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Self-consistent treatment of the full vectorial nonlinear optical pulse propagation equation in an isotropic medium

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Abstract

We derive a propagation equation for the pulse envelope of an electromagnetic field in an isotropic nonlinear dispersive media. The equation is first order in the propagation coordinate. We develop expressions valid without any additional assumptions on the form of the nonlinear polarization. Specific results are given for a Kerr-type nonlinear polarization in the form of a truncated nonlinear differential polynomial. We discuss the applicability of the expansion and determine the conditions for its validity; if and only if the counter-propagating wave is negligible is the expansion valid. We take into account a vectorial character of the electromagnetic field and show that it generates corrections of the same order as the nonparaxial terms.

1. Introduction

The propagation equation governing the evolution of the slowly varying envelope of the electric field of a light pulse of light is key to understanding nonlinear optical phenomena. The wave equation for an optical pulse is derived from Maxwell equations, but to save computational effort, one usually considers the slowly varying envelope of the electric field and develops a propagation equation which involves only the first derivative in the propagation direction. In the regime of very short pulses, strongly focused pulses and/or pulses with large intensities, great care must be taken in order to retain mathematical self-consistency in going beyond simple slowly varying envelope and paraxial approximations. There are many examples where simulation of pulse propagation beyond these approximations is necessary. One example is in near-field scanning optical microscopy [1], where an optical pulse (or beam) with transverse dimension a small fraction of a wavelength can be generated at the end of an optical fiber pulled to a narrow tip and coated with metal. The slowly varying envelope approximation (SVEA) cannot be used to propagate a pulse

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(beam) wherein forward and backward propagating components are both present and interact with one another. Another example is a very short duration pulse that is only a few optical cycles long. Starting from the pioneering work of Lax et al. [2], the conceptual and practical importance of describing such pulses was well recognized; it is described even in textbooks [3]. Many attempts has been made [4–13] to generalize a parabolic wave equation in a rigorous manner to include to all order corrections in the small parameters $\eta \equiv (\omega_0\tau_0)^{-1}$ and $\epsilon \equiv (k_0\sigma_0)^{-1}$. Here τ_0 is the pulse duration, ω_0 is the central frequency of the pulse, $k_0 = n(\omega_0)\omega_0/c$ is central wavevector magnitude in the medium, σ_0 is the transverse pulse width and $n_0 \equiv n(\omega_0)$ is the refractive index at the central frequency. Few publications addressed the issue of preserving a vectorial nature of the problem [10–13]. Here we present a first attempt to combine a short, strongly focused pulses regime with full vectorial aspect of the propagation.

The outline of the paper is as follows. In Section 2 we begin by considering the general electromagnetic wave equation derived from Maxwell's equations. In Section 2.1 we treat the case of a linear polarization, and we then introduce the slowly varying envelope concept in Section 2.2. We complete the derivation, first in the model scalar field case in Section 3, where we introduce dimensionless units in Section 3.1. We outline the expansion in the scalar wave equation case in Section 3.2, describe the normal-incidence boundary matching for the scalar wave case in Section 5, and derive the full equation in the general vectorial case in Section 4. A summary and conclusion is presented in Section 8.

It was shown by Brabec et al. [6] that it is meaningful to consider a slowly varying envelope of the electric field, $\mathbf{A}(\mathbf{r}, t)$, even down to the single optical cycle regime. Similarly, one can consider a slowly varying envelope for extremely focused optical beams or pulses. Since in these cases $\mathbf{A}(\mathbf{r}, t)$ may not be slowly varying as a function of its arguments, we prefer to call $\mathbf{A}(\mathbf{r}, t)$ the wave packet envelope (WPE) for the electric field.

