Efficient Solution of the Nonlinear Helmholtz Equation in 2D Photonic Crystals

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Abstract. The nonlinear Helmholtz equation models nonparaxial electromagnetic wave propagation in Kerr-type media and presents numerical challenges in two-dimensional photonic crystals due to strong nonlinearities, high wave numbers, and material discontinuities. This work presents an efficient and robust numerical framework combining a fourth-order finite difference scheme with multiple iterative methods, including fixed-point, frozen nonlinearity, Newton's, and modified Newton's methods. A key novelty contribution is the high-order discretization of nonlinear interfaces, enabling accurate treatment of discontinuous coefficients. Enhanced boundary conditions further ensure stability at high frequencies. Numerical experiments validate the accuracy of the scheme using analytical solutions, and demonstrate that the modified Newton's method provides superior convergence performance. The results offer an efficient and robust approach for simulating nonlinear wave propagation in complex periodic media and designing nonlinear photonic device.

Keywords: nonlinear Helmholtz equation; Kerr nonlinearity; Photonic Crystal; Finite difference method; Iterative method.

1. Introduction

Wave propagation in nonlinear optical media has gained significant interest due to its applications in optical switching, soliton transmission, and photonic crystal devices [1-6]. Kerr-type nonlinear media, where the refractive index depends on field intensity, exhibit key phenomena such as optical bistability [1], self-focusing [2], and spatial solitons [3-5]. These effects are typically governed by the nonlinear Helmholtz (NLH) equation derived from Maxwell's equations under monochromatic and linearly polarized wave assumptions [6].

Numerical methods for solving the NLH equation include high-order finite difference methods [7,8] finite elements methods [9-11], and pseudospectral methods [12]. High-order schemes are particularly effective for oscillatory solutions at large wave numbers [13]. Due to nonlinearity, iterative solvers such as fixed-point, frozen-nonlinearity, and Newton's method are commonly used [7,8,14]. A robust modified Newton's method improves convergence in strongly nonlinear regimes [12].

Nevertheless, solving the NLH equation in complex photonic structures remains challenging due to localized nonlinearities, material coefficients, and intricate 2D geometries [14]. While prior studies address simplified systems (e.g., layered media [15] or smooth refractive index domains), high-accuracy solutions for 2D periodic structures with discontinuous coefficients are less explored.

This study focuses on the 2D NLH equation in photonic crystals with embedded Kerr-type nonlinear regions. We propose a fourth-order finite difference scheme with iterative methods to address nonlinearity, high wavenumbers, and discontinuous material properties. Key innovations include precise boundary condition treatment, high-order discretization near interfaces, and analysis of nonlinear iteration convergence. Numerical experiments demonstrate the method's effectiveness in capturing nonlinear transmission and field enhancement effects within photonic crystals [15]. These results advance stable simulations of nonlinear wave phenomena in periodic media, supporting the development of future nonlinear photonic devices.

2. Model Formulation in Nonlinear Photonic Crystals

2.1 The nonlinear Helmholtz equation and boundary conditions

We consider the propagation of an electromagnetic field $u(x,y) \in \mathbb{C}$ in a 2D nonlinear photonic crystal, governed by the NLH equation [6]:

$$\Delta u + k_0^2 \left(\varepsilon + \gamma \, |u|^2 \right) u = 0, \tag{1}$$

where $\Delta u = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}$, u denotes the electric field, $k_0 = \dfrac{\omega}{c}$ is the free space wavenumber, and ω is the angular frequency, c is the speed of light in vacuum, ε is the relative permittivity, γ is the Kerr-type nonlinear coefficient. The medium consists of both linear and nonlinear regions, and the Kerr coefficient γ is nonzero only within a nonlinear subdomain $\Omega_0 \subset \Omega$.

The medium comprises periodic inclusions of alternating refractive indices, with the nonlinear region Ω_0 embedded centrally. The computational domain Ω includes material interfaces with discontinuous coefficients (see Fig.1).To accurately model wave propagation in a bounded two-dimensional photonic crystal domain $\Omega = [0,L] \times [0,H]$, we impose appropriate boundary and interface conditions as follows.

We consider a time-harmonic incident wave entering the computational domain from the left boundary $x = 0$, giving rise to both reflection and transmission. The total field on the left and right boundaries is expressed as:

$$u(0,y) = u_I(y) + u_R(y), \quad u(L,y) = u_T(y) e^{i\alpha_b L}, \quad \forall y \in \left[0,H\right], \tag{2}$$

where $u_L(y)$, $u_R(y)$ and $u_T(y)$ denote the transverse profiles of the incident, reflected and trans-mitted waves, respectively, The parameter α_b is the propagation constant in the background medium.

