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Abstract—An iterative finite difference beam propagation method based on the Crank–Nicholson scheme is presented to simulate continuous wave (CW) second-order nonlinear effects in optical waveguides with the depletion of the pump wave taken into account. This method is an extension of the linear finite-difference beam propagation method and preserves the same order of accuracy. Comparisons with the previously published explicit finite difference beam propagation method and the rectangular approximation method are presented. Quasi-phase matched difference frequency generation in AlGaAs and quasi-phase-matched second harmonic generation in LiNbO$_3$ are considered in the evaluation, showing that one iteration for the IFD-BPM is sufficient for the simulation with good accuracy and without increasing much computation time.

Index Terms—Difference frequency generation, finite-difference beam propagation method, quasi-phase matching, second harmonic generation, second-order nonlinear effects.

I. INTRODUCTION

SECOND-ORDER nonlinear effects in optical waveguides, especially with the quasi-phase-matching (QPM) technique [1]–[2], have extensive applications because of their versatile and efficient frequency conversion abilities. The quasi-phase-matched second harmonic generation (QPM-SHG) [3] can serve as a laser source in the visible region [4]. In particular, the generation of blue light by this technique [5]–[7] has potential applications in data storage and display technology. Other QPM second-order nonlinear effects like difference frequency generation (DFG) and sum frequency generation (SFG) are under intensive study for their use in difference frequency generation (DFG) and sum frequency generation networks [10]. Large nonlinear phase shifts induced by QPM second-order nonlinear effects like difference frequency generation (DFG) and sum frequency generation (SFG) are also under intensive study for their use in frequency tripling and quadrupling [8], mid-IR generation [9], and wavelength division multiplexing (WDM) networks [10]. Large nonlinear phase shifts induced by QPM second-order nonlinear effects require light intensities orders of magnitude lower than that required by the usual third-order nonlinearities [11]. This phase shift has also been proposed to implement all-optical switching [12] and pulse compression [13]. QPM devices have been successfully fabricated on ferroelectric materials such as LiNbO$_3$, LiTaO$_3$, and KTP [5]–[7] as well as on semiconductor materials such as AlGaAs [14], [15].

Theoretical modeling of the QPM nonlinear effects has increasing importance for the optimal implementation of the QPM devices. Precise analytical modeling of these second-order nonlinear devices is quite difficult especially when large or irregular geometrical variations exist and the depletion of the pump wave is not negligible. Many approximations need to be made for the analytical models [16]–[18]. For a general and accurate analysis, numerical methods are necessary. The beam propagation method (BPM) [19] is a powerful and flexible approach to design and simulate optical devices. Applications of BPM to linear devices have been studied extensively. Some researchers have extended this method to simulate second-order nonlinear effects, mostly SHG, in optical waveguides based on schemes such as fast Fourier transform (FFT) [20], finite element (FE) [21]–[23], and finite difference (FD) methods [24]–[28]. FFT-BPM is generally not preferred for its low efficiency and accuracy and its improvements are still under investigation [19], [29]. On the other hand, FD-BPM is more popular than FE-BPM for the former is more straightforward to implement.

Even in the numerical methods for SHG, most of the publications still make the assumption that the fundamental wave is independent of the propagation distance. This assumption greatly alleviates the difficulties in the treatment of the nonlinear terms. However, in devices where the conversion efficiency is high or where there is a geometrical variation of the waveguide structure, this assumption is not valid. The operator splitting method [30] has been used to deal with the nonlinearly coupled wave equations [27], [28]. In this method, the linear propagation and the nonlinear coupling effects are taken into consideration successively in each propagation step. When the operator splitting method converges with respect to the step size in the propagation direction, it could also lead to rather accurate results without much sophisticated manipulations. However, the nonlinear coupling terms therein are treated by assuming a constant coupling between different frequencies in each propagation step to linearize the equations. Then, eigenvector expansions are used to solve these equations, which eventually involve the calculations for trigonometric functions. The evaluation of these trigonometric functions will reduce the efficiency of the operator splitting method even with the approximations made in the linearization. The combination of the trapezoidal rule and direct iterations is suggested to improve both accuracy and efficiency because constant coupling is not assumed and only
simple arithmetic calculations are required. The convergence rate is fast and will be clearly shown in the following sections.