2. Wave equation

We begin with Maxwell equations. Upon using the Faraday and Ampére equations we obtain the wave equation (1) for the electric field vector in the usual fashion [14], and Gauss's Law (2) serves as a constraint equation:

$$-\nabla \times \nabla \times \mathbf{E}(\mathbf{r}, t) = \frac{1}{c^2}\partial_t^2[\mathbf{E}(\mathbf{r}, t) + 4\pi\mathbf{P}(\mathbf{r}, t)], \tag{1}$$

$$\nabla \cdot [\mathbf{E}(\mathbf{r}, t) + 4\pi\mathbf{P}(\mathbf{r}, t)] = 0. \tag{2}$$

Here the polarization has linear and nonlinear contributions, $\mathbf{P} = \mathbf{P}^{\mathrm{L}} + \mathbf{P}^{\mathrm{NL}}$. The linear and nonlinear parts of the polarization depend on details of the medium in which the light propagates. A particular contribution to the nonlinear polarization corresponding to a given frequency and wavevector may be singled out, depending on the nonlinear process that we wish to describe (e.g., second harmonic generation or self-focusing). Our discussion is initially quite general, without using a specific form of the nonlinear polarization. Later, as an illustration, we use the case of a Kerr nonlinearity.

2.1. Linear polarization

Let us consider only the linear polarization in Eq. (1). In a linear dispersive medium, the electric induction vector, $\mathbf{D}^{\mathrm{L}} = \mathbf{E} + 4\pi\mathbf{P}^{\mathrm{L}}$, can be described by the convolution of the electric field vector with a tensor response function $\hat{\boldsymbol{\varepsilon}}(t)$ [14]

$$\mathbf{D}^{\mathrm{L}}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}, t) + 4\pi\mathbf{P}^{\mathrm{L}}(\mathbf{r}, t) = \int_{-\infty}^{+\infty} \mathrm{d}\tau\, \hat{\boldsymbol{\varepsilon}}(t - \tau)\mathbf{E}(\mathbf{r}, \tau). \tag{3}$$

Although our method can in principle treat the anisotropic case, we restrict our discussion here to an isotropic medium to avoid tedious tensorial algebraic expressions. In the isotropic case, the dielectric tensor $\hat{\boldsymbol{\varepsilon}}$ is proportional to the unit matrix, and we can drop the tensorial indices in Eq. (3) leaving a scalar quantity $\hat{\boldsymbol{\varepsilon}} \equiv \varepsilon$. In the linear regime, the right-hand side (RHS) of Eq. (1) may be transformed to Fourier space as follows:

$$\frac{1}{c^2}\partial_t^2\left(\mathbf{E}(t) + 4\pi\mathbf{P}^{\mathrm{L}}(t)\right) = -\int_{-\infty}^{+\infty} \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega t}\,\frac{\omega^2}{c^2}\left(\tilde{\mathbf{E}}(\omega) + 4\pi\tilde{\mathbf{P}}^{\mathrm{L}}(\omega)\right)$$
$$= -\int_{-\infty}^{+\infty} \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega t}\left(\frac{\omega}{c}\right)^2 \varepsilon(\omega)\,\tilde{\mathbf{E}}(\omega) \equiv -\int_{-\infty}^{+\infty} \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega t}\, k^2(\omega)\,\tilde{\mathbf{E}}(\omega), \tag{4}$$

where $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{P}}$ are the Fourier transforms of $\mathbf{E}$ and $\mathbf{P}$. We also used the relation $k^2(\omega) = \varepsilon(\omega)(\omega/c)^2$ $(= n^2(\omega)(\omega c)^2)$ and Eq. (3) together with convolution theorem.

