

Modified nonlinear Schrödinger equation for frequency-dependent nonlinear profiles of arbitrary sign

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In recent times, materials exhibiting frequency-dependent optical nonlinearities, such as nanoparticle-doped glasses and other metamaterials, have gathered significant interest. The simulation of the propagation of intense light pulses in such media, by means of the nonlinear Schrödinger equation (NLSE), poses the problem in that straightforward inclusion of a frequency-dependent nonlinearity may lead to unphysical results, namely, neither the energy nor the photon number is conserved in general. Inspired by a simple quantum-mechanical argument, we derive an energy- and photon-conserving NLSE (pcNLSE). Unlike others, our approach relies only on the knowledge of the frequency-dependent nonlinearity profile and a generalization of Miller's rule for nonlinear susceptibility, enabling the simulation of nonlinear profiles of arbitrary frequency dependence and *sign*. Moreover, the proposed pcNLSE can be efficiently solved by the same numerical techniques commonly used to deal with the NLSE. Relevant simulation results supporting our theoretical approach are presented.

1. INTRODUCTION

Propagation of light pulses in nonlinear Kerr media, such as nonlinear optical fibers and waveguides, is usually modeled by the well-known nonlinear Schrödinger equation (NLSE) [1], which provides a powerful approximation based on the Maxwell equations. The usefulness of the NLSE stems from the existence of efficient numerical algorithms to solve it [1,2] and the fact that it has been proven to be accurate in a wide variety of cases. However, the NLSE may well reach the limits of its validity in various scenarios, and therefore, many attempts to introduce modifications extending its applicability, for instance to shorter pulses, have been proposed [3–10].

In the past few years, researchers in the field of nonlinear optics have shown an increased interest in new kinds of materials, such as nanoparticle-doped glasses [11–15] and other metamaterials [16–21]. The nonlinear refractive index of these media is strongly frequency dependent, giving rise to unusual phenomena such as solitons and modulation instability in the normal-dispersion regime, the existence of a zero-nonlinearity wavelength, and even a controllable self-steepening parameter

[14,17]. Modeling of light propagation in these peculiar media requires a modification of the NLSE taking into account the frequency dependence of the nonlinear coefficient [17,21–26]. A simple approach consists of preserving the NLSE and adding a wavelength dependence to the nonlinear coefficient. However, it is a well-established fact that, in general, this approach does not preserve either the energy or the photon number [25,27].

In this paper, we focus on the question of which conditions an NLSE-like equation should meet in order to satisfy fundamental physical constraints such as energy and photon-number conservation, even in the context of arbitrary frequency-dependent nonlinearities. By looking at four-wave-mixing (FWM) processes from a quantum mechanical point of view, we arrive at a modified equation that naturally conserves both quantities in lossless waveguides. A further simplification is obtained by assuming the validity of a generalized Miller's rule for nonlinear susceptibility [28]. This simplification enables the simulation of light propagation relying on the usual nonlinear parameter $\gamma(\omega)$ and avoiding more complex parameters that are difficult

to measure and scarcely found in the literature. It is worth mentioning that a generalization of the proposed approach may provide a way to extend the modified equation to include the Raman (delayed) response of the medium (see Ref. [29]).

We must note that there have been other approaches to the problem of energy and photon conservation in the presence of frequency-dependent nonlinearities. For instance, in Ref. [25], a modified NLSE was presented in the context of the analysis of mode profile dispersion. However, to the best of our knowledge, a method that makes use only of the nonlinear profile $\gamma(\omega)$, yielding physically sound results even when considering highly frequency-dependent nonlinearities of arbitrary sign, has not yet been presented elsewhere.

The remaining of the paper is organized as follows. In Section 2, we briefly review limitations of the NLSE to accurately model frequency-dependent nonlinearities. In Section 3, we derive a new photon-conserving NLSE (pcNLSE) that allows to model the propagation of light in waveguides with arbitrary nonlinearities. Section 4 presents extensive simulation results supporting the soundness of our approach. Finally, we close the paper with some conclusions in Section 5.

