Improved Three-Point Formulas Considering the Interface Conditions in the Finite-Difference Analysis of Step-Index Optical Devices

Yih-Peng Chiou, Yen-Chung Chiang, and Hung-Chun Chang, *Member, IEEE, Member, OSA*

***Abstract*—A general relation, considering the interface conditions, between a sampled point and its nearby points is derived. Making use of the derived relation and the generalized Douglas scheme, the three-point formulas in the finite-difference modeling of step-index optical devices are extended to fourth order accuracy irrespective of the existence of the step-index interfaces. With numerical analysis and numerical assessment, several frequently used formulas are investigated.**

***Index Terms*—Finite-difference method, generalized Douglas scheme, step-index optical waveguides.**

I. INTRODUCTION

WITH the rapid progress of computers, in both software and hardware, simulation programs or computer-aided design (CAD) tools for the design of optoelectronic devices have become more and more convenient and important. Among these CAD tools, the finite-difference method (FDM) is one of the most well-known numerical methods, which is widely used in the mode solvers and beam propagation methods (BPM's). Comprehensive reviews can be found in [1] and [2].

Since the differential equations are directly approximated with their corresponding difference equations in the FDM, the efficiency and accuracy of the FDM are greatly affected by its finite-difference (FD) formulas. Various formulations have been proposed to elevate the accuracy and efficiency in the modeling. The simplest FD formula is based on the scalar approximation. Stern [3] derived vectorial formulas based on graded index approximation, in which the dielectric interface conditions between different refractive indexes were matched by means of averaging the permittivity over meshes. As will be shown later, these formulas have $O(h^0)$ truncation errors where h is the grid spacing and $O(h^k)$ denotes that the order is kth power of h. It should be noted that the accuracy is not elevated when finer grid spacings are used. Besides, the interface is required to be in the middle between the sampled points, i.e., $p = q = h/2$ in Fig. 1. If the interface is not in the middle between the sampled points, the truncation errors would be large than $O(h^0)$. Vassallo [4] provided improvement of the FDM for step-index optical waveguides without averaging the permittivity over meshes. The resulting formulas were derived from the Taylor series expansion and from matching of interface conditions, and gave more accurate results. The truncation errors are usually $O(h)$ irrespective of the location of the interface with respect to the sampled points. If the interface is in the middle between the sampled points, then the truncation errors in Vassallo's formulas are $O(h^2)$. Usually, the truncation error of the commonly used three-point FD schemes can only be $O(h^2)$ at best. Formulations with higher order truncation errors can be obtained when higher order terms are retained in the derivation. The generalized Douglas (GD) scheme [5]–[7] was used in the BPM's to increase the accuracy of the FD formulas. The accuracy was elevated to $O(h^4)$ when the medium is homogeneous, i.e., the refractive indexes $n_{i-1} = n_i = n_{i+1}$ in Fig. 1. However, interface conditions were not treated. The accuracy was still $O(h^2)$ at best and was reduced to $O(h)$ when the interface is not in the middle between the sampled points or the discretization is nonuniform [7], i.e., $p \neq q$ or $h_- \neq h_+$ in Fig. 1. Yamauchi *et al.* [8] derived formulas under nonuniform discretization for the GD scheme and improved Vassallo's formulas to $O(h^2)$ accuracy irrespective of the location of the interface by means of evaluating higher order terms through the BPM. The above derivations all placed the interface between the sampled points. Lüsse *et al.* [9] derived another formulation by placing the interfaces exactly at the sampled points, i.e., $p = 0$ in Fig. 1. Hadley [10] derived quasifourth order equations by taking the interface conditions and nonuniformity of grid spacings into consideration. The higher order terms were evaluated through the BPM and a complicated averaging operator.

In this paper, formulas similar to Vassallo's [4] are derived simply by the Taylor series expansion and matching the interface conditions. The interfaces need not be located exactly at the sampled points, that is, they can be placed at the grids or elsewhere. Higher order terms are retained and the GD scheme is adopted. It is also found that higher order terms are not necessarily evaluated through the BPM and the complicated averaging operator as in [8] and [10], but they can be included in a more general and simple algebraic form. The resulting eigenvalue problems can be solved directly and efficiently, instead

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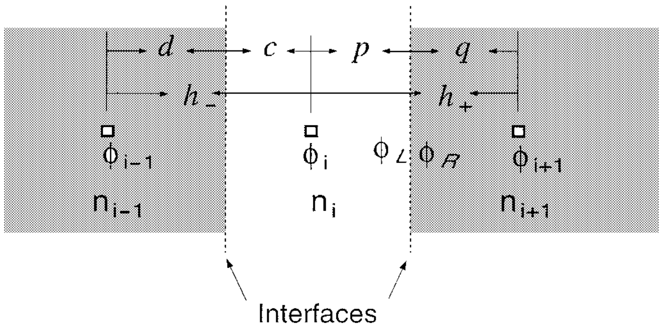

Fig. 1. Sketch of interfaces between sampled points.

of indirectly and inefficiently using the BPM. The derived formulas can also be applied to the BPM with little extra computation efforts, compared with the computation in the eigenvalue problem, in finding the coefficients.

Several formulations are derived in Section II, followed by a description of numerical implementation in Section III. In Section IV the formulation is assessed and applications to modal solutions for slab waveguides and multiple-quantum-well waveguides are numerically demonstrated. Section V gives the conclusion.

II. Formulation

A general relation between the sampled field ϕ_i and the fields nearby $\phi_{i\pm 1}$ as shown in Fig. 1 is derived in this section. It is found that Stern's [3] and Vassallo's [4] formulations are lower order cases of our derived formulation. Retaining the higher order terms and making use of the GD scheme, the truncation error of our formulation can be extended to $O(h^4)$ irrespective of the existence of the interfaces.