2.2. Slowly varying envelope

Using the results of the previous subsection, we can rewrite Eq. (1) as

$$-\nabla\times\nabla\times\mathbf{E}(\mathbf{r},t) = \frac{4\pi}{c^2}\partial_t^2\mathbf{P}^{\mathrm{NL}}(\mathbf{r},t) - \int_{-\infty}^{+\infty}\mathrm{d}\omega\,\mathrm{e}^{-\mathrm{i}\omega t}\,k^2(\omega)\tilde{\mathbf{E}}(\omega). \tag{5}$$

Now we use the concept of the WPE of the electric field $\mathbf{E}(\mathbf{r},t)$ and the nonlinear polarization $\mathbf{P}^{\mathrm{NL}}(\mathbf{r},t)$,

$$\mathbf{E}(\mathbf{r},t) = \mathrm{e}^{\mathrm{i}k_0 z - \mathrm{i}\omega_0 t}\mathbf{A}(\mathbf{r},t) + \text{c.c.}, \tag{6a}$$

$$\mathbf{P}^{\mathrm{NL}}(\mathbf{r},t) = \mathrm{e}^{\mathrm{i}k_0 z - \mathrm{i}\omega_0 t}\mathbf{R}(\mathbf{r},t) + \text{c.c.}, \tag{6b}$$

where ω_0 is central angular frequency of the pulse and $k_0 = k(\omega_0) = n(\omega_0)\omega_0/c$ is its central wavevector.

It is essential that the positive (i.e., $\mathrm{e}^{\mathrm{i}k_0 z - \mathrm{i}\omega_0 t}\mathbf{A}(\mathbf{r},t)$) and negative (the c.c. of $\mathrm{e}^{\mathrm{i}k_0 z - \mathrm{i}\omega_0 t}\mathbf{A}(\mathbf{r},t)$) spectral components be distinguishable if the concept of a WPE is to make sense. This is assured if $\tilde{\mathbf{A}}(\mathbf{k},\omega) \approx 0$ for all $\mathbf{k}$ and for all frequencies ω near zero frequency. This condition is in turn satisfied if the pulse is at least as long as an optical cycle and its central propagation direction is well defined.

If the electric field vector $\mathbf{E}$ and nonlinear polarization $\mathbf{P}^{\mathrm{NL}}$ satisfy Eq. (5), an analogous equation for their WPEs, $\mathbf{A}$ and $\mathbf{R}$, have the same structure provided we (a) make the following substitutions for the differential operators ∇ and ∂_t:

$$\nabla \to \tilde{\nabla} \equiv \begin{pmatrix} \partial_{\tilde{x}} \\ \partial_{\tilde{y}} \\ \partial_z + \mathrm{i}k_0 \end{pmatrix}, \tag{7a}$$

$$\partial_t \to \widetilde{\partial_t} \equiv \partial_t - \mathrm{i}\omega_0, \tag{7b}$$

and (b) we substitute $k^2(\omega)$ with $k^2(\omega+\omega_0)$ under the Fourier integral in Eq. (5). Next we expand $k(\omega+\omega_0)$ in a Taylor series,

$$k(\omega+\omega_0)\tilde{\mathbf{A}}(\omega) = \left(\sum_{j=0}\frac{\beta_j}{j!}\omega^j\right)\tilde{\mathbf{A}}(\omega), \tag{8}$$

where $\beta_j = \partial_\omega^j k(\omega)|_{\omega=\omega_0}$ and $\beta_0 = k(\omega_0) = (n(\omega_0)\omega_0)/c \equiv k_0$. Upon taking the inverse Fourier transform of Eq. (8), we can define a dispersion operator $\hat{D}$

$$\hat{D}(\partial_t)\mathbf{A}(t) \equiv \hat{D}\mathbf{A}(t) \equiv \left(\sum_{j=0}\frac{\beta_j}{j!}(\mathrm{i}\partial_t)^j\right)\mathbf{A}(t). \tag{9}$$

Finally, Eq. (5) takes the form

$$-\tilde{\nabla} \times \tilde{\nabla} \times \mathbf{A}(\mathbf{r}, t) = \frac{4\pi}{c^2} \tilde{\partial}_t^2 \mathbf{R}(\mathbf{r}, t) - \hat{D}^2 \mathbf{A}(t). \tag{10}$$