2. ON THE LIMITS OF THE NONLINEAR SCHRÖDINGER EQUATION

Let us recall that, in the frequency domain, the NLSE reads [1]

$$\begin{aligned} \frac{\partial \tilde{A}_\omega}{\partial z} &= i\beta(\omega)\tilde{A}_\omega + i\gamma(\omega)\mathcal{F}(|A|^2 A) \\ &= i\beta(\omega)\tilde{A}_\omega + i \iint \frac{\gamma(\omega)}{(2\pi)^2} \tilde{A}_{\omega'}^* \tilde{A}_{\omega-\mu} \tilde{A}_{\omega'+\mu} d\omega' d\mu, \end{aligned} \quad (1)$$

where z is the direction of propagation, A is the complex envelope of the electric field normalized such that $|A|^2$ is the optical power, $\tilde{A}_\omega = \mathcal{F}(A)$, and \mathcal{F} stands for the Fourier transform. Since we focus on the lossless case, the mode-propagation profile $\beta(\omega)$ is assumed to be real valued. The nonlinear coefficient $\gamma(\omega)$ is related to the third-order susceptibility $\chi^{(3)}$ and the effective area of the transverse mode. It is customary to assume that

$$\gamma(\omega) = \frac{n_2(\omega) \times (\omega + \omega_0)}{c A_{\text{eff}}(\omega)} \approx \gamma_0 + \gamma_1 \cdot \omega, \quad (2)$$

where ω_0 is the central frequency of the propagating pulse, c is the speed of light, and $n_2(\omega)$ and $A_{\text{eff}}(\omega)$ are the frequency-dependant nonlinear refractive index and mode effective area, respectively. In many cases, only the first-order approximation on the right-hand side is used [3,30–32]. Usually γ_1 is written as $\gamma_0 \tau_{\text{shock}}$, where [4,30,31] $\gamma_0 = \gamma(0)$, and

$$\tau_{\text{shock}} = \frac{1}{\omega_0} + \frac{d}{d\omega} \ln \left(\frac{n_2(\omega)}{A_{\text{eff}}(\omega)} \right) \Big|_{\omega=0}. \quad (3)$$

However, as it was shown by Blow and Wood [30], the conservation of the photon number requires that $\gamma_1 = \gamma_0/\omega_0$ in the approximation. This observation raises the main question we aim to answer in this paper: what are the requirements for an

arbitrary frequency-dependent nonlinear coefficient in order to guarantee the conservation of energy and photon number?

It is instructive to analyze the conservation of these quantities in Eq. (1) by means of a simple example and physical considerations. The nonlinear term of Eq. (1) models a process where two photons at frequencies ω_1 and ω_4 are annihilated, and simultaneously, two photons at frequencies ω_2 and ω_3 are created. Let us consider such a FWM process by setting $A = \sum_{m=1}^4 A_m(z) e^{-i\omega_m t}$, where the energy conservation in the annihilation and creation of photons requires that $\omega_1 + \omega_4 = \omega_2 + \omega_3$. By replacing A in Eq. (1), we can obtain the evolution of the total energy $E \propto \sum_{m=1}^4 |A_m|^2$ and the photon number $N \propto \sum_{m=1}^4 |A_m|^2 / (\omega_0 + \omega_m)$ along the z axis. It can be shown that these quantities evolve according to

$$\frac{\partial E}{\partial z} \propto (\gamma(\omega_1) - \gamma(\omega_2) - \gamma(\omega_3) + \gamma(\omega_4)) \Delta \quad (4)$$

and

$$\frac{\partial N}{\partial z} \propto \left(\frac{\gamma(\omega_1)}{\omega_0 + \omega_1} - \frac{\gamma(\omega_2)}{\omega_0 + \omega_2} - \frac{\gamma(\omega_3)}{\omega_0 + \omega_3} + \frac{\gamma(\omega_4)}{\omega_0 + \omega_4} \right) \Delta, \quad (5)$$

