

Propagating Modes in Optical Waveguides Terminated by Perfectly Matched Layers

Ya Yan Lu and Jianxin Zhu

Abstract— For numerical simulations of optical waveguides, perfectly matched layers (PMLs) are widely used to truncate the unbounded transverse directions. However, a PML induces some undesired side-effects to the propagating modes in the waveguide. In general, the propagation constant becomes complex, so that the mode may grow or decay exponentially along the waveguide axis. Through a perturbation analysis, we obtain approximate formulas for the propagation constants of PML-terminated planar waveguides.

Index Terms— Optical waveguides, propagating modes, perfectly matched layers, perturbation methods.

I. INTRODUCTION

For numerical simulations of light waves propagating in open optical wave-guiding structures, the perfectly matched layer (PML) [1] is widely used for truncating unbounded domains. While the PML technique was originally developed for time domain problems, its application in frequency domain is particularly simple using the complex coordinate stretching [2], [3] interpretation. The PML technique has been used in the beam propagation method [4], [5] and the eigenmode expansion method [6] for optical waveguide modeling.

A PML of a finite thickness is usually analyzed [1], [7] by its reflection to incident plane waves. For waveguides, a small reflection coefficient of the PML does not guarantee the accuracy of the solution, since the field must propagate a large distance (compared with the wavelength) along the waveguide axis and the small errors induced by the PML may accumulate over the large propagation distance leading to unacceptable solutions.

Although a PML is mostly used in analyzing z -varying wave-guiding structures, such as tapers, bends, Y -branches, waveguide gratings, etc, we believe it is helpful to study the effect of a PML on straight waveguides. A propagating mode in a straight waveguide depends on the waveguide axis z as $e^{i\beta z}$, where β is the real propagation constant. When a PML is used to truncate the transverse variables, β is changed to $\hat{\beta}$. If $\hat{\beta}$ is real, we just have a phase error. However, $\hat{\beta}$ is usually complex. This implies that the propagating mode may blow up or be damped while it propagates along the waveguide axis. Clearly, this side-effect of the PML must be carefully controlled. For that, we need to know how $\hat{\beta}$ depends on the location and the parameters of the PML. Numerical methods can certainly be used to calculate $\hat{\beta}$, but a perturbation result is more convenient, since

it gives an explicit relationship between $\hat{\beta}$ and the PML configuration. We develop perturbation results for planar waveguides terminated by PMLs in the following sections.

II. THE TE CASE

Consider a planar waveguide given by the refractive index profile $n(x)$, where x is the transverse variable and z is the waveguide axis. Away from the waveguide core, we assume that the medium is homogeneous. That is $n(x) = n_1$ if $x < b_1$ and $n(x) = n_2$ if $x > b_2$, for some constants b_1 and b_2 satisfying $b_1 \leq 0 \leq b_2$. A transverse electric (TE) propagating mode is given by $\phi(x)e^{i\beta z}$, where ϕ and β satisfy

$$\frac{d^2\phi}{dx^2} + k_0^2 n^2(x) \phi = \beta^2 \phi, \quad (1)$$

$$\phi(x) \rightarrow 0 \quad \text{as} \quad |x| \rightarrow \infty \quad (2)$$

and k_0 is the free space wavenumber.

To have a PML, we choose c_1, c_2 satisfying $c_1 \leq b_1 < b_2 \leq c_2$ and introduce the new variable

$$\hat{x} = \int_0^x s(\xi) d\xi, \quad s(x) = 1 + i\sigma(x), \quad (3)$$

where σ is a function satisfying $\sigma(x) > 0$ for $x < c_1$ and $x > c_2$, and $\sigma(x) = 0$ otherwise. The requirement of a positive σ in the PML is related to our assumed time dependence of $e^{-i\omega t}$, where ω is the angular frequency.