3. Scalar approximation

In this section we assume that **A** and **R** are linearly polarized along the x direction

$$\mathbf{A} = \hat{\mathbf{e}}_x A \quad \text{and} \quad \mathbf{R} = \hat{\mathbf{e}}_x R, \tag{11}$$

i.e., we explicitly neglect longitudinal (along propagation direction) component of the electric field. Within this approximation Eq. (10) reduces to

$$\tilde{\nabla}^2 A = \frac{4\pi(\partial_{\tilde{t}} - \mathrm{i}\omega_0)^2}{c^2} R - \hat{D}^2 A, \tag{12}$$

where $A = A(\mathbf{r}, t)$ is a scalar function. We can rewrite Eq. (12) as follows:

$$\partial_z A = \frac{1}{2\mathrm{i}k_0} \left[(k_0^2 - \hat{D}^2) A - \Delta_\perp A + \frac{4\pi}{c^2} (\partial_t - \mathrm{i}\omega_0)^2 R - \partial_z^2 A \right]. \tag{13}$$

Eq. (13) also applies to the case of a planar waveguide in the y–z plane if all derivatives with respect to x are ignored. In this case, due to the boundary conditions, both the electric field vector and the polarization vector have nonzero components only along the x direction for TE modes.

Eq. (13) is the starting point for our perturbative analysis of the scalar wave equation case. In the next section we introduce the dimensionless variables used for deriving the expansion.

3.1. Dimensionless parameters

Throughout the rest of the paper we take time in units of the initial temporal pulse duration τ_0, and x and y in units of the initial transverse pulse width σ_0, and z in units of $1/k_0$, where $k_0 = k(\omega_0)$. Dimensionless variables are very useful for the estimates of the contribution of different terms in the expansion that we present below. Furthermore, we introduce the small dimensionless parameters ϵ and η, that are our expansion parameters. They determine the contribution of higher order terms in our expansion. Our change of variables is defined by:

$$\mathbf{r}_\perp = \sigma_0 \tilde{\mathbf{r}}_\perp, \tag{14a}$$

$$t = \tau_0 \tilde{t}, \tag{14b}$$

$$z = \frac{1}{k_0} \tilde{z}. \tag{14c}$$

As long as we measure time and space in the units defined by (14a), the magnitude of the temporal derivatives of amplitude A and its derivatives with respect to $\tilde{x}$ and $\tilde{y}$ (perpendicular spatial variables) for a Gaussian-shaped pulse are of the same order as the amplitude of the pulse itself, $\mathrm{O}(\partial_{\tilde{t}} A) = \mathrm{O}(\partial_{\tilde{x}} A) = \mathrm{O}(\partial_{\tilde{y}} A) = \mathrm{O}(A) = \mathrm{O}(1)$. We also define two dimensionless parameters:

$$\epsilon = (k_0 \sigma_0)^{-1}, \tag{15a}$$

$$\eta = (\omega_0 \tau_0)^{-1}. \tag{15b}$$

These parameters give the perpendicular pulse dimension in natural units of $1/k_0$ and the pulse duration in natural units of $1/\omega_0$. The dispersion parameter η characterizes the temporal extent of the pulse; the shorter the pulse, the larger the parameter η. The diffraction parameter ε characterizes the transverse spatial extent of the pulse.

In terms of the dimensionless variables in Eq. (15a), Eq. (13) is written as

$$\partial_{\tilde{z}}A = \underbrace{\frac{i}{2}\left(\frac{\hat{D}^2(\omega_0\eta\partial_{\tilde{t}})}{k_0^2} - 1\right)A + i\frac{\varepsilon^2}{2}\Delta_{\tilde{\perp}}A}_{\hat{L}A} + \underbrace{\frac{-4\pi i(\eta\partial_{\tilde{t}} - i)^2}{2n_0^2}R}_{\hat{N}R} + \frac{i}{2}\partial_{\tilde{z}}^2 A. \tag{16}$$

We defined the operators $\hat{L}$ and $\hat{N}$ in order to introduce a compact notation. Both operators are linear, and both commute with $\partial_{\tilde{z}}$, since they do not depend on z.