with $\Delta = 4\text{Im}(A_1^* A_2 A_3 A_4^* e^{i\Delta k z})$, $\Delta k = k_1 + k_4 - k_2 - k_3$, and $k_m = \beta(\omega_m) + \sum_{n=1}^4 (2 - \delta_{mn}) \gamma(\omega_m) |A_n|^2$. From these expressions, we can deduce that energy conservation is satisfied only if $\gamma(\omega) = \gamma_0 + \gamma_1 \omega$, whereas the conservation of the number of photons requires $\gamma(\omega) = \gamma_a(\omega_0 + \omega) + \gamma_b(\omega_0 + \omega)^2$, where $\gamma_{0,1,a,b}$ are arbitrary constants. The simultaneous conservation of both quantities is obtained only in the particular case of $\gamma(\omega) = \gamma_0 + (\gamma_0/\omega_0)\omega$. In other words, in order to guarantee the conservation of energy and photon number, the nonlinear coefficient must be equal to (and not just approximated by) a linear function of frequency with a single free parameter (γ_0). From Eq. (3), it is clear that this linear relationship implies that the ratio of the nonlinear refractive index to the mode effective area ($n_2(\omega)/A_{\text{eff}}(\omega)$) must be frequency independent, a condition that has already been shown inadequate in many situations [31].

This simple analysis shows that the NLSE cannot satisfactorily deal with a frequency-dependent nonlinear refractive index and mode effective area while conserving the energy and number of photons. For this reason, many researchers have looked into variations of Eq. (1) starting from first principles [8,25,26]. In this paper, we propose an extended version of Eq. (1) that allows for an arbitrary $\gamma(\omega)$, where both the effective area and the nonlinear coefficient are frequency-dependent functions. Most importantly, the resulting equation can be solved with the very same efficient algorithms that are customarily used to solve Eq. (1).

3. PHOTON-CONSERVING NONLINEAR SCHRÖDINGER EQUATION

Since dispersion does not affect the conserved quantities, and for the sake of simplicity, let us consider a dispersionless fiber ($\beta(\omega) = 0$). Following the quantum mechanical approach to the NLSE proposed by Lai and Haus [33], we assume that this

equation can be derived as a mean-value evolution from the Schrödinger propagation equation

$$\frac{\partial}{\partial z}|\psi\rangle = i\hat{H}|\psi\rangle, \quad (6)$$

where $|\psi\rangle$ is the quantum state of light, and

$$\hat{H} = \iiint \frac{\kappa}{2} \hat{a}_{\omega_1}^\dagger \hat{a}_{\omega_2}^\dagger \hat{a}_{\omega_1-\mu} \hat{a}_{\omega_2+\mu} d\omega_1 d\omega_2 d\mu, \quad (7)$$

where \hat{a}_ω and \hat{a}_ω^\dagger are the annihilation and creation operators, and κ is the nonlinear interaction associated with the third-order susceptibility $\chi^{(3)}$. In this way, we ensure the conservation of the number of photons, since the derived equation includes a combination of all possible FWM parametric processes. Note, however, that we have neglected a term involving the combination of operators $\hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \hat{a}$, related to third-harmonic generation, as is customary in modelling propagation in fiber optics [1]. We introduce the frequency dependence of the nonlinearity by assuming that κ depends on the four frequencies involved. In order to ensure conservation of energy, we must require only \hat{H} to be hermitian. It can be easily shown that this condition is satisfied only if $\kappa_{\omega_1, \omega_2, \omega_3, \omega_4} = \kappa_{\omega_4, \omega_3, \omega_2, \omega_1}^*$. The mean value of the field-operator $\hat{A}_\omega \propto \hat{a}_\omega \sqrt{\omega_0 + \omega}$ [29] can be calculated by the Heisenberg equations of motion and reads