A. General Formulation Considering the Interface Conditions

Consider the magnetic field ϕ_i at a sampled point and the fields nearby, ϕ_{i-1} and ϕ_{i+1}, as shown in Fig. 1, where ϕ_L and ϕ_R represent fields at just to the left and just to the right sides of the interface, respectively. Using the Taylor series expansion, ϕ_L is expressed as

$$\begin{aligned}\phi_L &= \phi_i + \frac{p}{1!}\,\frac{\partial \phi_i}{\partial x} + \frac{p^2}{2!}\,\frac{\partial^2 \phi_i}{\partial x^2} + \frac{p^3}{3!}\,\frac{\partial^3 \phi_i}{\partial x^3} \\ &\quad + \cdots + \frac{p^j}{j!}\,\frac{\partial^j \phi_i}{\partial x^j} + \cdots \\ &= \sum_{j=0}^{\infty} \frac{p^j}{j!}\,\frac{\partial^j \phi_i}{\partial x^j}. \end{aligned} \tag{1}$$

When (1) is differentiated m times successively and multiplied with p^m, we can express the derivatives of ϕ_L in terms of the derivatives of ϕ_i as

$$p^m \frac{\partial^m \phi_L}{\partial x^m} = \sum_{j=0}^{\infty} \frac{p^{m+j}}{j!}\,\frac{\partial^{m+j}\phi_i}{\partial x^{m+j}}. \tag{2}$$

When the first s terms are retained in (1) and higher order terms (H.O.T.) are ignored, we have

$$p^m \frac{\partial^m \phi_L}{\partial x^m} = \sum_{j=0}^{s-m-1} \frac{p^{m+j}}{j!}\,\frac{\partial^{m+j}\phi_i}{\partial x^{m+j}} + O(h^s). \tag{3}$$

Equation (3) can be rewritten in a matrix form as

$$\begin{bmatrix} \phi_L \\ p\phi_L' \\ p^2\phi_L'' \\ p^3\phi_L^{(3)} \\ \vdots \\ p^s\phi_L^{(s-1)} \end{bmatrix} = \begin{bmatrix} 1 & \frac{1}{1!} & \frac{1}{2!} & \frac{1}{3!} & \cdots & \frac{1}{s!} \\ 0 & 1 & \frac{1}{1!} & \frac{1}{2!} & \cdots & \frac{1}{(s-1)!} \\ 0 & 0 & 1 & \frac{1}{1!} & \cdots & \frac{1}{(s-2)!} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \phi_i \\ p\phi_i' \\ p^2\phi_i'' \\ p^3\phi_i^{(3)} \\ \vdots \\ p^s\phi_i^{(s-1)} \end{bmatrix} + O(h^s) \tag{4}$$

or denoted as

$$\overline{\phi}_L = \overline{\overline{M}}_{Li} \cdot \overline{\phi}_i + O(h^s) \tag{5}$$

where ϕ' and ϕ'' denote the first and second derivatives, respectively, and $\phi^{(j)}$ denotes the jth derivative. Similarly, ϕ_{i+1} and its derivatives can be expressed in terms of ϕ_R and its derivatives as

$$q^m \frac{\partial^m \phi_{i+1}}{\partial x^m} = \sum_{j=0}^{s-m-1} \frac{q^{m+j}}{j!}\,\frac{\partial^{m+j}\phi_R}{\partial x^{m+j}} + O(h^s) \tag{6}$$

or denoted as

$$\overline{\phi}_{i+1} = \overline{\overline{M}}_{+R} \cdot \overline{\phi}_R + O(h^s). \tag{7}$$

The interface conditions require that

$$\phi_R = \phi_L \tag{8}$$

$$\phi_R' = \theta \phi_L' \tag{9}$$

where

$$\theta = \begin{cases} 1, & \text{for transverse electric (TE) case} \\ n_{i+1}^2/n_i^2, & \text{for transverse magnetic (TM) case.} \end{cases} \tag{10}$$

Making use of the Helmholtz equation, the relation between the higher order derivatives of ϕ_R and ϕ_L can be obtained. The Helmholtz equation for ϕ is

$$\beta^2 \phi = \left(\frac{\partial^2}{\partial x^2} + k_0^2 n^2\right)\phi \tag{11}$$

where β is the propagation constant, k_0 is the wave number in free space, and n is the refractive index. From (8) and (11), we have

$$\left(\frac{\partial^2}{\partial x^2}+k_0^2 n_{i+1}^2\right)\phi_R=\left(\frac{\partial^2}{\partial x^2}+k_0^2 n_i^2\right)\phi_L \tag{12}$$

or

$$\phi_R^{''}=\phi_L^{''}+\eta\phi_L \tag{13}$$

where $\eta = k_0^2(n_i^2 - n_{i+1}^2)$ and n_i and n_{i+1} are the refractive indexes of two adjacent regions, as shown in Fig. 1. Repeating the similar process successively, higher order derivatives of ϕ_R can be expressed in terms of ϕ_L and its derivatives as

$$\phi_R^{(3)}=\theta\phi_L^{(3)}+\theta\eta\phi_L^{'} \tag{14}$$

$$\phi_R^{(4)}=\phi_L^{(4)}+2\eta\phi_L^{''}+\eta^2\phi_L \tag{15}$$

$$\phi_R^{(5)}=\theta(\phi_L^{(5)}+2\eta\phi_L^{(3)}+\eta^2\phi_L^{'}) \tag{16}$$

$$\vdots$$

or denoted as

$$\overline{\phi}_R=\overline{\overline{M}}_{RL}\cdot\overline{\phi}_L. \tag{17}$$

From (5), (7), and (17), ϕ_{i+1} and its derivatives can be expressed in terms of ϕ_i and its derivatives as

$$\begin{aligned}\overline{\phi}_{i+1}&=\overline{\overline{M}}_{+R}\cdot\overline{\overline{M}}_{RL}\cdot\overline{\overline{M}}_{Li}\cdot\overline{\phi}_i+O(h^s)\\&\equiv\overline{\overline{M}}_{+}\cdot\overline{\phi}_i+O(h^s)\end{aligned} \tag{18}$$

where

$$\overline{\overline{M}}_{+}=\overline{\overline{M}}_{+R}\cdot\overline{\overline{M}}_{RL}\cdot\overline{\overline{M}}_{Li}. \tag{19}$$

Note that (17) is exact without any truncation error while (5) and (7) have $O(h^s)$ truncation errors, which reveals that the truncation errors will not increase with the interface conditions being included and that the truncation errors are from the neglect of higher order terms of the Taylor series expansions. Also, when (17) is multiplied with 1/θ, we have the E-field formulation, which reveals that the E-field and the H-field formulations are equivalent, and the accuracy and efficiency are the same for these two formulations.