To obtain an equation for the PML mode $\hat{\phi}e^{i\hat{\beta}z}$, we replace x by \hat{x} in (1). This leads to

$$\frac{1}{s(x)} \frac{d}{dx} \left[\frac{1}{s(x)} \frac{d\hat{\phi}}{dx} \right] + k_0^2 n^2(x) \hat{\phi} = \hat{\beta}^2 \hat{\phi}. \quad (4)$$

The x -axis is truncated at d_1 and d_2 satisfying $d_1 < c_1$ and $c_2 < d_2$. The following simple condition is often used:

$$\hat{\phi} = 0, \quad \text{at} \quad x = d_1 \quad \text{and} \quad d_2. \quad (5)$$

Our perturbation result can be written as

$$\hat{\beta}^2 \approx \beta^2 - \frac{4(\epsilon_1 w_1 v_1 + \epsilon_2 w_2 v_2)}{(b_2 - b_1)^2 (2 + w_1/v_1 + w_2/v_2)}, \quad (6)$$

where w_1, w_2, v_1 and v_2 are dimensionless quantities given by

$$w_j = \frac{(b_2 - b_1)\phi^2(b_j)}{\int_{b_1}^{b_2} \phi^2 dx},$$

$$v_j = (b_2 - b_1)\gamma_j, \quad \gamma_j = \sqrt{\beta^2 - k_0^2 n_j^2},$$

for $j = 1, 2$. Notice that w_j is the ratio between the intensity at b_j and the average intensity in the core ($b_1 < x < b_2$), γ_j is the decay rate of the propagating mode in the homogeneous medium ($x < b_1$ or $x > b_2$), $1/\gamma_j$ is the length scale over which the field decays by a factor of e , and v_j is the ratio between the width of the core and that length scale. The PML parameters are involved in the ϵ_1 and ϵ_2 only. We have

$$\epsilon_1 = e^{2\gamma_1(\hat{d}_1 - b_1)}, \quad \epsilon_2 = e^{-2\gamma_2(\hat{d}_2 - b_2)}, \quad (7)$$

$$\hat{d}_j = \int_0^{d_j} s(x) dx = d_j + i \int_0^{d_j} \sigma(x) dx, \quad (8)$$

for $j = 1, 2$. If we let $\epsilon_j = |\epsilon_j|e^{i\theta_j}$, then

$$|\epsilon_j| = e^{-2\gamma_j|d_j - b_j|}, \quad \theta_j = -2\gamma_j \left| \int_0^{d_j} \sigma(x) dx \right|,$$

for $j = 1, 2$. In terms of $\hat{\beta}$ itself, we have

$$\hat{\beta} \approx \beta - \frac{2(\epsilon_1 w_1 v_1 + \epsilon_2 w_2 v_2)}{\beta(b_2 - b_1)^2(2 + w_1/v_1 + w_2/v_2)}. \quad (9)$$

In particular, the imaginary part of $\hat{\beta}$ is given by

$$\text{Im}(\hat{\beta}) = -\frac{2(|\epsilon_1|w_1v_1 \sin \theta_1 + |\epsilon_2|w_2v_2 \sin \theta_2)}{\beta(b_2 - b_1)^2(2 + w_1/v_1 + w_2/v_2)}.$$

It is clear that $\hat{\beta}$ is usually complex due to the presence of the PML function σ . On the other hand, the size of the perturbation is mainly determined by $|\epsilon_j|$ which does not depend on σ . If the original propagating mode decays slowly in the homogeneous medium n_j , i.e. γ_j is small, we need to use a large $|d_j|$ to reduce the side-effect of the PML. The PML function σ is used to annihilate the radiation modes that propagate to infinity.

To validate our perturbation result, we first consider a symmetric slab waveguide. The width of the core is $0.2 \mu\text{m}$, the refractive index is 3.3 in the core and 3.17 in the cladding. The PMLs correspond to the intervals (d_1, c_1) and (c_2, d_2) , where $d_2 = -d_1 = 2\mu\text{m}$, $c_2 = -c_1 = 1.8 \mu\text{m}$ and $b_2 = -b_1 = 0.1 \mu\text{m}$. The PML function is defined by

$$\sigma(x) = \frac{C_j \tau^3}{1 + \tau^2}, \quad \tau = \frac{x - c_j}{d_j - c_j} \quad (10)$$

for $j = 1, 2$ and a constant $C = C_1 = C_2$. For the free space wavelength $\lambda = 1.55 \mu\text{m}$, the TE mode of the original unbounded waveguide has a real propagation constant $\beta \approx 12.9129687 (\mu\text{m})^{-1}$. When a PML is used, we have a complex propagation constant $\hat{\beta}$. In Table I, we compare the perturba-

TABLE I
EXACT AND APPROXIMATE VALUES OF $\hat{\beta}$.