From Eq. (16) we obtain a series expansion of $\partial_{\tilde{z}}A$ in the small parameters η and ϵ^2. The two parameters η and ϵ^2 are already identified, but as we show later, there is one additional parameter (that we call δ) that is needed in the nonlinear case. Its particular form depends on the form of the nonlinear polarization.

3.2. Expansion in terms of η, ϵ and δ

3.2.1. Linear polarization case

If the magnitude of the electric field is small and we can neglect the nonlinearity in Eq. (16), this equation simplifies to

$$\partial_{\tilde{z}}A = \hat{L}A + \frac{i}{2}\partial_{\tilde{z}}^2 A. \tag{17}$$

It then has an formal analytic solution of the form

$$\partial_{\tilde{z}}A = \left(\pm i\sqrt{1 - 2i\,\hat{L}} - i\right)A, \tag{18}$$

where + and − correspond to forward and backward propagating waves. The forward linear propagation operator is described by

$$\hat{\mathscr{L}} = i\sqrt{1 - 2i\,\hat{L}} - i, \tag{19}$$

where both small parameters η and ϵ are hidden in the definition of $\hat{L}$. When the pulse is very wide compared with $1/k_0$, diffraction becomes small. In the plane wave limit $\epsilon \to 0$, we can simply neglect all the terms beyond the zeroth order in ϵ to obtain a one-dimensional equation (also valid for one-dimensional pulse propagation in optical fibers). Using Eqs. (16) and (19) we find

$$\hat{\mathscr{L}} \to i\frac{\hat{D}(\omega_0\eta\partial_{\tilde{t}})}{k_0} - i, \tag{20}$$

where

$$\hat{D}(\omega_0\eta\partial_{\tilde{t}}) = \left(\sum_{j=0}\frac{\beta_j}{j!}(i\omega_0\eta\partial_t)^j\right). \tag{21}$$

Eq. (20) justifies the name linear dispersion operator for $\hat{D}$ introduced in Section 2.2. The operator $\hat{D}$ can be truncated at any power of η to yield a partial differential equation for the propagation dynamics. Second and third order expansions are standard textbook examples. An almost equally simple exercise consists of expanding $\hat{\mathscr{L}}$ in a series in η and ϵ. In this case we obtain a linear partial differential propagation equation in the independent variables z, t, x and y. Upon expanding Eq. (20) to fourth order in η and ϵ we find

$$\hat{\mathscr{L}} = -\frac{\omega_0\beta_1}{k_0}\eta\partial_{\tilde{t}} - \frac{i}{2}\frac{\beta_2\omega_0^2}{k_0}\eta^2\partial_{\tilde{t}}^2 + \frac{1}{6}\frac{\beta_3\omega_0^3}{k_0}\eta^3\partial_{\tilde{t}}^3 + \frac{i}{24}\frac{\beta_4\omega_0^4}{k_0}\eta^4\partial_{\tilde{t}}^4 + \left(\frac{i}{2} + \frac{1}{2}\frac{\beta_1\omega_0}{k_0}\eta\partial_{\tilde{t}} + \frac{i\omega_0^2}{2}\left(\frac{1}{4}\frac{\beta_2}{k_0} - \frac{\beta_1^2}{k_0^2}\right)\eta^2\partial_{\tilde{t}}^2\right)\epsilon^2\nabla_{\perp}^2 - \frac{i}{8}\epsilon^4\nabla_{\perp}^4 + O(\max(\eta,\epsilon)^5). \tag{22}$$