In this paper, we present an iterative finite difference beam propagation method (IFD-BPM) based on the Crank–Nicholson scheme [29]–[31]. This method can simulate continuous wave second-order nonlinear effects with consistent second-order accuracy. Instead of using the operator splitting method, the nonlinear coupling terms are treated as nonhomogeneous source terms [31]. We will show that improper treatment of these terms will lower the order of accuracy. Comparisons with the previously published explicit finite difference beam propagation method (EFD-BPM) [25]–[26] and the rectangular approximation method (RA) are presented. Two cases will be considered in these evaluations: QPM-DFG in AlGaAs and QPM-SHG in LiNbO₃. We will focus mainly on the 2-D case, which is sufficient for lucid manifestation of these algorithms and comparisons among them.

II. FORMULATIONS

Propagation of light in the presence of the second-order nonlinear polarization can be described by

\[
\begin{align*}
\nabla^2 E &= \mu_0 \varepsilon_0 \frac{\partial^2 E}{\partial z^2} + \mu_0 \frac{\partial^2 P}{\partial z^2} \\
\frac{\partial P}{\partial z} &= \varepsilon_0 \left( \chi^{(1)} E + \chi^{(2)} EE \right)
\end{align*}
\]

(1a) (1b)

where \(E\) and \(P\) are the electric field and the polarization; \(\chi^{(1)}\) and \(\chi^{(2)}\) are the linear and the second-order susceptibilities; \(\varepsilon_0\) and \(\mu_0\) are the permittivity and the permeability in vacuum. Our formulation is restricted to the scalar wave equation which is a fair approximation for most optoelectronic devices. It can be easily extended to the semivectorial simulation. Second-order nonlinear effects are three-photon processes, so there are in general three different frequencies involved. However, in SHG, there is a degeneracy in frequency and only two wavelengths need to be considered. Since SHG is a special case of the second-order nonlinear effects, the formulation here is given for the general three-frequency case. Reduction to the degenerate situation is straightforward.

The total electric field composed of three monochromatic waves can be expressed in the phasor notation as

\[
E = \frac{1}{2} \left\{ E_1(x, z) e^{j(\omega_1 t - k_{10} \overline{n}_1 z)} + E_2(x, z) e^{j(\omega_2 t - k_{20} \overline{n}_2 z)} + E_3(x, z) e^{j(\omega_3 t - k_{30} \overline{n}_3 z)} \right\} + c.c.
\]

(2)

where \(\omega_1, \omega_2, \text{ and } \omega_3\) are the angular frequencies of the three waves and \(\omega_3 = \omega_1 + \omega_2\) for energy conservation; \(k_{10}, k_{20}, \text{ and } k_{30}\) are their wavevectors in vacuum; \(\overline{n}_1, \overline{n}_2, \text{ and } \overline{n}_3\) are the reference indexes and usually set to be the effective indexes of the waveguide modes of interest. The waves are assumed to propagate along the \(z\)-direction. Substituting (2) into (1) and equating terms with the same frequency yield

\[
2j k_{10} \overline{n}_1 \frac{\partial E_1}{\partial z} = \frac{\partial^2 E_1}{\partial z^2} + k_{10}^2 (\overline{n}_1^2 - \overline{n}_2^2) E_1 + k_{10}^2 \chi^{(2)} e^{-j\Delta k z} E_3 E_1^* \]

(3a)

\[
2j k_{20} \overline{n}_2 \frac{\partial E_2}{\partial z} = \frac{\partial^2 E_2}{\partial z^2} + k_{20}^2 (\overline{n}_2^2 - \overline{n}_3^2) E_2 + k_{20}^2 \chi^{(2)} e^{-j\Delta k z} E_3 E_2^* \]

(3b)

\[
2j k_{30} \overline{n}_3 \frac{\partial E_3}{\partial z} = \frac{\partial^2 E_3}{\partial z^2} + k_{30}^2 (\overline{n}_3^2 - \overline{n}_1^2) E_3 + k_{30}^2 \chi^{(2)} e^{-j\Delta k z} E_1 E_2 \]

(3c)

where

\[
\Delta k = k_{10} \overline{n}_1 - k_{20} \overline{n}_2 - k_{30} \overline{n}_3
\]

\[
\overline{n}_i^2 = 1 + \chi^{(1)}, \quad i = 1, 2, 3.
\]

Paraxial approximations are made to derive (3). The Kleinman’s symmetry [32] is assumed so that \(\chi^{(2)}\) is independent of frequency. This assumption is valid when the applied field frequencies are far from the resonant frequencies of the medium. This means no energy transfer to the nonlinear medium, so the energy in the light field is conserved, as described by the Manley-Rowe relations [32]. \(\chi^{(2)}\) can be frequency-dependent in the simulation. The Kleinman’s symmetry is assumed for the evaluation of numerical schemes which will be clear in Section III.