$$\frac{\partial \langle \hat{A}_\omega \rangle}{\partial z} = i \iint \Gamma_{\omega, \omega', \mu} \langle \hat{A}_{\omega'}^\dagger \hat{A}_{\omega-\mu} \hat{A}_{\omega'+\mu} \rangle d\omega' d\mu, \quad (8)$$

where

$$\Gamma_{\omega, \omega', \mu} = \frac{(\kappa_{\omega, \omega', \omega-\mu, \omega'+\mu} + \kappa_{\omega', \omega, \omega'+\mu, \omega-\mu}) \sqrt{\omega_0 + \omega}}{2\sqrt{(\omega_0 + \omega')(\omega_0 + \omega - \mu)(\omega_0 + \omega' + \mu)}}. \quad (9)$$

Equation (8) can be written classically as

$$\frac{\partial \tilde{A}_\omega}{\partial z} = i \iint \Gamma_{\omega, \omega', \mu} \tilde{A}_{\omega'}^* \tilde{A}_{\omega-\mu} \tilde{A}_{\omega'+\mu} d\omega' d\mu. \quad (10)$$

A Hamiltonian-based approach has already been used by Amiranashvili and colleagues [8,9]. However, since we resort to a quantum-mechanically inspired derivation, the conservation of energy and number of photons is straightforwardly guaranteed by Eq. (10). Although this equation is similar to the nonlinear term of the NLSE, there is a fundamental difference that explains the failure of the latter to preserve those quantities: the nonlinear coefficient Γ depends on the four frequencies involved in the FWM interaction, while γ depends only on ω . This fact suggests that $\gamma(\omega)$ does not provide enough information to completely describe a frequency-dependent FWM process, as the knowledge of the function $\Gamma_{\omega, \omega', \mu}$ is required. As a matter of fact, this is expected from semi-classical and quantum-mechanical derivations of $\chi^{(3)}$ [28,34].

One problem with Eq. (10) is the lack of hard-to-conduct measurements of the four-frequency dependence of Γ . Indeed, a full characterization of Γ would imply measurements of FWM for all possible combinations of the four wavelengths intervening in Eq. (10). On the contrary, it is easier to find measurements of $\gamma(\omega)$. Consequently, we propose a reasonable way