We have shown above how to obtain a differential propagation equation upon expanding the linear propagation operator defined in Eq. (19). However, this method is not easily generalized to the nonlinear case. Therefore we introduce an alternative expansion method, that can be generalized to the nonlinear case, consisting of the recursive substitution of the z-derivatives on the RHS of Eq. (17). The details of the generalization to the nonlinear scalar case will be presented in the next section, and the nonlinear vectorial case will be discussed towards the end of this paper. The main idea of the method is to construct a series of approximations for $\partial_{\tilde{z}}A$ using Eq. (16), which in the linear case reduces to

$$\partial_{\tilde{z}}A - \hat{L}A = \frac{i}{2}\partial_{\tilde{z}}(\partial_{\tilde{z}}A). \tag{23}$$

Let $[\partial_{\tilde{z}}A]^{(j)}$ be the jth order approximation to $\partial_{\tilde{z}}A$. We define the recurrence equations:

$$[\partial_{\tilde{z}}A]^{(1)} - \hat{L}A = 0, \tag{24a}$$

$$[\partial_{\tilde{z}}A]^{(2)} - \hat{L}A = \frac{i}{2}\partial_{\tilde{z}}([\partial_{\tilde{z}}A]^{(1)}) = \frac{i}{2}\partial_{\tilde{z}}(\hat{L}A) = \frac{i}{2}\hat{L}\partial_{\tilde{z}}A = \frac{i}{2}\hat{L}[\partial_{\tilde{z}}A]^{(1)} = W_1(\hat{L})[\partial_{\tilde{z}}A]^{(1)} = \frac{i}{2}\hat{L}^2A, \tag{24b}$$

where in (24b) we first used (24a), then we commuted the $\hat{L}$ and $\partial_{\tilde{z}}$ operators, used the first order approximation of $\partial_{\tilde{z}}A$, and noted that the left-hand side of (24b) is equivalent to a polynomial of $\hat{L}$ ($W_1(\hat{L}) \equiv (i/2)\hat{L}$) acting on $[\partial_{\tilde{z}}A]^{(1)}$. For higher order j we define $[\partial_{\tilde{z}}A]^{(j+1)}$ by

$$[\partial_{\tilde{z}}A]^{(j+1)} - \hat{L}A = \frac{i}{2}\partial_{\tilde{z}}([\partial_{\tilde{z}}A]^{(j)}) = W_j(\hat{L})[\partial_{\tilde{z}}A]^{(j)}. \tag{25}$$

As a result of subsequent substitutions, the RHS of Eq. (25) eventually becomes equal to a polynomial of $\hat{L}$ ($W_j(\hat{L})$) operators acting on $[\partial_{\tilde{z}}A]^{(j)}$. The functions $[\partial_{\tilde{z}}A]^{(j)}$ defined in this way form a sequence of approximations for $\partial_{\tilde{z}}A$. In the previous paragraph we mentioned that derivatives with respect to x, y, t of the WPE are the same order of magnitude as the pulse itself. We identified two quantities η and ϵ that determine the temporal and spatial extent of the pulse with respect to the central frequency and wavelength, respectively. We use these quantities as small expansion parameters. The difference between $\partial_{\tilde{z}}A$ and $[\partial_{\tilde{z}}A]^{(j)}$ is of order η^j and ϵ^{2j}. This can be understood from the following arguments. First, to simplify the notation we define a universal parameter $f = \max(\eta, \epsilon^2)$, and use f for our estimates. It follows from equations (24a) that:

$$O([\partial_{\tilde{z}}A]^{(1)}) = O(f), \tag{26}$$

and we can estimate the difference $([\partial_{\tilde{z}}A]^{(j+1)} - [\partial_{\tilde{z}}A]^{(j)})$ using Eq. (25)

$$\begin{aligned} O\Big(([\partial_{\tilde{z}}A]^{(j+1)} - [\partial_{\tilde{z}}A]^{(j)})\Big) &= O\Big(\partial_{\tilde{z}}([\partial_{\tilde{z}}A]^{(j)} - [\partial_{\tilde{z}}A]^{(j-1)})\Big) = O\Big(f([\partial_{\tilde{z}}A]^{(j)} - [\partial_{\tilde{z}}A]^{(j-1)})\Big) \\ &= O\Big(f^2([\partial_{\tilde{z}}A]^{(j-1)} - [\partial_{\tilde{z}}A]^{(j-2)})\Big) = \cdots = O(f^{j+1}). \end{aligned} \tag{27}$$