In the finite difference scheme, the spatial domain is divided into small regions by placing a grid over the domain. Uniform grid is used in this work. The step sizes along the \(x\) and the \(z\) directions are denoted by \(\Delta x\) and \(\Delta z\) with \(m\) and \(s\) representing the indexes along these two directions, respectively. For example, \(E_{m,s}^{n}\) represents the electric field at the point \((x_m, z_s) = (m \cdot \Delta x, s \cdot \Delta z)\). For concise expressions, we define the following finite difference operators and variables:

\[
L_{m,s} E_{m,s}^{n} = \frac{1}{\Delta x^2} \left( E_{m-1,s}^{n} - 2E_{m,s}^{n} + E_{m+1,s}^{n} \right) \]

(4a)

\[
F_{i,s}^{n} = \frac{k_{i0}^2 (\overline{n}_i^2 - \overline{n}_s^2)}{\overline{n}_s^3}, \quad i = 1, 2, 3 \]

(4b)

\[
F_{i,s}^{n} = k_{i0}^2 \chi^{(2)} (\overline{n}_i^2 - \overline{n}_s^2) e^{-j\Delta k_i z_s}, \quad i = 1, 2 \]

(4c)

\[
F_{3,s}^{n} = k_{30}^2 \chi^{(2)} (\overline{n}_3^2 - \overline{n}_s^2) e^{-j\Delta k_3 z_s} \]

(4d)

Note that \(\chi^{(2)}\) and \(\overline{n}_i\) are functions of position. In the remainder of this section, we will describe the actual implementations of the methods that are compared in this paper.

A. Scheme I: EFD-BPM

Using the explicit finite difference beam propagation method (EFD-BPM) to model linear devices has been discussed in detail in [33], where only fields in previous steps are required to simulate the propagation of the beam. The stability requirement gives an upper limit of the step size along the propagation direction, \(\Delta z\). This method can also be applied to the vectorial simulation with extra restrictions on the minimum transverse step sizes, \(\Delta x\) and \(\Delta y\) [34]. Extensions of the EFD-BPM to model SHG in optical waveguides have been presented in [25] and [26]. The nonlinear phase shift and the output depletion of the fundamental field are studied in those works. The modification of this algorithm for the general three-frequency situation in our case is straightforward with the same order of accuracy. In our notations, it is described.
by the following equations:

\[
\frac{j k_0 n_1}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) \equiv (L_x + L_{01}) E_{m}^{n,s} + F_{1}^{m,s} E_{0}^{n,m} E_{2}^{n,m,s} \quad (5a)
\]

\[
\frac{j k_0 n_2}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) \equiv (L_x + L_{02}) E_{2}^{n,m,s} + F_{2}^{m,s} E_{2}^{n,m} E_{3}^{n,m,s} \quad (5b)
\]

\[
\frac{j k_0 n_3}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) \equiv (L_x + L_{03}) E_{3}^{n,m,s} + F_{3}^{m,s} E_{3}^{n,m} E_{1}^{n,m,s} \quad (5c)
\]

The central difference method [35] is used for the first derivative in \( z \), which is second-order accurate. This is a three-level scheme in which fields in three successive steps are involved in the computation.