The relations between the above-mentioned fields can be illustrated as

$$\phi_{i+1}\underset{\overline{\overline{M}}_{+R}}{\overset{\mathrm{TSE}}{\longleftrightarrow}}\phi_R\underset{\overline{\overline{M}}_{RL}}{\overset{\mathrm{MBC}}{\longleftrightarrow}}\phi_L\underset{\overline{\overline{M}}_{Li}}{\overset{\mathrm{TSE}}{\longleftrightarrow}}\phi_i \tag{20}$$

where TSE denotes *Taylor Series Expansion* and MBC denotes *Matching the Boundary Condition*. Similarly, ϕ_{i-1} and its derivatives can be expressed in terms of ϕ_i and its derivatives as

$$\overline{\phi}_{i-1}=\overline{\overline{M}}_{-}\cdot\overline{\phi}_i+O(h^s). \tag{21}$$

Considering the first rows of $\overline{\overline{M}}_{\pm}$, we have

$$\phi_{i\pm1}=\overline{V}_{\pm}\cdot\overline{\phi}_i+O(h^s) \tag{22}$$

where $\overline{V}_+$ and $\overline{V}_-$ are the first rows of $\overline{\overline{M}}_+$ and $\overline{\overline{M}}_-$, respectively.

B. Scalar Approximation and Graded-Index Approximation

The simplest three point formula is based on the scalar approximation, and the vectorial nature is ignored. The second derivative is the same as that in a homogeneous medium and is expressed as

$$\phi_i^{''}\approx\frac{2h_+\phi_{i-1}-2(h_-+h_+)\phi_i+2h_-\phi_{i+1}}{h_-h_+(h_-+h_+)} \tag{23}$$

and reduced to

$$\phi_i^{''}\approx\frac{\phi_{i-1}-2\phi_i+\phi_{i+1}}{h^2} \tag{24}$$

when the grid spacing is uniform $(h=h_-=h_+)$. Equations (23) and (24) are good approximations when the index contrast is low but fail when the index contrast is high. Besides, the vectorial nature is not included.

Stern [3] derived a vectorial formulation and similar formulation can be derived from the graded-index approximation, which was frequently used later in the optical waveguide simulation [11]–[13]. In their derivation, $h_- = h_+ \equiv h$, $p = q = h/2$, $s = 2$, and the second derivatives are assumed to be continuous. Thus, the formulation is the same as (24) for TE cases and

$$\begin{aligned}\phi_i^{''}\approx&\frac{2n_i^2}{(n_{i-1}^2+n_i^2)h^2}\phi_{i-1}\\&-\left(\frac{2n_i^2}{(n_{i-1}^2+n_i^2)h^2}+\frac{2n_i^2}{(n_{i+1}^2+n_i^2)h^2}\right)\phi_i\\&+\frac{2n_i^2}{(n_{i+1}^2+n_i^2)h^2}\phi_{i+1}\end{aligned} \tag{25}$$

for TM cases. Since the second derivatives are assumed to be continuous, the truncation error in (22) is $O(h^2)$ for $s = 2$ and thus the truncation errors of (24) and (25) are $O(h^2)/h^2 = O(h^0)$, which means that the truncation errors would not decrease with the grid size with the existence of the interfaces. Equations (24) and (25) may be a good approximation in the modeling of structures with graded index or low index contrast but they are not suitable in the modeling of step-index structures.

C. Improved Formulation with $O(h^2)$ Truncation Errors

Vassallo [4] derived an improved formulation by making use of the Helmholtz equation. Equivalently, $s = 4$ in the derivation. From (22), we have

$$\phi_{i-1}=a_0\phi_i+a_1\phi_i^{'}+a_2\phi_i^{''}+a_3\phi_i^{(3)}+O(h^4) \tag{26}$$

$$\phi_{i+1}=b_0\phi_i+b_1\phi_i^{'}+b_2\phi_i^{''}+b_3\phi_i^{(3)}+O(h^4) \tag{27}$$

where the coefficients a_j's and b_j's are $O(h^j)$ and are given in the Appendix. $\phi_i^{''}$ is obtained by ignoring $\phi_i^{(3)}$ and eliminating $\phi_i^{'}$

$$\phi_i^{''} \approx \frac{b_1\phi_{i-1} + (b_0\, a_1 - a_0\, b_1)\phi_i - a_1\phi_{i+1}}{a_2\, b_1 - b_2\, a_1}. \tag{28}$$

Since the coefficients of $\phi_i^{''}$ and $\phi_i^{(3)}$ are $O(h^2)$ and $O(h^3)$, respectively, the approximation in (28) is $O(h^3)/h^2 = O(h)$. Interestingly, when

$$h_- = h_+ = h \tag{29}$$

and

$$p = 0, \quad p = h, \quad \text{or} \quad p = q = h/2 \tag{30}$$

the coefficients would have such relation $a_3 = (h^3/3!)a_1 + O(h^4)$ and $b_3 = (h^3/3!)b_1 + O(h^4)$, as shown in the Appendix. Eliminating $\phi_i^{'}$ would result in eliminating $\phi_i^{(3)}$ simultaneously and the approximation in (28) is thus $O(h^4)/h^2 = O(h^2)$.

D. Improved Formulation of Higher Order Accuracy

In this subsection the improved formulation is derived based on the GD scheme. Again, $\phi_{i\pm1}$ can be expressed in terms of ϕ_i and its derivatives as

$$\begin{aligned}\phi_{i-1} &= e_0\phi_i + e_1\phi_i^{'} + e_2\phi_i^{''} \\ &\quad + e_3\phi_i^{(3)} + e_4\phi_i^{(4)} + e_5\phi_i^{(5)} + O(h^6)\end{aligned} \tag{31}$$

$$\begin{aligned}\phi_{i+1} &= f_0\phi_i + f_1\phi_i^{'} + f_2\phi_i^{''} \\ &\quad + f_3\phi_i^{(3)} + f_4\phi_i^{(4)} + f_5\phi_i^{(5)} + O(h^6)\end{aligned} \tag{32}$$

where the coefficients e_j's and f_j's are $O(h^j)$ and given in the Appendix. If the higher order terms containing $\phi_i^{(3)}$, $\phi_i^{(4)}$, and $\phi_i^{(5)}$ in (31) and (32) are ignored, then $\phi_i^{'}$ and $\phi_i^{''}$ can be solved as

$$\begin{aligned}\phi_i^{'} &\approx \frac{f_2\phi_{i-1} + (f_0\, e_2 - e_0\, f_2)\phi_i - e_2\phi_{i+1}}{e_1\, f_2 - f_2\, e_1} \\ &= s_-\phi_{i-1} + s_0\phi_i + s_+\phi_{i+1} \\ &\equiv D_x\phi_i\end{aligned} \tag{33}$$

$$\begin{aligned}\phi_i^{''} &\approx \frac{f_1\phi_{i-1} + (f_0\, e_1 - e_0\, f_1)\phi_i - e_1\phi_{i+1}}{e_2\, f_1 - f_2\, e_1} \\ &= t_-\phi_{i-1} + t_0\phi_i + t_+\phi_{i+1} \\ &\equiv D_x^2\phi_i.\end{aligned} \tag{34}$$