C	Exact $\hat{\beta}$	Approximate $\hat{\beta}$ by (9)
10	12.911848 + 0.00118 i	12.911860 + 0.00110 i
20	12.913038 + 0.00159 i	12.912955 + 0.00156 i
50	12.914025 - 0.00100 i	12.914097 - 0.00108 i

tion results of $\hat{\beta}$ with the exact results obtained numerically for

a number of different values of C . It is clear that the perturbation results are quite accurate. For $C = 10$, after propagating $100 \mu\text{m}$, the magnitude of the propagating mode will be reduced by about 11%. For $C = 50$, the magnitude will increase by about 10.5%. To reduce the perturbing effect of the PML, we can put the PMLs further away from the core. If the distance between the PMLs and the core is increased by $1 \mu\text{m}$, the magnitude of the mode will change for only about 1% over the distance of $100 \mu\text{m}$.

For another example, we consider a slab waveguide given by $n = 3.3$ in the core (that is, $b_1 < x < b_2$, where $b_2 = -b_1 = 0.4 \mu\text{m}$), $n = 3.17$ in the substrate ($x < b_1$) and $n = 1$ for $x > b_2$. For the TE mode, the exact propagation constant $\beta \approx 13.1089992$. For the PMLs, we choose $d_1 = -1.6 \mu\text{m}$, $c_1 = -1.4 \mu\text{m}$, $c_2 = 0.5 \mu\text{m}$ and $d_2 = 0.65 \mu\text{m}$. The PML function σ is given in (10) with $C_1 = 10$ and $C_2 = 5$. The exact propagation constant of the modified mode is $\hat{\beta} = 13.109132 + 0.00035318 i$. Once again, the perturbation result is quite accurate. Using (9), we obtain $\hat{\beta} \approx 13.109130 + 0.00035343 i$.

III. THE DERIVATION

The perturbation result (6) can be derived in a few simple steps. First, we reduce the linear eigenvalue problems (1,2) and (4,5) to nonlinear eigenvalue problems on the interval (b_1, b_2) . For the original propagating mode, we have

$$\frac{d\phi}{dx}(b_1) = \gamma_1(\mu)\phi(b_1), \quad \frac{d\phi}{dx}(b_2) = -\gamma_2(\mu)\phi(b_2), \quad (11)$$

where $\mu = \beta^2$. In the above, we make explicit the dependence of γ_j on μ . That is, $\gamma_j(\mu) = \sqrt{\mu - k_0^2 n_j^2}$. For x between d_j and b_j , Eq. (4) can be written as $d^2 \hat{\phi}/d\hat{x}^2 = \gamma_j^2(\hat{\mu})\hat{\phi}$, where $\hat{\mu} = \hat{\beta}^2$. We can write down its general solution and let it satisfy the boundary condition (5). This gives rise to

$$\frac{d\hat{\phi}}{dx}(b_1) = q_1(\hat{\mu})\hat{\phi}(b_1), \quad \frac{d\hat{\phi}}{dx}(b_2) = -q_2(\hat{\mu})\hat{\phi}(b_2), \quad (12)$$

where

$$q_j(\hat{\mu}) = \gamma_j(\hat{\mu}) \frac{1 + \epsilon_j(\hat{\mu})}{1 - \epsilon_j(\hat{\mu})}, \quad j = 1, 2.$$

Notice that ϵ_j defined in (7) is a function of μ . Here μ is replaced by $\hat{\mu}$. Equations (1,11) and (4,12) are the nonlinear eigenvalue problems, where ϕ and $\hat{\phi}$ are the eigenfunctions, μ and $\hat{\mu}$ are the eigenvalues.