**B. Scheme II: Rectangular Approximation (RA)**

The implicit second-order-accurate Crank-Nicolson scheme is often used to solve parabolic partial differential equations. In the initial-boundary-value problem, it is unconditionally stable for proper boundary conditions [31], [36]. This is a two-level scheme and, in the linear case, it results in a tridiagonal system of linear equations which can be solved simultaneously with a good efficiency [29]-[30]. However, in the presence of nonlinearities, the nonlinear coupling terms cannot be exactly splitted to yield a linear system of equations. A simple way to handle this problem is to “lag” part of the nonlinear terms. For example, in a Kerr medium, the refractive index depends on the local light intensity [32], [37], and leads to intensity-dependent nonlinear terms. These terms in the current step are then approximated by the known fields in the previous step [24]. With this approximation, the BPM is implemented like in the linear case. Similar ideas can be found in other places [35], [38] on solving the diffusion equation with a source term that is evaluated in the previous step. Applying this approximation and the Crank-Nicolson scheme to (3) gives

\[
\frac{2j k_0 n_1}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) = \frac{1}{2} \left( L_x + L_{01} \right) \left( E_{1}^{n,m,s} + s^{n+1} \right) + F_{1}^{m,s} E_{3}^{n,m,s} E_{2}^{n,m,s} \quad (6a)
\]

\[
\frac{2j k_0 n_2}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) = \frac{1}{2} \left( L_x + L_{02} \right) \left( E_{2}^{n,m,s} + s^{n+1} \right) + F_{2}^{m,s} E_{3}^{n,m,s} E_{1}^{n,m,s} \quad (6b)
\]

\[
\frac{2j k_0 n_3}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) = \frac{1}{2} \left( L_x + L_{03} \right) \left( E_{3}^{n,m,s} + s^{n+1} \right) + F_{3}^{m,s} E_{1}^{n,m,s} E_{2}^{n,m,s} \quad (6c)
\]

Equation (6) can also be derived from the conservation-law approach [31], which involves integration of the partial differential equations. Then, we will be able to see that this scheme is only first-order accurate in \( z \). The reduction of order in accuracy is due to the approximation used in integrating the nonlinear source terms over the cell centered at \((x,z) = (m \cdot \Delta x, (s + \frac{1}{2}) \cdot \Delta z)\) by the rectangular rule.

**C. Scheme III: IFD-BPM**

From the above discussions for scheme II, if we want to have a scheme that is consistently second-order accurate, the nonlinear source terms should be integrated by other methods, for example, the trapezoidal rule. The resulting difference equations then involve undetermined nonlinear source terms in the next step. Many iterative schemes [30], [31], [35] can be used to solve this problem. Among them, the fixed-point iteration [35] is chosen for the IFD-BPM. It has the advantage of great simplicity and requires the minimal modification from the linear BPM, compared with other iterative methods.

The IFD-BPM is described as follows. First, one set of solution is obtained by the RA scheme (scheme II) and denoted by \( E_{m+1}^{n,s+1} \) which is our initial guess of the electric fields in the following step. Note that \( E_{m+1}^{n,s+1} \) can also be assigned by other methods, e.g., Scheme I or its two-level version. The way of the initial guess influences the rate of convergence, but the difference is minor. Therefore, we use only scheme II to obtain \( E_{m+1}^{n,s+1} \). This iterative algorithm can be written as

\[
\frac{2j k_0 n_1}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) = \frac{1}{2} \left[ \left( L_x + L_{01} \right) \left( E_{1}^{n,m,s} + E_{1}^{n,m,s+1} \right) + F_{1}^{m,s} E_{3}^{n,m,s} E_{2}^{n,m,s} + F_{3}^{m,s+1} E_{2}^{n,m+1} \left( E_{m+1}^{n,s+1} \right) \right] \quad (7a)
\]

\[
\frac{2j k_0 n_2}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) = \frac{1}{2} \left[ \left( L_x + L_{02} \right) \left( E_{2}^{n,m,s} + E_{2}^{n,m,s+1} \right) + F_{2}^{m,s} E_{3}^{n,m,s} E_{1}^{n,m,s} + F_{3}^{m,s+1} E_{3}^{n,m+1} \left( E_{m+1}^{n,s+1} \right) \right] \quad (7b)
\]

\[
\frac{2j k_0 n_3}{\Delta z} (E_{m+1}^{n,s+1} - E_{m}^{n,s}) = \frac{1}{2} \left[ \left( L_x + L_{03} \right) \left( E_{3}^{n,m,s} + E_{3}^{n,m,s+1} \right) + F_{3}^{m,s} E_{1}^{n,m,s} E_{2}^{n,m,s} + F_{3}^{m,s+1} E_{3}^{n,m+1} \left( E_{m+1}^{n,s+1} \right) \right] \quad (7c)
\]

where the superscript \( t \) is the iteration count and \( E_{m+1}^{n,s+1(t)} \) represents the \( t \)th iteration field. Now, these equations can be solved readily because there is no undetermined nonlinear terms. This procedure is executed repeatedly until the difference between successive iterations is smaller than a given tolerance value. This iterative scheme is convergent for all cases studied. The rate of convergence is fast as will be shown in Section III.