Following the procedure in Section II-C, it can be found that, usually, $\phi_i^{'} = D_x\phi_i + O(h^2)$ and $\phi_i^{''} = D_x^2\phi_i + O(h)$. Also, $\phi_i^{''} = D_x^2\phi_i + O(h^2)$ when (29) and (30) are satisfied. Eliminating $\phi_i^{'}$ in (31) and (32) by the linear combination $((31)\, f_1 - (32)\, e_1)/(e_2\, f_1 - f_2\, e_1)$, we have (35) shown at the bottom of the page or denoted as

$$\begin{aligned}D_x^2\phi_i &= t_-\phi_{i-1} + t_0\phi_i + t_+\phi_{i+1} \\ &= \left(1 + g_1\frac{\partial}{\partial x} + g_2\frac{\partial^2}{\partial x^2} + g_3\frac{\partial^3}{\partial x^3}\right)\phi_i^{''} + O(h^4)\end{aligned} \tag{36}$$

which is approximated with

$$D_x^2\phi_i \approx (1 + g_1\, D_x + g_2\, D_x^2)\phi_i^{''} \tag{37}$$

or

$$\phi_i^{''} \approx \frac{D_x^2\phi_i}{1 + g_1\, D_x + g_2\, D_x^2}. \tag{38}$$

Since g_j is $O(h^{j+2}/h^2) = O(h^j)$, $\partial/\partial x = D_x + O(h^2)$, and $\partial^2/\partial^2 x = D_x^2 + O(h)$, the approximation in (37) and (38) are, at worst, $O(h^3)$. Similarly, when (29) and (30) are satisfied, the coefficients would have such relation $e_5 = (h^5/5!)e_1 + O(h^6)$ and $f_5 = (h^5/5!)f_1 + O(h^6)$, as shown in the Appendix. Eliminating $\phi_i^{'}$ would result in eliminating $\phi_i^{(5)}$ simultaneously. Besides, $\partial/\partial x = D_x + O(h^2)$, $\partial^2/\partial x^2 = D_x^2 + O(h^2)$, and g_1 and g_2 are $O(h^2)$. Therefore, formulas with $O(h^4)$ accuracy is obtained when (29) and (30) are satisfied.

III. Implementation

Substituting (38) into the Helmholtz equation

$$\phi^{''} + k_0^2 n^2\phi = \beta^2\phi \tag{39}$$

leads to

$$\frac{D_x^2\phi_i}{1 + g_1\, D_x + g_2\, D_x^2} + k_0^2 n^2\phi_i = \beta^2\phi_i \tag{40}$$

or

$$\begin{aligned}D_x^2\phi_i &+ k_0^2 n^2(1 + g_1\, D_x + g_2\, D_x^2)\phi_i \\ &= \beta^2(1 + g_1\, D_x + g_2\, D_x^2)\phi_i.\end{aligned} \tag{41}$$

Combining all sampled points together from (41), we have an algebraic equation

$$[\mathbf{A} + k_0^2\mathbf{N}^2(\mathbf{C} - \mathbf{I})]\boldsymbol{\Phi} = \beta^2\mathbf{C}\boldsymbol{\Phi} \tag{42}$$

or denoted as

$$\mathbf{A}^{'}\boldsymbol{\Phi} = \beta^2\mathbf{C}\boldsymbol{\Phi} \tag{43}$$

$$\begin{aligned}&\frac{f_1\phi_{i-1} + (f_0\, e_1 - e_0\, f_1)\phi_i - e_1\phi_{i+1}}{e_2\, f_1 - f_2\, e_1} \\ &\quad = \phi_i^{''} + \frac{(f_3\, e_1 - e_3\, f_1)\phi_i^{(3)} + (f_4\, e_1 - e_4\, f_1)\phi_i^{(4)} + (f_5\, e_1 - e_5\, f_1)\phi_i^{(5)}}{e_2\, f_1 - f_2\, e_1} + O(h^4)\end{aligned} \tag{35}$$

where $\mathbf{A}' = \mathbf{A} + k_0^2\mathbf{N}^2(\mathbf{C}-\mathbf{I}), \mathbf{N}^2 = \mathrm{diag}(n_1^2, n_2^2, \cdots n_j^2, \cdots)$, $\mathbf{A}$ results from the operator $D_x^2 + k_0^2 n^2$, $\mathbf{C}$ results from the operator $(1 + g_1 D_x + g_2 D_x^2)$, and $\mathbf{I}$ is an identity matrix. The matrices $\mathbf{A}$, $\mathbf{C}$, and $\mathbf{A}'$ are all tridiagonal. Note that when the GD scheme is not adopted, $\mathbf{C} = \mathbf{I}$ and the formulation reduces to Vassallo's [4]. The eigenvalue problem in (43) can be solved efficiently with the shifted-inverse power method [14].

Substituting β^2 with $\partial^2/\partial z^2$ in (41) and assuming the envelope approximation $\phi = \Phi \exp(-jk_0\overline{n}z)$, where $\overline{n}$ is the reference refractive index, we have

$$D_x^2\Phi_i + k_0^2 n^2(1 + g_1 D_x + g_2 D_x^2)\Phi_i = \left(\frac{\partial^2}{\partial z^2} - 2jk_0\overline{n}\frac{\partial}{\partial z} - k_0^2\overline{n}^2\right) \cdot (1 + g_1 D_x + g_2 D_x^2)\Phi_i. \quad (44)$$

This formulation can also be applied to the beam propagation method directly as described in [7] and [8].