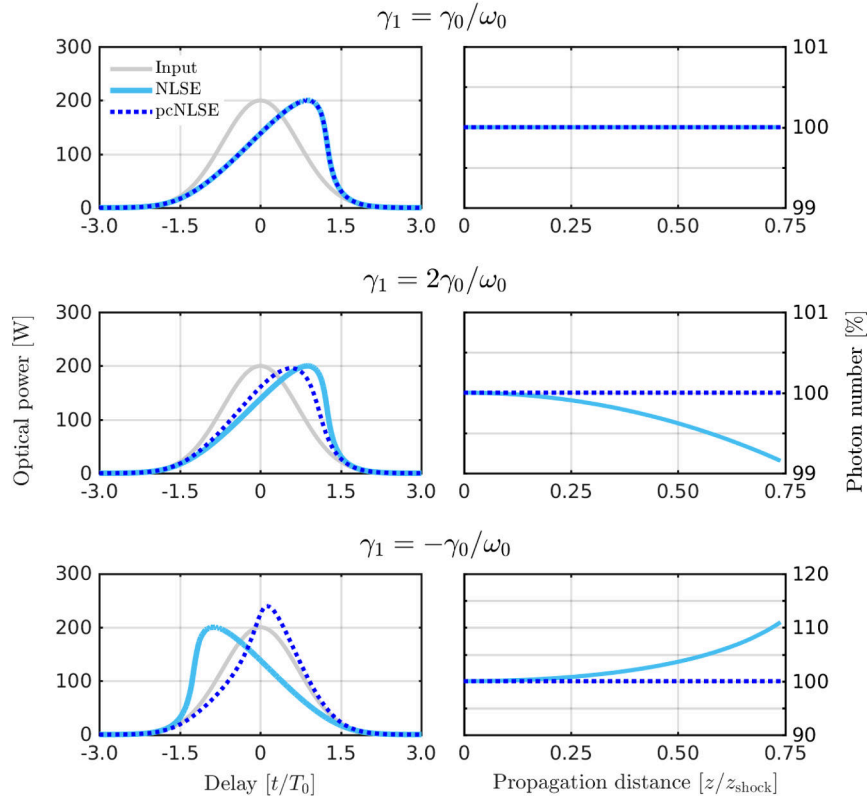


Fig. 1. Self-steepening in a nonlinear frequency-dependent waveguide for three different values of the self-steepening parameter γ_1 : pulses @ $0.75z_{\text{shock}}$ (left) and evolution of the photon number (right). While the NLSE preserves the photon number only in the first case, the pcNLSE preserves it in all cases.

to approximate Γ from a known $\gamma(\omega)$. We expect Eq. (10) and the nonlinear term of Eq. (1) to be equivalent, at least in the case of self-phase modulation (SPM), i.e., when the four frequencies involved in FWM are the same. This requirement leads to the simple relation

$$\kappa_{\omega,\omega,\omega,\omega} = \frac{\gamma(\omega) \times (\omega_0 + \omega)}{(2\pi)^2}. \quad (11)$$

Any κ that satisfies this relation and the hermiticity condition guarantees the conservation of energy and photon number and leads to an equation that is consistent with the expected behavior of a light pulse propagating in a waveguide under the sole effect of SPM. In order to choose a single κ satisfying both requirements, we take as a guide the generalized Miller's rule [28,34], which has been shown to be accurate for a broad range of media [35–38]. It states that $\chi_{\omega_1,\omega_2,\omega_3,\omega_4}^{(3)} \propto \chi_{\omega_1}^{(1)} \chi_{\omega_2}^{(1)} \chi_{\omega_3}^{(1)} \chi_{\omega_4}^{(1)}$. Analogously, we propose

$$\kappa_{\omega_1,\omega_2,\omega_3,\omega_4} \equiv \text{Re}(r_{\omega_1} r_{\omega_2} r_{\omega_3} r_{\omega_4}^*), \quad (12)$$

where r_ω is a possibly complex function. It must be remarked that hermiticity is automatically satisfied with this choice. Substituting Eq. (12) into Eq. (11), we find that $r_\omega = \sqrt[4]{\gamma(\omega) \times (\omega_0 + \omega)} / \sqrt{2\pi}$. Using this expression for κ in Eq. (8) and including the linear dispersion term, we obtain a very simple pcNLSE:

$$\frac{\partial \tilde{A}_\omega}{\partial z} = i\beta(\omega)\tilde{A}_\omega + i\bar{\gamma}(\omega)\mathcal{F}(C^*B^2) + i\bar{\gamma}^*(\omega)\mathcal{F}(B^*C^2), \quad (13)$$

where the variables are defined as $\tilde{B}_\omega = \sqrt[4]{\gamma(\omega)/(\omega + \omega_0)}\tilde{A}_\omega$ and $\tilde{C}_\omega = (\sqrt[4]{\gamma(\omega)/(\omega + \omega_0)})^*\tilde{A}_\omega$, and the effective nonlinear coefficient is $\bar{\gamma}(\omega) = \sqrt[4]{\gamma(\omega) \times (\omega + \omega_0)^3}/2$.

It is worthy to note that Eq. (13) can be solved by the same efficient numerical algorithms as the standard NLSE, such as the split-step Fourier method. Furthermore, Eq. (13) is valid for negative values of $\gamma(\omega)$ (such as those exhibited by some metamaterials [16–21]) without compromising the imposed photon-number conservation and SPM-consistency constraints. This constitutes a very important feature of the present approach.