The corresponding first-order radiation conditions on the normal derivatives are given by:

$$\frac{\partial u}{\partial x}(0,y) = 2i\alpha_0 u_I(y) - i\alpha_0 u(0,y), \quad \frac{\partial u}{\partial x}(L,y) = i\alpha_b u(L,y), \quad \forall y \in \left[0,H\right], \tag{3}$$

where α_0 corresponds to the incident wave's wavenumber component in the x-direction. These conditions are derived from matching plane wave solutions and represent a refined form of nonreflecting boundary approximations [16].

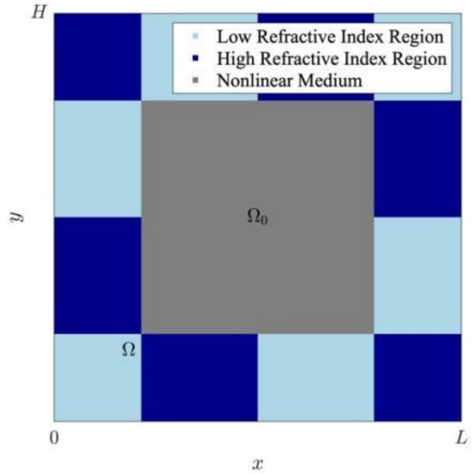

Fig. 1 2D Square Photonic Crystal with Linear and Nonlinear Media

The photonic structure is assumed to be periodic in the vertical direction, so we enforce periodic boundary conditions [17]:

$$u(x,0) = u(x,H), \quad \frac{\partial u}{\partial y}(x,0) = \frac{\partial u}{\partial y}(x,H), \quad \forall x \in [0,L]. \tag{4}$$

Therefore, (1) is followed by,

$$\begin{gathered}\Delta u + k_0^2\left(\varepsilon(x,y)+\gamma(x,y)|u|^2\right)u = 0, \quad (x,y)\in\Omega,\\ u(0,y)=u_I(y)+u_R(y), \quad \partial_x u(0,y)=2i\alpha_0 u_I(y)-i\alpha_0 u(0,y),\\ u(L,y)=u_T(y)e^{i\alpha_b L}, \quad \partial_x u(L,y)=i\alpha_b u(L,y),\\ u(x,0)=u(x,H), \quad \partial_y u(x,0)=\partial_y u(x,H).\end{gathered} \tag{5}$$

2.2 Iterative methods

To solve the NLH equation, several iterative methods can be employed. For simplicity, we rewrite the problem as follows:

$$Lu+\mathscr{N}(u)=0, \tag{6}$$

where $\mathscr{L}=\Delta+k_0^2\varepsilon$ is a linear operator and $\mathscr{N}(u)=k_0^2\gamma|u|^2u$ represents the nonlinear term. The nonlinearity in $\mathscr{N}(u)$ necessitates iterative linearization.

The *fixed-point iteration* reformulates the problem into a contractive mapping:

$$u^{(m+1)}=\mathscr{L}^{-1}\left(-\mathscr{N}(u^{(m)})\right), \tag{7}$$

where $u^{(m+1)}$ is the next iteration. In this approach, the solution is updated by directly applying the inverse of the linear operator to the nonlinear residual from the previous iterate. Nevertheless, its convergence is generally slow and may fail in regimes where the nonlinear effects are significant.

A closely related but more commonly used approach is the *frozen nonlinearity iteration*, which improves stability by fixing the nonlinear coefficient at each step:

$$\mathscr{L}u^{(m+1)}+k_0^2\varepsilon|u^{(m)}|^2u^{(m+1)}=0. \tag{8}$$

While this method is simple and easy to implement, its convergence rate is typically linear and may deteriorate in strongly nonlinear regimes.

To improve convergence, *Newton's method* is employed. We define the nonlinear residual operator $\mathscr{F}(u)$ as

$$\mathscr{F}(u,\bar{u}):=\mathscr{L}u+k_0^2\gamma u^2\bar{u}. \tag{9}$$

At each iteration, one seek can update $u^{(m+1)}=u^{(m)}+\delta u$ such that $\mathscr{F}(u^{(m+1)})\approx 0$. Applying a Taylor expansion of $\mathscr{F}$ yields the linearized equation:

$$\mathscr{F}(u^{(m)},\bar{u}^{(m)})+\frac{\partial\mathscr{F}}{\partial u}(u^{(m)},\bar{u}^{(m)})\,\delta u+\frac{\partial\mathscr{F}}{\partial\bar{u}}(u^{(m)},\bar{u}^{(m)})\,\delta\bar{u}=0. \tag{10}$$

Consequently, the update equation takes the form:

$$\left[\mathscr{L}+2k_0^2\gamma|u^{(m)}|^2\right]u^{(m+1)}+k_0^2\gamma(u^{(m)})^2\,\bar{u}^{(m+1)}=2k_0^2\gamma|u^{(m)}|^2u^{(m)}. \tag{11}$$

It is worth noting that while Newton's method converges quadratically near the solution but is sensitive to the initial guess.