IV. Numerical Results

A. Assessment of the Formulation

The investigated structure is a symmetric slab waveguide. The core and cladding indexes are $n_{\mathrm{core}} = 3.3704$ and $n_{\mathrm{clad}} = 3.2874$ for GaAs and $Ga_{0.82}Al_{0.18}As$, respectively. The waveguide width is $D = 2$ μm and the wavelength is $\lambda = 1.55$ μm. The effective index for the TE mode of this waveguide is $n_{\mathrm{eff}} = 3.35795671005961$, and the transverse wave numbers in the core and cladding are $k_x/k_0 = \sqrt{n_{\mathrm{core}}^2 - n_{\mathrm{eff}}^2} = 0.28896709041585$ and $\alpha_x/k_0 = \sqrt{n_{\mathrm{eff}}^2 - n_{\mathrm{clad}}^2} = 0.68457874579999$, respectively. In the assessment of the formulation the magnitudes of the fields, ϕ_i and $\phi_{i\pm1}$ are assigned with exact values and then k_x or α_x are evaluated using (24), (25), (28), and (38). For example

$$\tau_{\mathrm{calculated}} = \frac{D_x^2\phi_i}{(1 + g_1 D_x + g_2 D_x^2)\phi_i} \quad (45)$$

for our formulation, where $\tau = -k_x^2$ in the core region and $\tau = \alpha_x^2$ in the cladding region. The relative error in the transverse wave number is defined as

$$\epsilon_{k_x} = \left|\frac{k_{x,\,\mathrm{calculated}} - k_{x,\,\mathrm{exact}}}{k_0(n_{\mathrm{core}} - n_{\mathrm{clad}})}\right| \quad (46)$$

in the core region, or

$$\epsilon_{\alpha_x} = \left|\frac{\alpha_{x,\,\mathrm{calculated}} - \alpha_{x,\,\mathrm{exact}}}{k_0(n_{\mathrm{core}} - n_{\mathrm{clad}})}\right| \quad (47)$$

in the cladding region.

Fig. 2 shows ϵ_{k_x} for the TE case with respect to the grid size for uniform grids, i.e., $n_{i-1} = n_i = n_{i+1} = n_{\mathrm{core}}$ and $h_- = h_+ = h$ in Fig. 1, where 3pt. denotes that three-point formulation is adopted and 5pt. formulation is adopted. All the sampled points are in the core region. It can be seen that the slopes are two and four for $O(h^2)$ and $O(h^4)$ formulations, respectively. Note that ϵ_{k_x} calculated using the five-point scheme is slightly larger than that calculated using the $O(h^4)$ three-point scheme. ϵ_{α_x} in the cladding region is of the same order as ϵ_{k_x} (not shown). The truncation error of our formulation is exactly

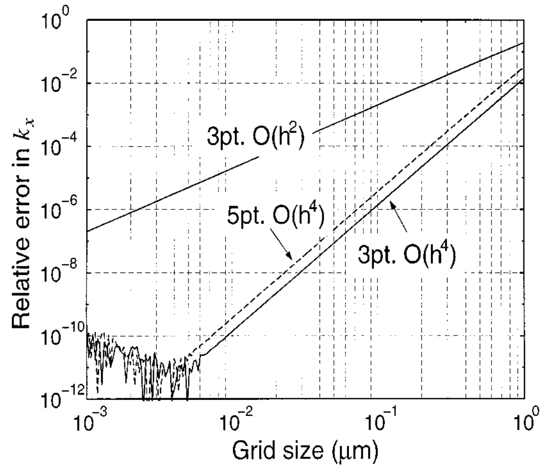

Fig. 2. Relative error in the transverse wave number with respect to the grid size: uniform grid size.

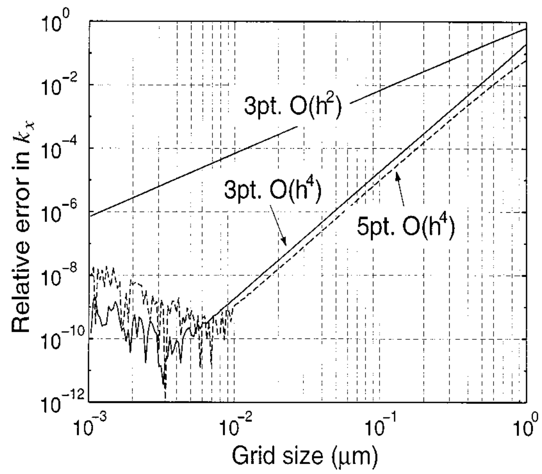

Fig. 3. Relative error in the transverse wave number with respect to the grid size: nonuniform grid size.

$O(h^4)$. The distorted behavior of ϵ_{k_x} for $\Delta x < 7 \times 10^{-3}$ is due to finite digits in the computer.

Fig. 3 shows the relative error with respect to the average grid size for nonuniform grids, i.e., $n_{i-1} = n_i = n_{i+1} = n_{\mathrm{core}}$ and $h_- \neq h_+$ in Fig. 1. The three sampled points again are all in the core region. The average grid size is defined as

$$\Delta x = \frac{h_- + h_+}{2} = h_+ \frac{1 + R}{2} \quad (48)$$

where the ratio $R = 20$ in this case. ϵ_{k_x} is larger than that in the case of uniform grids, but still behaves as $O(h^4)$. It can be seen that ϵ_{k_x} calculated using the five-point scheme is slightly smaller than that calculated using the $O(h^4)$ three-point scheme. ϵ_{α_x} in the cladding region is again of the same order as ϵ_{k_x}.