Based on the nonlinear eigenvalue problems, we can derive an exact relationship between β , $\hat{\beta}$, ϕ and $\hat{\phi}$. Multiplying (1) and (4) by $\hat{\phi}$ and ϕ , respectively, and using integration by part and the boundary conditions (11,12), we obtain

$$(\hat{\mu} - \mu) \int_{b_1}^{b_2} \hat{\phi} \phi dx = \sum_{j=1}^2 [\gamma_j(\mu) - q_j(\hat{\mu})] \hat{\phi}(b_j) \phi(b_j).$$

We can approximately solve $\hat{\mu}$ based on $q_j(\hat{\mu}) \approx q_j(\mu) + (\hat{\mu} - \mu)q'_j(\mu)$. Therefore,

$$(\hat{\mu} - \mu) \left[\int_{b_1}^{b_2} \hat{\phi} \phi dx + \sum_{j=1}^2 q'_j(\mu) \hat{\phi}(b_j) \phi(b_j) \right]$$

$$\approx \sum_{j=1}^2 [\gamma_j(\mu) - q_j(\mu)] \hat{\phi}(b_j) \phi(b_j).$$

To the leading order, we have $\hat{\phi} \approx \phi$. Assuming that ϵ_1 and ϵ_2 are small, we obtain $\gamma_j(\mu) - q_j(\mu) \approx -2\gamma_j(\mu)\epsilon_j(\mu)$ and $q_j'(\mu) \approx \gamma_j'(\mu) = 1/[2\gamma_j(\mu)]$. These further approximations give rise to (6).

IV. EXTENSIONS

In this section, we present perturbation results for a few other cases, include a different boundary condition for the PML, a real coordinate stretching for reducing the side-effects and the corresponding results for the transverse magnetic (TM) case.

As an alternative to the boundary condition (5), we consider

$$\begin{aligned} \frac{1}{s(d_1)} \frac{d\hat{\phi}}{dx}(d_1) &= a_1 \hat{\phi}(d_1), \\ \frac{1}{s(d_2)} \frac{d\hat{\phi}}{dx}(d_2) &= -a_2 \hat{\phi}(d_2), \end{aligned}$$

where a_1 and a_2 are constants. Following the same procedure, we obtain the following perturbation result:

$$\hat{\beta}^2 \approx \beta^2 - \frac{4(\epsilon_1 u_1 w_1 v_1 + \epsilon_2 u_2 w_2 v_2)}{(b_2 - b_1)^2 (2 + w_1/v_1 + w_2/v_2)}, \quad (13)$$

where ϵ_j , w_j and v_j are the same as before and

$$u_j = \frac{a_j - \gamma_j}{a_j + \gamma_j}, \quad \text{for } j = 1, 2.$$

Notice that if $a_j = \gamma_j$, the perturbation term is zero. In fact, we have $\hat{\beta} = \beta$ exactly [8]. Since γ_j depends on β , we can choose the constant a_j to preserve one (but only one) mode. Nevertheless, such a boundary condition can be useful for modeling single-mode waveguides.

If the original propagating mode decays to zero slowly as $|x| \rightarrow \infty$, it is useful to incorporate a real coordinate stretching in (3) [9], [10]. We introduce a function $\delta(x)$ such that $\delta(x) \geq 1$ and define the PML function s by

$$s(x) = \delta(x) + i\sigma(x). \quad (14)$$

The new perturbation results are given as in (6) and (13) with the following modifications:

$$\begin{aligned} \hat{d}_j &= \int_0^{d_j} \delta(x) dx + i \int_0^{d_j} \sigma(x) dx, \\ |\epsilon_j| &= e^{-2\gamma_j} \left| \int_0^{d_j} \delta(x) dx - b_j \right|. \end{aligned}$$

It is clear that the perturbation effect of the PML can be reduced by increasing the real part δ .