Moreover, *a modified Newton's method* was introduced in [12], in which $\bar{u}^{m+1}$ is replaced by $\bar{u}^m$ in equation (11), leading to the following form:

$$\mathscr{L}u^{(m+1)}+2k_0^2\gamma|u^{(m)}|^2u^{(m+1)}=k_0^2\gamma|u^{(m)}|^2u^{(m)}. \tag{12}$$

Although only linearly convergent, it simplifies implementation and remains effective in strongly nonlinear or multistable regimes.

For convenience, the four iterative methods introduced above can be reformulated as a general expression

$$\mathscr{L}u^{(m+1)}+a_1^{(m)}u^{(m+1)}+b_1^{(m)}\bar{u}^{(m+1)}=a_2^{(m)}u^{(m)}. \tag{13}$$

Table 1 presents the values of the coefficients $a_1^{(m)}$, $b_1^{(m)}$ and $a_2^{(m)}$ corresponding to the four iterative schemes discussed above.

Table 1. Coefficients of $a_1^{(m)}$, $b_1^{(m)}$, $a_2^{(m)}$

Iterative Method	$a_1^{(m)}$	$b_1^{(m)}$	$a_2^{(m)}$
Fixed-point	0	0	$-k_0^2\gamma|u^{(m)}|^2$
Frozen nonlinearity	$k_0^2\gamma|u^{(m)}|^2$	0	0

Newton	$2k_0^2\gamma\,\vert u^{(m)}\vert^2$	$k_0^2\gamma(u^{(m)})^2$	$2k_0^2\gamma\,\vert u^{(m)}\vert^2$
Modified Newton	$2k_0^2\gamma\,\vert u^{(m)}\vert^2$	0	$k_0^2\gamma\,\vert u^{(m)}\vert^2$

2.3 Fourth-order Finite Difference Discretization

We consider a computational domain $\Omega = [0,L] \times [0,H]$, discretized using a uniform Cartesian grid with spacing $x_i = i\,\Delta x, \quad i = 0,1,\ldots,N_x, \quad y_j = j\,\Delta y, \quad j = 0,1,\ldots,N_y$.

For interior points (i,j), where $2 \le x \le N_x - 2 \quad 2 \le y \le N_y - 2$, the Laplacian operator is discretized using a standard fourth-order central finite difference stencil:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{(i,j)} \approx \frac{-u_{i+2,j} + 16u_{i+1,j} - 30u_{i,j} + 16u_{i-1,j} - u_{i-2,j}}{12\,\Delta x^2}, \tag{14}$$

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{(i,j)} \approx \frac{-u_{i,j+2} + 16u_{i,j+1} - 30u_{i,j} + 16u_{i,j-1} - u_{i,j-2}}{12\,\Delta y^2}. \tag{15}$$

Let $u \in \mathbb{C}^n$ and $\bar{u} \in \mathbb{C}^n$ denote the column vectors of the real and imaginary parts of the field values at all interior points, and $n = (N_x - 3)(N_y - 3)$, then the discretized system corresponding to the unified iterative scheme reads:

$$\begin{aligned} &-\frac{u_{i+2,j}^{(m+1)} - 16u_{i+1,j}^{(m+1)} + 30u_{i,j}^{(m+1)} - 16u_{i-1,j}^{(m+1)} + u_{i-2,j}^{(m+1)}}{12\,\Delta x^2} \\ &-\frac{u_{i,j+2}^{(m+1)} - 16u_{i,j+1}^{(m+1)} + 30u_{i,j}^{(m+1)} - 16u_{i,j-1}^{(m+1)} + u_{i,j-2}^{(m+1)}}{12\,\Delta y^2} \\ &+k_0^2 n_0^2 u_{i,j}^{(m+1)} + a_1^{(m)} u_{i,j}^{(m+1)} + b_1^{(m)} \bar{u}_{i,j}^{(m+1)} = a_2^{(m)} u_{i,j}^{(m)} \end{aligned} \tag{16}$$

Let the values $u_{i,j}^{(m+1)}$ and their imaginary parts over all interior grid points be stored in column vectors $u^{(m+1)}$ and $\bar{u}^{(m+1)}$ respectively, the discretized system can be expressed compactly as:

$$\left[\mathscr{A} + A_1^{(m)}\right] u^{(m+1)} + B_1^{(m)} \bar{u}^{(m+1)} = A_2^{(m)} u^{(m)}, \tag{17}$$

where $\mathscr{A}$ denotes the fourth-order Laplacian operator, and $A_1^{(m)}$, $B_1^{(m)}$, $A_2^{(m)}$ encode the nonlinear coefficients evaluated at the m-th iteration.