Fig. 4 shows the relative error with respect to the grid size for an interface lying between sampled points, that is, $n_{i-1} = n_i = n_{\mathrm{core}}$, $n_{i+1} = n_{\mathrm{clad}}$, $h_- = h_+ = h$ and $p = q = h/2$ in Fig. 1. It can be seen that the truncation error of our formulation is also $O(h^4)$ even if the interfaces exist. The accuracy of our formulation is close to that of the uniform grid size as shown in Fig. 2. The transverse wave vector cannot be well approximated using the graded-index approximation whose truncation error is

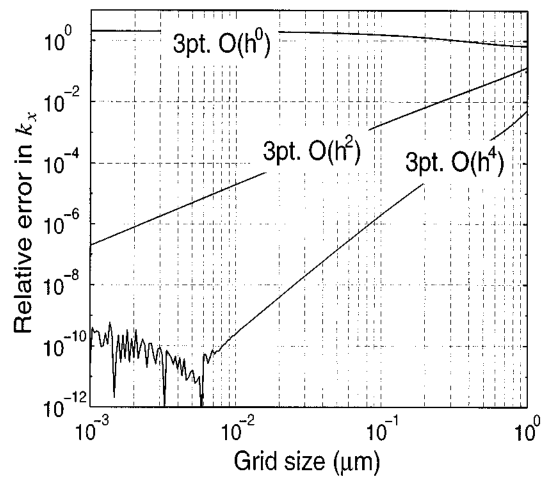

Fig. 4. Relative error in the transverse wave number with respect to the grid size: interfaces lying between sampled points.

only $O(h^0)$ and cannot be reduced with smaller grid size due to the existence of the interface.

As shown in Figs. 2–4, the accuracy is greatly enhanced when higher-order formulation is adopted. Or on the other side, the efficiency is elevated because coarser grids can be used. For example, the grid size of the $O(h^4)$ formulation can be about ten times larger that of the $O(h^2)$ formulation at $\epsilon_{k_x} = 10^{-4}$. All the above results are for TE cases. The TM cases have also been assessed, the results being close to those for the TE cases for the same parameters.

From the above assessment of the numerical error, the derivation in Section II is confirmed and the truncation error of our derived formulation is indeed $O(h^4)$. We have applied the derived formulation to various parameters, which also validates our derivation.

B. Application to Mode Solvers: Slab Waveguides

First, a weakly guiding waveguide is investigated. The structure is the same as that considered in [10]. The wavelength is 1.55 μm and the waveguide width is $D = 2$ μm. The core and cladding relative permittivities are $n_{\rm core}^2 = 11.088$ and $n_{\rm clad} = 11.044$, respectively. The exact effective index is $n_{\rm eff,\,exact} = 3.32578847351789$. The transparent boundary condition [15] is adopted.

Fig. 5(a) and (b) shows the field profiles calculated using the $O(h^4)$ formulation for large grid sizes $\Delta x = 2$ and 1 μm, respectively. The solid curves are the analytical field profiles and the circles are the results calculated using our formulation. The numerical effective indexes are $n_{\rm eff,\,calculated} = 3.32581388171437$ and 3.32578998973725 for $\Delta x = 2$ and 1 μm, respectively. In this case the propagation constant and the modal profile can be calculated accurate to four digits even though only one sampled point is placed in the core. It seems that our formulation may be more "economic" than that of Hadley's [10] which requires a sampled point at the each interface. Our results are accurate to the same order as those of [10] with slightly smaller error when the grid sizes are the same.

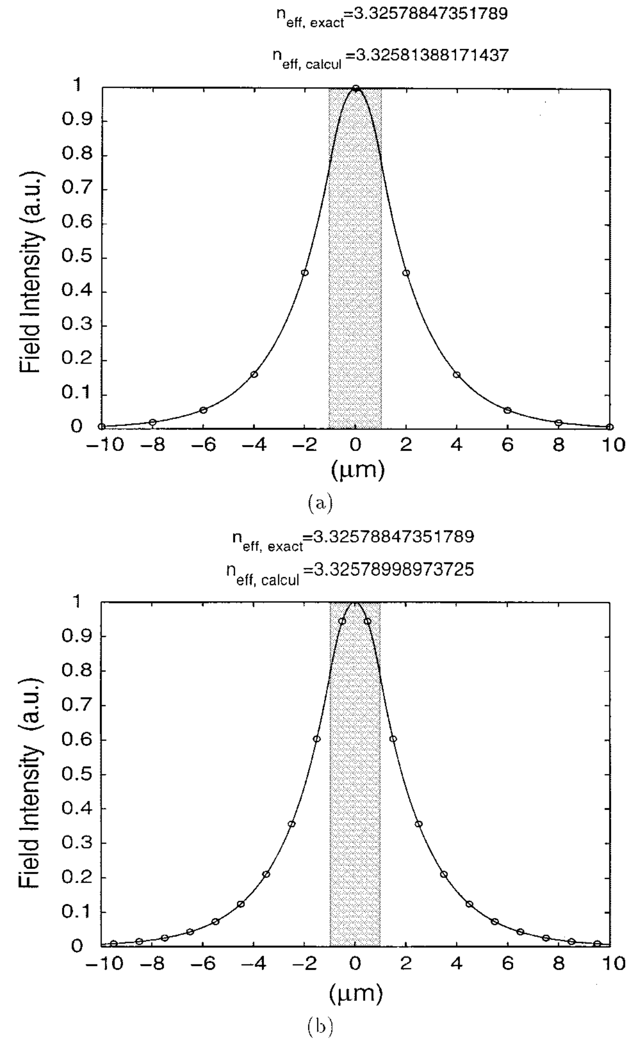

Fig. 5. Field profiles for grid size Δx = (a) 2 μm and (b) 1 μm.

Fig. 6 shows the relative error in the reduced propagation constant with respect to the grid size. The reduced propagation constant is defined as [10]

$$\tilde{n} = \frac{n_{\rm eff} - n_{\rm clad}}{n_{\rm core} - n_{\rm clad}}. \tag{49}$$

The dashed curve is calculated using an $O(h^0)$ scheme across the interface and an $O(h^2)$ scheme elsewhere. It can be seen that such rough approximation yields worse results for large grid sizes, while the effect of inaccurate sampled points near the interface is less weighted due to much more $O(h^2)$ sampled points for small grid sizes. If the interface conditions are considered, the results become better for large grid sizes. It can be seen that the truncation error of our formulation is indeed $O(h^4)$. The grid size with $O(h^4)$ truncation errors can be ten times larger or more than that with $O(h^2)$ truncation errors, resulting in great reduction of the computation effort.