As a final remark, when considering a fiber with constant n_2 and a frequency-dependent effective area A_{eff} , we can simplify Eq. (13) to

$$\frac{\partial \tilde{A}_\omega}{\partial z} = i\beta(\omega)\tilde{A}_\omega + i\frac{n_2 \times (\omega_0 + \omega)}{c\sqrt[4]{A_{\text{eff}}(\omega)}}\mathcal{F}(|G|^2 G), \quad (14)$$

with $\tilde{G}_\omega = \tilde{A}_\omega / \sqrt[4]{A_{\text{eff}}(\omega)}$. This equation is equivalent to an approximation also in Ref. [25] that takes into account the frequency-dependent nature of A_{eff} . Also, if we consider a fiber with constant n_2 and constant A_{eff} , the pcNLSE reduces to the standard NLSE [Eq. (1)], as expected.

4. SIMULATION RESULTS

We now compare results from Eq. (13) to those obtained with the NLSE. First, we focus on the self-steepening of short pulses

under arbitrary shock parameters (γ_1), a relevant case in the study of metamaterials where γ_1 can be “engineered” to take either positive or negative values [17]. Furthermore, a negative γ_1 is often used to model the nonlinear profile of many novel materials, such as silver-nanoparticle-doped photonic crystal fibers (SNPCFs) [13–15]. Both Eq. (1) and Eq. (13) were numerically solved using the split-step Fourier method [1]. The waveguide parameters are $\beta(\omega) = 0$ and $\gamma(\omega) = \gamma_0 + \gamma_1\omega$, where $\gamma_0 = 1.2 \times 10^{-3}/\text{Wm}$, and γ_1 takes three different values: $\gamma_1 = \gamma_0/\omega_0$, $\gamma_1 = 2\gamma_0/\omega_0$, and $\gamma_1 = -\gamma_0/\omega_0$. The input is a Gaussian pulse $A(t) = \sqrt{P_0}e^{-t^2/2T_0^2}$, with $P_0 = 200$ W, $T_0 = 0.1$ ps, and central frequency ω_0 corresponding to a wavelength $\lambda_0 = 1550$ nm. The propagation distance is measured in terms of the shock distance, defined as $z_{\text{shock}} = 0.39 T_0/(|\gamma_1| P_0)$ [1]. Figure 1 shows simulation results for the three different values of γ_1 . As expected, when $\gamma_1 = \gamma_0/\omega_0$, the pcNLSE matches completely the standard NLSE, and both equations preserve the number of photons. For any other values of γ_1 , the NLSE fails to preserve this quantity. The pcNLSE, however, does conserve

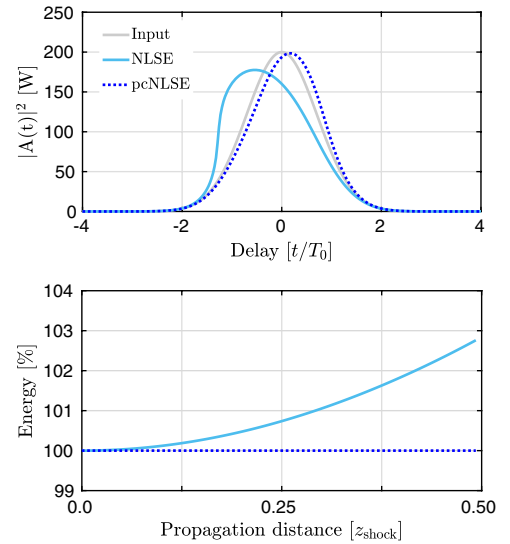


Fig. 2. Pulse propagation in a waveguide with a quadratic nonlinear profile as predicted by the NLSE and the pcNLSE: pulses @ $0.5z_{\text{shock}}$ (top) and evolution of the pulse energy (bottom). Pulse energy is referred to as the input value. Unlike the pcNLSE, the NLSE predicts an unphysical increase in energy.