To impose the mixed Robin boundary conditions on $x = 0$ and $x = L$ and the periodic conditions on $y = 0$ and $y = H$, we introduce both the physical boundary values and the two layers of ghost-point values into a single vector $\mathbf{u}_b = \left[u_{0,j},\, u_{1,j},\, u_{N_x-1,j},\, u_{N_x,j},\, u_{i,0},\, u_{i,1},\, u_{i,N_y-1},\, u_{i,N_y}\right]^T \in \mathbb{C}^{n_b}$, and the boundary condition is discretized as

$$\mathscr{D}u + \mathscr{D}_0 u_b = h\cdot \tag{18}$$

Taking into account the finite difference discretizations for both interior domain and boundary conditions, the resulting system can be expressed as:

$$\begin{pmatrix} \mathscr{A} + A_1^{(m)} & B_1^{(m)} & 0 \\ \mathscr{D} & 0 & \mathscr{D}_0 \end{pmatrix} \begin{pmatrix} u^{(m+1)} \\ \bar{u}^{(m+1)} \\ u_b^{(m+1)} \end{pmatrix} = \begin{pmatrix} A_2^{(m)} u^{(m)} \\ h \end{pmatrix}. \tag{19}$$

3. Numerical experiments

In this section, we conduct numerical experiments on a 2D nonlinear photonic crystal structure, where a Kerr-type nonlinear medium is embedded in the central region. The overall geometry exhibits both periodicity and material discontinuities, distinguishing it from previously studied models that typically involve layered media or smoothly varying refractive indices [7,8,14].

We now verify the accuracy of the proposed fourth-order finite difference scheme in a 2D photonic crystal structure. Let the computational domain be defined as $\Omega = [8,8]^2$ and the nonlinear Kerr region be $\Omega_0 = [4,4]^2$, we consider the case where the nonlinearity parameter is given by $\varepsilon = k_0^{-2}$, and compare the numerical solution with the analytical expression [18]:

$$E_{\text{exact}}(x,y) = \frac{5\sqrt{2}\, e^{iy\sqrt{k_0^2+25}}}{\sqrt{\varepsilon}\, k_0 \cosh(5x)}.$$

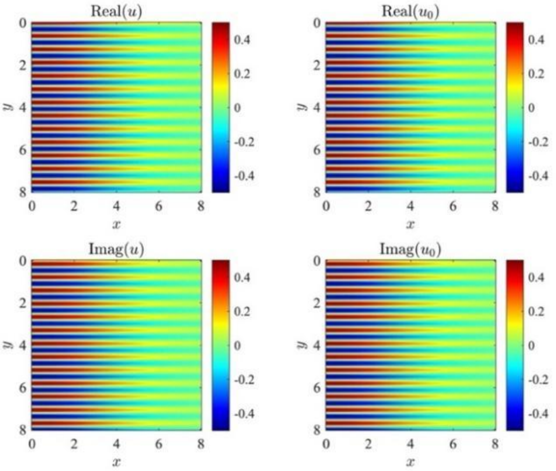

Fig. 2 Comparison between numerical solutions u and exact solutions u_0

As shown in Fig.2, the solution exhibits high-frequency oscillations. Nevertheless, the numerical results show excellent agreement with the exact solution in both the real and imaginary components.

Table 2. Comparison of iteration numbers for different iterative methods

k_0	5	10	20	40	80
Fixed-point	1057	438	135	38	/
Frozen nonlinearity	10	12	/	/	/
Newton	87	111	93	110	124
Modified Newton	11	57	11	10	10

Table 2 shows that the fixed-point method converges slowly, while Newton-type methods are sign-ificantly more efficient. In particularly, the modified Newton method maintains consistently low iteration numbers across all values of k_0 presented in the table above, indicating superior robustness and convergence performance for NLH equation.

4. Summary

This paper presents a fourth-order finite difference framework for solving the 2D NLH equation in photonic crystals with localized Kerr-type nonlinearities. Compared to previous studies on layered or smooth media, we consider a more complex geometry with periodic structure and discontinuous coefficients.

Numerical validation using analytical solutions confirms the method's accuracy and efficiency. The fourth-order scheme maintains high fidelity in highly oscillatory regimes, while iterative comparisons show Newton-type methods—especially the modified Newton's approach—achieve robust convergence across wavenumbers, outperforming slower fixed-point iterations.

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