C. Application to Mode Solvers: Multiple-Quantum-Well Waveguides

The modal characteristics of multiple-quantum-well (MQW) optical waveguides have attracted considerable attention because of their distinctive features and potential applications in

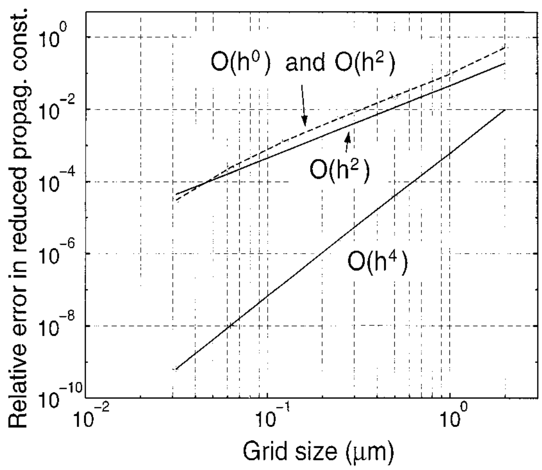

Fig. 6. Relative error in the reduced propagation constant with respect to the grid size for different three-point formulations.

photonic devices. Unfortunately, those complicated structures are difficult to analyze using conventional FD techniques since the refractive index varies significantly and the widths of wells and barriers are very small and usually not uniform. The equivalent index methods [16] or the finite element methods [17] are often employed. The situation changes when the formulation of high accuracy is applied. The grid size is much more flexible and the accuracy can be much higher than those of conventional FD schemes.

The modal characteristics of a complicated MQW waveguide is investigated to show the excellent performance of our formulation. Fig. 7 shows the index distribution. The wavelength is $\lambda = 1.55$ μm, and the widths of wells and barriers are $D_{\text{well}} = 0.007$ μm and $D_{\text{barr}} = 0.012$ μm, respectively. The refractive indexes of the wells, barriers, and claddings are $n_{\text{well}} = 3.3704$, $n_{\text{barr}} = 3.2874$, and $n_{\text{clad}} = 3.2224$ for GaAs, $Ga_{0.82}Al_{0.18}As$, and $Ga_{0.68}Al_{0.32}As$, respectively. There are 55 wells and 56 barriers in the MQW structure. The exact effective propagation constants are $n_{\text{eff, exact}} = 3.28736376034$ and 3.28552369073 for TE and TM modes, respectively. Only one sampled point is placed at the center of each well or barrier. The grid size is 0.0095 μm in the MQW region and 0.01 μm in the cladding region. Fig. 8 shows the calculated field distribution which is indistinguishable from the analytical one. The calculated effective propagation constants are $n_{\text{eff, calculated}} = 3.28736376027$ and 3.28552369081 for TE and TM modes, respectively, which are both correct to ten digits even nonuniform grid sizes are used under such strongly guiding structure.

V. Conclusion

We have derived improved three-point formula for the finite-difference analysis of step-index optical waveguides. A general relation is derived from the Taylor series expansion and matching the interface conditions. From the relation, the truncation errors are not from matching the boundary conditions but from the truncation of the higher order terms in the Taylor series expansion. Also, the E-field and the H-field formulations are actually equivalent. Making use of the the general relation and the Generalized Douglas scheme the improved formulation is derived. It is found that the frequently adopted formulations of Stern's [3] and Vassallo's [4] are lower-order cases of our derived formulation.

We have assessed the frequently used formulations and our derived formulation for various parameters. Our formulation is indeed $O(h^4)$ in the uniform discretization cases irrespective of the existence of the interfaces. The graded-index approximation

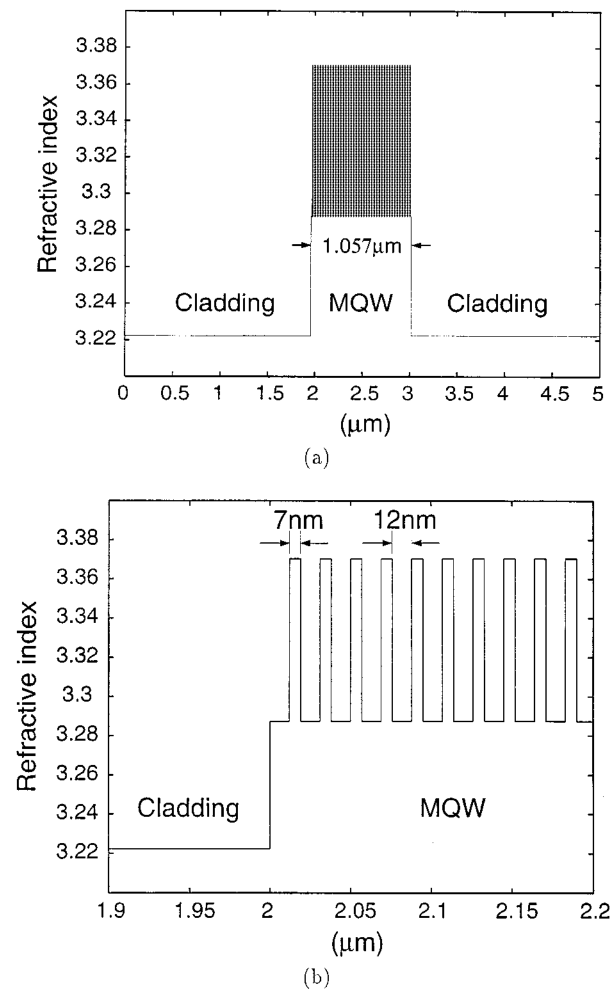

Fig. 7. Refractive index profile of the investigated MQW optical waveguide.

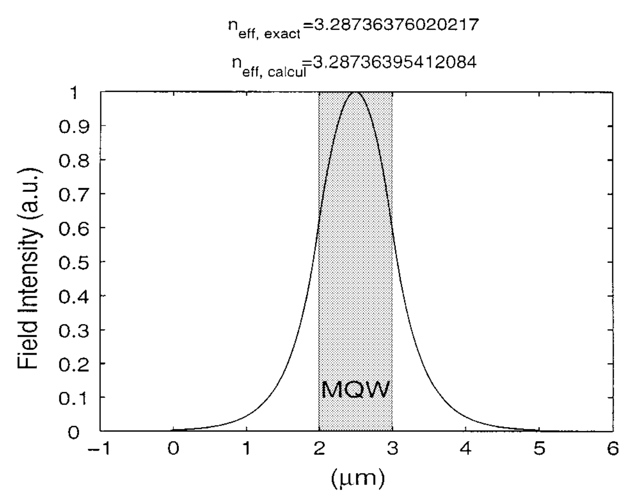

Fig. 8. Field profile in the MQW optical waveguide.

is not suitable for cases with high refractive index contrast ratio since the accuracy is only $O(h^0)$. When the discretization is nonuniform, the accuracy is reduced, especially in cases with high refractive contrast ratio.