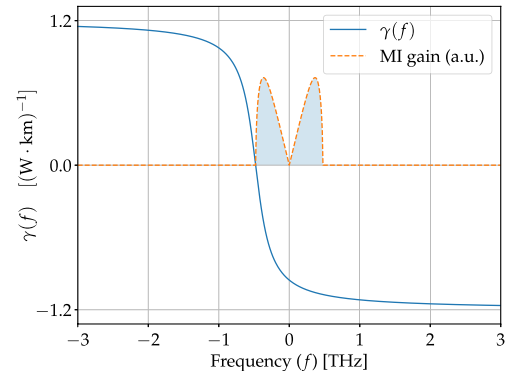


Fig. 3. Nonlinear profile and corresponding MI gain.

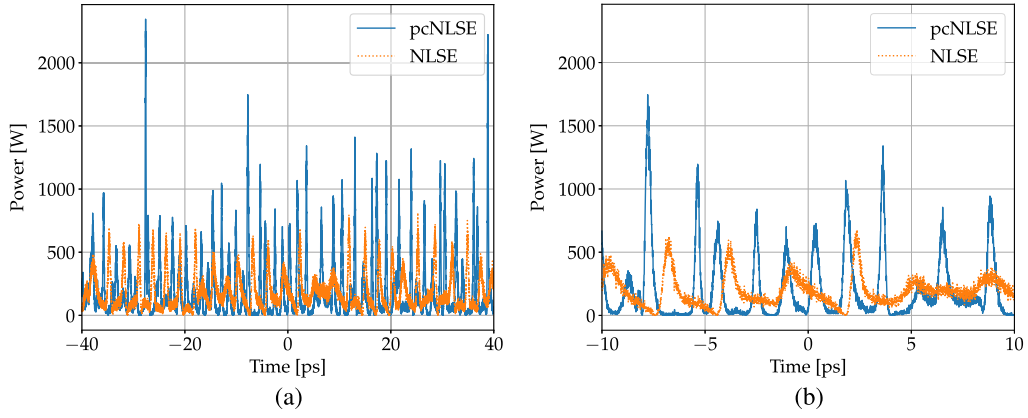


Fig. 4. Power versus time at a $900 L_D$ distance (a) and detail (b).

the photon number for any self-steepening parameter, as it is expected for such a parametric process. Notably, in all cases, the pcNLSE predicts a lagging pulse peak due to self-steepening.

In a more general case, with a nonlinear profile that is not a linear function of frequency, the NLSE may lead to unphysical results that do not preserve either the photon number or the energy, whereas the pcNLSE preserves both. This is shown in Fig. 2, where we add a quadratic term to the nonlinearity, $\gamma(\omega) = \gamma_0 + \gamma_1(\omega) + \gamma_2\omega^2/2$, representing a nonlinear profile used in the numerical analysis of the propagation in metamaterial waveguides [17,18,20]. Figure 2 shows results for parameters $\gamma_0 = 1.2 \times 10^{-3}/\text{W m}$, $\gamma_1 = -9.8 \times 10^{-7}\text{ps}/\text{W m}$, and $\gamma_2 = 3.2 \times 10^{-9}\text{ps}^2/\text{W m}$. Equation (1), unlike Eq. (13), predicts the energy of the output pulse to be unphysically 3% higher than that of the input pulse.

Finally, to further illustrate how significantly different predictions may arise by using the pcNLSE and the NLSE, we choose a context where the frequency dependence and sign of $\gamma(\omega)$ play a central role: modulation instability (MI) in nonlinear metamaterials [18,20]. Figure 3 presents a particularly interesting setting in which there is a zero-nonlinearity wavelength (ZNW), and a pump is applied in the negative nonlinearity region. Figure 3 also shows the MI gain spectrum predicted by a standard first-order linear stability analysis based on the usual NLSE (see, e.g., Ref. [39]) for $\beta(\omega) = \beta_2\omega^2/2$, $\beta_2 = 9.6 \times 10^{-3} \text{ ps}^2/\text{m}$, and