The perturbation results of a transverse magnetic (TM) mode can be similarly derived. For the original TM mode $\phi(x)e^{i\beta z}$ and the modified mode $\hat{\phi}(x)e^{i\hat{\beta}z}$, the governing equations are

$$\begin{aligned} n^2(x) \frac{d}{dx} \left[\frac{1}{n^2(x)} \frac{d\phi}{dx} \right] + k_0^2 n^2(x) \phi &= \beta^2 \phi, \quad \text{and} \\ \frac{n^2(x)}{s(x)} \frac{d}{dx} \left[\frac{1}{s(x)n^2(x)} \frac{d\hat{\phi}}{dx} \right] + k_0^2 n^2(x) \hat{\phi} &= \hat{\beta}^2 \hat{\phi}, \end{aligned}$$

respectively. We can derive the following exact integral relationship:

$$(\hat{\mu} - \mu) \int_{b_1}^{b_2} \frac{1}{n^2} \phi \hat{\phi} dx = \sum_{j=1}^2 \frac{1}{n_j^2} [\gamma_j(\mu) - q_j(\hat{\mu})] \phi(b_j) \hat{\phi}(b_j).$$

The final results can still be written as (6) and (13), if we define a new w_j by

$$w_j = \frac{(b_2 - b_1) \phi^2(b_j)}{n_j^2 \int_{b_1}^{b_2} \phi^2/n^2 dx}, \quad \text{for } j = 1, 2.$$

V. CONCLUSIONS

For open wave-guiding structures, the PML technique is widely used for terminating the unbounded transverse directions. Unfortunately, the propagation constant $\hat{\beta}$ of a propagating mode is usually complex when PML is used. The existence of an imaginary part of $\hat{\beta}$ implies that the mode may decay or grow exponentially along the waveguide axis. Although $\text{Im}(\hat{\beta})$ is usually small, it can still be a serious problem, if we have to simulate the propagation over a large distance. The perturbation result developed in this paper reveals the relationship between the PML parameters and the propagation constant. If the original propagating mode decays slowly in an unbounded transverse direction (i.e., γ_j is small), we should use the modified PML (14), otherwise a larger $|d_j|$ is needed to keep the side-effect of the PML under control.

REFERENCES

- [1] J. P. Berenger, "A Perfectly matched layer for the absorption of electromagnetic-waves", *J Comput Phys*, 114(2): 185-200, 1994.
- [2] W. C. Chew and W. H. Weedon, "A 3D perfectly matched medium from modified Maxwells equations with stretched coordinates", *Microwave and Optical Technology Letters*, 7(13): 599-604, 1994.
- [3] C. M. Rappaport, "Perfectly matched absorbing boundary-conditions based on anisotropic lossy mapping of space", *IEEE Microwave and Guided Wave Letters*, 5(3): 90-92, 1995.
- [4] W. P. Huang, C. L. Xu, W. Lui and K. Yokoyama, "The perfectly matched layer (PML) boundary condition for the beam propagation method", *IEEE Photonics Technology Letters*, 8(5): 649-651, May 1996.
- [5] C. Vassallo and F. Collino, "Highly efficient absorbing boundary conditions for the beam propagation method", *Journal of Lightwave Technology*, 14(6): 1570-1577, 1996.
- [6] H. Derudder, D. De Zutter and F. Olyslager, "Analysis of waveguide discontinuities using perfectly matched layers", *Electronics Letters*, 34(22): 2138-2140, 1998.
- [7] D. Yevick D, J. Yu and F. Schmidt, "Analytic studies of absorbing and impedance-matched boundary layers", *IEEE Photonics Technology Letters*, 9(1): 73-75 Jan. 1997
- [8] P. L. Ho and Y. Y. Lu, "A Mode-Preserving Perfectly Matched Layer for Optical Waveguides", *IEEE Photonics Technology Letters*, Vol. 15, No. 9, pp. 1234-1236, Sept. 2003.
- [9] B. Chen, D. G. Fang and B. H. Zhou, "Modified Berenger PML Absorbing boundary-condition for FD-TD meshes", *IEEE Microwave and Guided Wave Letters*, 5(11): 399-401, 1995.
- [10] J. Y. Fang and Z. H. Wu, "Generalized perfectly matched layer - an extension of Berengers perfectly matched layer boundary-condition", *IEEE Microwave and Guided Wave Letters*, 5(12): 451-453, 1995.