**III. RESULTS AND DISCUSSIONS**

The total power at \( z = s + \Delta z \) is defined as:

\[
\frac{\Delta x}{\eta_p} \sum_{p} \sum_{m} \left| E_{m}^{n,p} \right|^2
\]
where \( r_0 \) is the free space impedance, the summation, \( p_k \), runs over all frequencies and the summation, \( m_k \), runs over the discretization points along the \( x \)-direction. Note that the unit of the total power defined here is \( W/m \) because we are focusing on the 2-D case. As mentioned in section II, by assuming the Kleinman’s symmetry, the total power in the light field is conserved along the direction of propagation if the integration over the entire transverse plane is carried out. However, in the BPM, the computation window is of finite size and proper boundary conditions should be posed in order that the total power in this window can be conserved. Throughout this paper, the zero (Dirichlet) boundary condition is used. It can be proven that, under such boundary condition, there is no energy flux leaving the boundaries and the power in the computation window is conserved [39]. The size of the window is chosen to be large enough so that no appreciable wave is reflected at the boundaries to interfere with the field inside the window. Since power conservation is a fundamental property even in the discrete numerical configuration, we take it as a self-consistent criterion to evaluate the performance of the three schemes. We define the normalized total power deviation (NTPD) as

\[
NTPD = \left| \frac{\text{total power in current step} - \text{initial total power}}{\text{initial total power}} \right|
\]  

(8)

which is expressed in decibel.

Two cases will be studied to compare schemes mentioned in Section II. One is QPM-DFG and the other is QPM-SHG. The waveguides in these cases are straight with periodically modulated nonlinear coefficients. The index profile of the waveguide and the periodic variation of \( \chi^{(2)} \) along the \( z \)-axis are shown in Fig. 1, where \( \omega_s, n_g, n_c, \) and \( \Delta \) are the width of the waveguide, the refractive indexes of the guiding and the cladding layers, and the period of the modulated \( \chi^{(2)} \) grating, respectively. The duty cycle of the \( \chi^{(2)} \) grating is defined as

\[
\text{duty cycle} = \frac{p}{\Lambda}.
\]

In the two cases studied, first-order QPM with a 50% duty cycle is used.

A. Case I: QPM-DFG

In this case, QPM-DFG in AlGaAs [14] is studied. The zincblende semiconductor possesses nonzero second-order nonlinear susceptibility tensor elements \( \chi^{(2)}_{ijk} \) with all different \( i, j, \) and \( k \). The beam propagates along [110] with the polarization along [001] and [1\text{1}0\text{0}]. The wavelengths and refractive indexes for the pump, the signal, and the idler waves are 0.91 \( \mu m \), 1.55 \( \mu m \), 2.204 \( \mu m \), 3.2736, 3.13984, and 3.10567, respectively. The effective index method (EIM) [40] can be used to reduce the 3-D geometry to the 2-D case by assigning an effective index profile. For evaluation purposes, the index difference \( \Delta n = n_g - n_e = 0.002 \) is used throughout this paper. This value is of typical order for most of the integrated optical waveguides. \( \chi^{(2)} \) is 275 pm/V for AlGaAs. The initial fields are the fundamental modes with power levels of 4 W, 1 mW, and 1 mW for the pump, the signal, and the idler waves, respectively. The width of the waveguide, \( \omega_s \), is 4 \( \mu m \) and the computation window is 40 \( \mu m \) with \( \Delta x = 0.2 \mu m \) and \( \Delta z = 0.1 \mu m \). The same grid sizes are used for all schemes compared. For the EFD-BPM, a stability criterion is required and so limits the maximum value of \( \Delta z \). In this case, the EFD-BPM is unstable for \( \Delta z \geq 0.2 \mu m \) while the other two schemes are stable even with a very large \( \Delta z \). An additional calculation using \( \Delta z = 0.01 \mu m \) is also performed by the EFD-BPM. Instead of a tolerance control loop, we fix the number of iteration from one to four in the IFD-BPM to investigate the rate of convergence.