$\gamma(\omega) = \frac{-1.2[(\text{W-km})^{-1}]}{\pi/2} \arctan(\omega + 3)$, a sigmoid function with zero nonlinearity at $\simeq -0.5 \text{ THz}$. As it can be readily observed, there is MI gain in the normal dispersion regime whenever $\gamma(\omega)$ is negative. Figures 4–6 compare the results of the pcNLSE and the NLSE when a 200 W CW pump is applied. Figure 4 presents the results of a single noise realization in the time domain at $z = 900 L_D$, where the dispersion length $L_D = \beta_2/T_0^2$ is calculated for the average $T_0 \simeq 0.4 \text{ ps}$ as obtained from Fig. 4. We used additive white Gaussian noise with a fixed number of photons per mode. It must be remarked that, although exactly the same input (noise realization and pump) was used in both cases, very different results are obtained. In particular, the pcNLSE predicts some pulses of a much higher intensity than those expected from the NLSE. Figure 5 shows the spectral density predicted by both equations at the same distance, obtained by averaging results from 50 noise realizations. Not only the spectrum resulting from the NLSE falls off much faster than that predicted by the pcNLSE, but there is also a significant difference in the position of the MI peak gain, which is correlated to the difference in the beating frequency observed in the pulses in Fig. 4. Both the higher intensity pulses and slower power spectrum fall-off in the case of the pcNLSE with respect to the NLSE can be related to the fact that the former conserves the number of photons and the latter does not. Indeed, Fig. 6 shows how the number of photons varies with distance. Almost 15% of

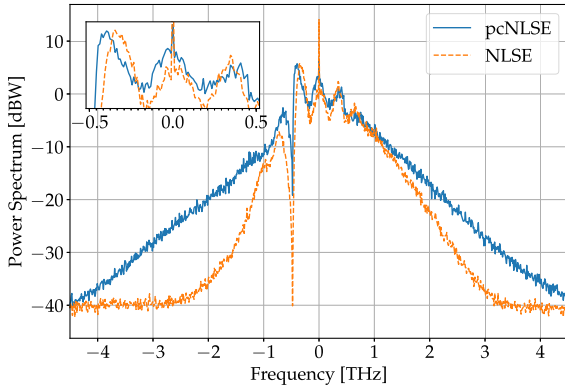


Fig. 5. Power spectra averaged over 50 noise realizations at a $900 L_D$ propagated distance.

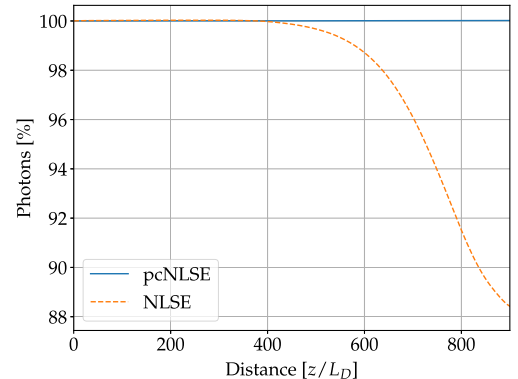


Fig. 6. Percentage of the total number of photons conserved as a function of propagated distance.

photons disappear after $900L_D$ when using the standard NLSE, leading to clearly unphysical results.

5. CONCLUSION

We presented an approach that enables the simulation of light propagation through media with peculiar nonlinearities. By departing only from the knowledge of the medium nonlinear profile (i.e., $\gamma(\omega)$), we arrive at an equation (pcNLSE) that circumvents the problem of photon-number conservation, an artifact present in the commonly adopted approach of modifying the NLSE by the addition of a frequency dependence to the mode effective area. Moreover, our proposed approach, whose results rely solely on the validity of a generalized Miller's rule, also allows for the study of nonlinear profiles of an arbitrary sign. Finally, the introduced pcNLSE can be solved by the same well-known and efficient numerical algorithms used for solving the NLSE, thus readily putting forth a powerful tool to assess nonlinear propagation in new and interesting media.

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