = G$, and the obtained solution acts as a reference.

In Fig. 6, we plot the numerical solutions of $u(L, z)$ for $h = 1/4$ (\mu m) and $h = 1/128$ (\mu m). We conclude that the numerical solution obtained by the new treatment is consistent with the reference one in the focused domain $[0, H]$, and a reasonably good solution is already obtained with $h = 1/4$ (\mu m).

In Table 2, we list the relative errors (compared with the “exact” solution in $L^2$ norm) of the numerical solutions of $u(L, z)$ for different range step sizes. In every case, the transverse operator is discretized by the finite difference method with 200 equidistant nodes, and 20 eigenfunctions are retained in the local base transformation.

Example 5

To further check the validity of our method, in this example, we consider another inhomogeneous waveguide with a refractive-index profile:

$$n^2(x, z) = \begin{cases} 
3.2^2 \left[ 1 - 0.02 e^{\pi/L} \left( \frac{z - 0.5}{2} \right)^2 \right], & 0 \leq z \leq 2.5 \text{ (\mu m)}; \\
3.0^2, & z > 2.5 \text{ (\mu m)}.
\end{cases}$$

Fig. 5. Comparison of optical propagation by the two methods at $x = L$.

Fig. 6. Comparison of optical propagation with different range steps by the new treatment at $x = L$.

| Table 1. Relative Errors for Different Step Sizes by Two Methods |
|-----------------|------|------|------|------|------|
| $b$ (\mu m)     | 5    | 2.5  | 1.25 | 0.625| 0.315|
| AOM             | 3.24e−03| 6.88e−03| 8.87e−03| 5.26e−02| 2.8196|
| New             | 5.21e−13| 1.36e−12| 3.31e−12| 7.32e−12| 1.51e−11|

| Table 2. Relative Errors for Different Range Step Sizes by the New Treatment |
|-----------------|-------|------|------|------|------|
| $b$ (\mu m)     | 1/4   | 1/8  | 1/16 | 1/32 | 1/64 |
| Error           | 8.74e−03| 4.39e−03| 2.04e−03| 8.72e−04| 2.90e−04|
APPENDIX A: DEFINITION AND PROOFS

Definition: The operator $L^\ast(x)$ is called the adjoint operator of $L(x)$ if
\[ \langle L\phi, \psi \rangle = \langle \phi, L^\ast \psi \rangle \quad \text{or} \quad \int_0^{D_1} \overline{\psi} L \phi \, dz = \int_0^{D_1} L^\ast \overline{\psi} \phi \, dz, \]
(A1)

for any $\phi$ and $\psi$ in $L^2(0, D_1)$.

By the definition and integration by parts, we have
\[ \int_0^{D_1} \overline{\psi} L \phi \, dz = \int_0^{D_1} \left( \frac{d}{dz} \left( \frac{1}{s(z)} \frac{d}{dz} \left( \frac{\overline{\phi}}{s(z)} \right) \right) + \kappa^2 \overline{\phi} \right) \phi \, dz \]
\[ + \overline{\psi} \left. \frac{d\phi(z)}{dz} \right|_{0}^{D_1} \phi(z) \left. \frac{d}{dz} \left( \frac{\overline{\phi}(z)}{s(z)} \right) \right|_{0}^{D_1}. \]
(A2)

Using the boundary conditions in Eq. (5) and letting $\overline{\psi}(0) = 0$ and $\overline{L}^0 \overline{\phi}(D_1) = 0$, we get
\[ \overline{L}^\ast \overline{\phi} = \frac{d}{dz} \left( \frac{1}{s(z)} \frac{d}{dz} \left( \frac{\overline{\phi}}{s(z)} \right) \right) + \kappa^2 \overline{\phi}. \]

By Eq. (A3), the eigenfunctions $\{\phi_j(z)\}$ of $L^\ast$ can be obtained easily from $\phi_j(z)$; that is
\[ \overline{\psi}(z) = s(z) \phi_j(z). \]

Proof: Here we give details of the theoretical derivation for Eq. (25). If we look at
\[ \langle L \phi, \psi \rangle = \langle \phi, L^\ast \psi \rangle, \]
(A5)

which means that
\[ \int_0^{D_1} \overline{\psi}(z)Lu(z) \, dz = \int_0^{D_1} u(z)L^\ast \overline{\psi}(z) \, dz. \]
(A6)

Suppose $L$ and $L^\ast$ are discretized as matrices $D$ and $M$, respectively, and $W$ is the weight matrix determined by the numerical quadrature formula. The left and right parts of Eq. (A6) can be approximated by $(WDu, v)$ and $(Wu, Mv)$, respectively, where vectors $u$, $v$ are the discrete version of the functions $u(z)$ and $v(z)$; and $(\cdot, \cdot)$ is the ordinary inner product in Euclidean space.

We have
\[ (WDu, v) = (Wu, Mv) + \epsilon \]
\[ \Rightarrow (Wu, (W^H)^{-1}D^H W^H v) = (Wu, Mv) + \epsilon \]
\[ \Rightarrow (Wu, (W^H)^{-1}D^H W^H v - Mv) = \epsilon. \]

Letting the order $n$ of the matrices tending to infinity, we get
\[ \lim_{n \to \infty} (Wu, (W^H)^{-1}D^H W^H v - Mv) = 0. \]

(A7)

Since $u(z)$ and $v(z)$ are arbitrary functions satisfying the boundary conditions in the Hilbert space, $(W^H)^{-1}D^H W^H$ and $M$ must be two kinds of approximations of the same operator. Letting $\phi$ be the eigenvector of $M$, this means
\[ M\phi = \lambda \phi. \]

(A8)

Since $(W^H)^{-1}D^H W^H$ and $M$ are both differential matrices of the operator $L^\ast$, we have
\[ (W^H)^{-1}D^H W^H \phi \approx \lambda \phi; \]

(A9)
that is
\[ D^H W^H \varphi \approx \lambda W^H \varphi. \quad (A10) \]
Thus,
\[ \xi \approx W^H \varphi, \quad (A11) \]
where \( \xi \) is the eigenvector of \( D^H \).

From
\[ (W \varphi, \varphi) = (\varphi, W^H \varphi), \quad (A12) \]
we have
\[ \int_0^D \bar{\varphi}(z) \varphi(z) \, dz \approx (W \varphi, \varphi) \approx (\varphi, \xi), \quad (A13) \]
where \( \varphi \) is the eigenvector of the matrix \( D \).

**Funding.** National Natural Science Foundation of China (NSFC) (11371319, 91130004); Zhejiang Provincial Natural Science Foundation of China (LY13A010002).

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