Fig. 2 shows the individual power levels versus the propagation distance, defined as power diagram, for the three waves. Since the powers calculated by the RA scheme and the IFD-BPM with different iteration counts have very little difference in the scale used, only the result computed by the IFD-BPM with one iteration is shown in Fig. 2(a). Fig. 2(b) shows the power diagram for the EFD-BPM with \( \Delta z = 0.1 \mu m \). The power calculated by the EFD-BPM after 25 000 \( \mu m \) obviously violates the power conservation law. Fig. 3 shows the normalized total power deviations (NTPD) along the propagation direction for different schemes. In Fig. 3, curves a and b represent the results obtained by the EFD-BPM with \( \Delta z = 0.1 \) and 0.01 \( \mu m \). Curves c and d represent the results obtained by the RA scheme and the IFD-BPM, respectively. The differences among the NTPD curves for the IFD-BPM with different iteration counts are almost indistinguishable even in the log scale, so only the curve for one iteration is shown. Although there are some local increases and decreases of the NTPD curve for the IFD-BPM, it is upper bounded at about \(-50\) dB. The NTPD curve for the RA scheme rises fast at the beginning and then has a slower increase. However, it does not seem to be bounded. As to the EFD-BPM, the deviation increases substantially after 25 000 \( \mu m \) of propagation even with \( \Delta z = 0.01 \mu m \). Although none of these schemes exactly conserve power, the total power deviation accumulates much faster in the EFD-BPM than in the RA scheme and the IFD-BPM.
In principle, more counts of iteration for the IFD-BPM should give better accuracy. In practice, the number of iteration counts cannot be large in order to save the computation time. To realize the required iteration counts, we calculate the normalized signal-power difference, defined by the absolute signal power difference between the forth count and the prior count divided by the forth count signal power. The normalized signal-power differences for one, two, three iteration counts are shown in Fig. 4. Difference curves for the RA scheme and the EFD-BPM with the same \( \Delta z \) are also shown in the figure for comparison. We can see from the figure that the normalized signal-power difference for the first iteration is already as small as -60 dB and decreases for about 30 dB after each successive iteration. The calculation also shows that the signal power calculated by this iterative scheme does converge to a limit that is determined by the accuracy of the discretization. Fig. 4 also shows that one iteration is already much better than the other two schemes.

For a closer investigation of the convergence rate of the IFD-BPM, the time-averaged signal field profiles of each iteration after propagating 30,000 \( \mu \text{m} \) are shown in Fig. 5. It is evident in this figure that the field also converges well only after one iteration. Combined with the 50 dB reduction of the normalized power difference for the first iteration, as shown in Fig. 4, it suggests that one iteration be sufficient to yield good accuracy.

**B. Case II: QPM-SHG**

In this part, we concentrate on the QPM-SHG in LiNbO\(_3\). The wavelengths and the refractive indexes of the fundamental and the second harmonic (SH) waves are 0.808, 0.404, 2.17503, and 2.32679 \( \mu \text{m} \), respectively. The width of the waveguide, \( w \), is 4 \( \mu \text{m} \). The largest susceptibility tensor...
element of LiNbO$_3$, $\chi^{(2)}_{\text{LiNbO}_3}$ is 68.8 pm/V. The initial power levels of the fundamental and the SH waves are 4 and 0 W. The size of the computation window is still 40 µm with $\Delta z = 0.2$ µm. However, in order to have a stable EFD-BPM, $\Delta z$ is changed to 0.08 µm for all schemes. Again, the choice of the same $\Delta z$ for all schemes is to compare these schemes on the same ground. An additional simulation with $\Delta z = 0.01$ µm is also performed for the EFD-BPM.