The improved formulation has been applied to the mode solver of slab waveguides and multiquantum waveguides, which shows its preference in accuracy and efficiency. The derived formulation can be applied not only to the analysis of optical waveguides, but also to other electromagnetic simulations for structures with step index.

APPENDIX

The parameters b_j's in (27) are as follows:

$$\begin{aligned} b_0 &= 1 + \frac{q^2\eta}{2} + O(h^4) \\ b_1 &= p + \frac{pq^2\eta}{2} + \theta\left(q + \frac{q^3\eta}{6}\right) + O(h^4) \\ b_2 &= \frac{p^2}{2} + \frac{q^2}{2} + \theta pq + O(h^4) \\ b_3 &= \frac{p^3}{6} + \frac{pq^2}{2} + \theta\left(\frac{p^2q}{2} + \frac{q^3}{6}\right) + O(h^4). \end{aligned} \tag{50}$$

Replacing p, q, and n_{i+1} with $-c$, $-d$, and n_{i-1}, respectively, a_j's can be obtained. Specifically, when $p = 0$ and $q = h$, b_j's become

$$\begin{aligned} b_0 &= 1 + \frac{h^2\eta}{2} + O(h^4) \\ b_1 &= \theta\left(h + \frac{h^3\eta}{6}\right) + O(h^4) \\ b_2 &= \frac{h^2}{2} + O(h^4) \\ b_3 &= \theta\left(\frac{h^3}{6}\right) + O(h^4) \\ &= \frac{h^2}{3!}b_1 + O(h^4). \end{aligned} \tag{51}$$

Or when $p = h/2$ and $q = h/2$, b_j's become

$$\begin{aligned} b_0 &= 1 + \frac{h^2\eta}{8} + O(h^4) \\ b_1 &= \frac{h}{2} + \frac{h^3\eta}{16} + \theta\left(\frac{h}{2} + \frac{h^3\eta}{6}\right) + O(h^4) \\ b_2 &= \frac{h^2}{4} + \theta\frac{h^2}{4} + O(h^4) \\ b_3 &= \frac{h^3}{12}(1+\theta) + O(h^4) \\ &= \frac{h^2}{3!}b_1 + O(h^4). \end{aligned} \tag{52}$$

The parameters b_j's in (27) are as follows:

$$\begin{aligned} f_0 &= 1 + \frac{q^2\eta}{2} + \frac{q^4\eta^2}{24} + O(h^6) \\ f_1 &= p + \frac{pq^2\eta}{2} + \frac{pq^4\eta^2}{24} \\ &\quad + \theta\left(q + \frac{q^3\eta}{6} + \frac{q^5\eta^2}{120}\right) + O(h^6) \\ f_2 &= \frac{p^2}{2} + \frac{q^2}{2} + \frac{p^2q^2\eta}{4} + \frac{q^4\eta}{12} \\ &\quad + \theta\left(pq + \frac{pq^3\eta}{6}\right) + O(h^6) \\ f_3 &= \frac{p^3}{6} + \frac{pq^2}{2} + \frac{p^3q^2\eta}{12} + \frac{pq^4\eta}{12} \\ &\quad + \theta\left(\frac{p^2q}{2} + \frac{q^3}{6} + \frac{pq^3\eta}{12} + \frac{q^5\eta}{60}\right) \\ &\quad + O(h^6) \\ f_4 &= \frac{p^4}{24} + \frac{p^2q^2}{4} + \frac{q^4}{24} \\ &\quad + \theta\left(\frac{p^3q}{6} + \frac{pq^3}{6}\right) + O(h^6) \\ f_5 &= \frac{p^5}{120} + \frac{p^3q^2}{12} + \frac{pq^4}{24} \\ &\quad + \theta\left(\frac{p^4q}{24} + \frac{p^2q^3}{12} + \frac{q^5}{120}\right) + O(h^6). \end{aligned} \tag{53}$$

Replacing p, q, and n_{i+1} with $-c$, $-d$, and n_{i-1}, respectively, e_j's can be obtained. Specifically, when $p = 0$ and $q = h$, f_j's become

$$\begin{aligned} f_0 &= 1 + \frac{h^2\eta}{2} + \frac{h^4\eta^2}{24} + O(h^6) \\ f_1 &= \theta\left(h + \frac{h^3\eta}{6} + \frac{h^5\eta^2}{120}\right) + O(h^6) \\ f_2 &= \frac{h^2}{2} + \frac{h^4\eta}{12} + O(h^6) \\ f_3 &= \theta\left(\frac{h^3}{6} + \frac{h^5\eta}{60}\right) + O(h^6) \\ f_4 &= \frac{h^4}{24} + O(h^6) \\ f_5 &= \theta\left(\frac{h^5}{120}\right) + O(h^6) \\ &= \frac{h^4}{5!}f_1 + O(h^6). \end{aligned} \tag{54}$$

Or when $p = h/2$ and $q = h/2$, f_j's become

$$\begin{aligned} f_0 &= 1 + \frac{h^2\eta}{8} + \frac{h^4\eta^2}{384} + O(h^6) \\ f_1 &= \frac{h}{2} + \frac{h^3\eta}{16} + \frac{h^5\eta^2}{768} \\ &\quad + \theta\left(\frac{h}{2} + \frac{h^3\eta}{48} + \frac{h^5\eta^2}{3840}\right) + O(h^6) \\ f_2 &= \frac{h^2}{4} + \frac{h^4\eta}{64} + \frac{h^4\eta}{192} \\ &\quad + \theta\left(\frac{h}{4} + \frac{h^4\eta}{96}\right) + O(h^6) \\ f_3 &= \frac{h^3}{12} + \frac{h^5\eta}{192} + \theta\left(\frac{h^3}{12} + \frac{h^5\eta}{320}\right) + O(h^6) \\ f_4 &= \frac{h^4}{48}(1+\theta) \\ f_5 &= \frac{h^5}{240}(1+\theta) \\ &= \frac{h^4}{5!}f_1 + O(h^6). \end{aligned} \tag{55}$$

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