Fig. 6(a) shows the power diagram obtained by the IFD-BPM with one iteration. Similar to case I, the differences among successive iterations for the IFD-BPM and the RA scheme are very small. The results obtained by the EFD-BPM with $\Delta z = 0.08$ µm is highly oscillatory and is not suitable for a clear illustration. Hence, we present the power diagram with $\Delta z = 0.01$ µm in Fig. 6(b). It is evident that even with a much smaller $\Delta z$, the power conservation law is still significantly violated in the EFD-BPM. Fig. 7 shows the NTPD curves. Curves a and b represent the results obtained by the EFD-BPM with $\Delta z = 0.08$ and 0.01 µm. Curves c and d represent the results obtained by the RA scheme and the IFD-BPM, respectively. The behavior of the NTPD curve for the RA scheme is essentially the same as in case I. The NTPD curve of the IFD-BPM in this case is different from its counterpart in case I. However, it is still upper bounded at around $\sim 40$ dB. As to the EFD-BPM, the errors of the total power accumulate almost at the same speed for the two $\Delta z$ values used. The broadening of the NTPD curve for the EFD-BPM with $\Delta z = 0.08$ µm is an indication of the oscillatory behavior of the computed fields. Oscillation often occurs in the EFD-BPM in modeling second-order nonlinear processes. Fig. 8 shows that the convergence rate of the IFD-BPM in this case is similar to that in case I, i.e., 50 dB reduction of the normalized signal power difference after the first iteration and 30 dB for the following iteration counts. The oscillatory characteristic of the EFD-BPM is also evident in this figure. Fig. 9 shows the time-averaged SH field profiles of each iteration after propagating 30000 µm. They are identical in the scale used, including the one obtained by the RA scheme.

In our simulations, with the same grid sizes, the EFD-BPM is about two times faster than the RA scheme and four times faster than the IFD-BPM with one iteration. Although explicit schemes are faster than implicit schemes, it is generally not preferred when the accuracy is taken into account. The performance of the EFD-BPM is not satisfactory even with a ten times smaller $\Delta z$ which requires ten times longer computation time. Further decrease of the grid sizes in an attempt to reach better performance of the EFD-BPM will totally eliminate its speed advantage. In our evaluation, the grid sizes are chosen so that the EFD-BPM is stable in the linear and the nonlinear case. For the linear case, if the EFD-BPM is stable, it also conserves power [33]. However, for the nonlinear case studied here, even if the grid sizes well satisfy the stability criterion, the total power is not conserved well. Severe violation of the power conservation law of the EFD-BPM may be caused by the evaluation of the nonlinear coupling terms from the previous step, which result in worse estimations of these terms. Since these terms are “sources” or “sinks” of the fields under consideration, the errors in these terms will lead to incorrect transformations of energy among the frequencies. Therefore, the total power is not conserved.

The same problem also happens to the RA scheme, but is not as severe as in the EFD-BPM. As to the IFD-BPM, the nonlinear terms are integrated by the trapezoidal rule. The errors are on the third order and do not accumulate as fast as the other two schemes. Consequently, the IFD-BPM is more reliable.

For short propagation distances, the EFD-BPM might also give accurate results. However, in practical simulations, the transparent boundary condition (TBC) [39] is often used in
wave is taken into consideration. This method is based on the widely used linear FD-BPM with the same second-order accuracy and good stability. Very few efforts are required to transform the linear version to the nonlinear case. Comparisons with the previously published nonlinear beam propagation methods, the EFD-BPM and the RA scheme, show the better reliability and adherence to the energy conservation law of the IFD-BPM. QPM-DFG in AlGaAs and QPM-SHG in LiNbO\textsubscript{3} are considered in the evaluation. The fast convergence of this scheme after only one iteration assures the efficiency without sacrificing the accuracy. The IFD-BPM should be very helpful in the design and evaluation of second-order nonlinear devices that have crucial applications in a broad range of fields.

**IV. CONCLUSION**

In conclusion, we presented an iterative finite difference beam propagation method to model second-order nonlinear effects in optical waveguides where the depletion of the pump order to reduce the computation window and the computation time. Thus, the power conservation law is no longer a useful criterion to monitor the performance of this scheme. As a result, it is difficult to judge whether or not the results are acceptable. Therefore, as long as the status of power conservation cannot be monitored, the RA scheme should be adopted in a preliminary simulation for its relatively slower accumulation of errors compared to the EFD-BPM. For a more accurate simulation, the IFD-BPM should be used. From the two cases studied in this work, it seems that the IFD-BPM converges well just after the first iteration, which assures the efficiency of this iterative scheme. As mentioned in section II, the initial guess in the IFD-BPM can be assigned by other methods. If scheme I is used instead, the rate of convergence is close to that obtained by using the RA scheme and more than one-fourth of the computation time could be saved for the calculation of only one iteration.

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**REFERENCES**


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