The sequence of approximations $[\partial_{\tilde{z}}A]^{(j)}$ should be geometrically convergent due to (27), and in the limit it satisfies Eq. (17), hence $\lim_{j\to\infty}[\partial_{\tilde{z}}A]^{(j)} = \partial_{\tilde{z}}A$. We stress that in order to simplify the notation and make the above discussion more transparent we have introduced a united parameter f. However, expansion in the parameters η and ϵ can be made more or less independently. Upon truncating the series expansion and neglecting terms with powers of η and ϵ higher than five, our new expansion procedure recovers exactly the result of Eq. (22).

3.2.2. Nonlinear generalization

We now generalize the expansion method introduced at the end of the previous subsection to the nonlinear case. Specifically, we derive a perturbative expansion of Eq. (16). Our method is general and can be applied to any type of nonlinearity, but we find it instructive to present the derivation for a specific example first. We assume a form of $\mathbf{R}$ corresponding to a Kerr-type nonlinearity, a nonlinear polarization that in scalar case takes the form

$$R(\mathbf{r},t) = \chi |A(\mathbf{r},t)|^2 A(\mathbf{r},t). \tag{28}$$

The order of magnitude of the nonlinear term may be denoted as $\mathrm{O}(\hat{N}R) = \mathrm{O}(\chi |A|^2 A)$. Therefore in the nonlinear case there is one extra parameter $\delta = \chi |A|^2$, that we need to add to the two expansion parameters introduced previously. Again to simplify notation we redefine f to include this new parameter

$$f = \max(\eta, \epsilon^2, \delta). \tag{29}$$

With this new f we can estimate the order of magnitude of the full nonlinear operator in Eq. (16), in analogy to the linear case

$$\mathrm{O}(\hat{L}A + \chi \hat{N}(|A|^2 A)) = \mathrm{O}(f). \tag{30}$$

Now we can proceed with our expansion procedure. We introduce recurrence equations, which are a direct generalization of Eqs. (24a). The nonlinear term is an explicit function of the WPE; it depends on z and does not commute with $\partial_{\tilde{z}}$. Moreover, it is a function of A and A^*. Hence, we need to define a recurrence series of approximations $[\partial_{\tilde{z}}A]^{(j)}$ as follows:

$$[\partial_{\tilde{z}}A]^{(1)} - \left(\hat{L}A + \chi \hat{N}(|A|^2 A)\right) = 0, \tag{31a}$$

$$[\partial_{\tilde{z}}A]^{(2)} - \left(\hat{L}A + \chi \hat{N}(|A|^2 A)\right) = \frac{\mathrm{i}}{2}\partial_{\tilde{z}}([\partial_{\tilde{z}}A]^{(1)}) = \frac{\mathrm{i}}{2}\left(\hat{L}[\partial_{\tilde{z}}A]^{(1)} + \chi \hat{N}(2|A|^2[\partial_{\tilde{z}}A]^{(1)} + A^2[\partial_{\tilde{z}}A]^{(1)^*})\right), \tag{31b}$$

and in general

$$[\partial_{\tilde{z}}A]^{(j+1)} - \left(\hat{L}A + \chi \hat{N}(|A|^2 A)\right) = \partial_{\tilde{z}}([\partial_{\tilde{z}}A]^{(j)}). \tag{32}$$

Note that we have to substitute the complex conjugate of $[\partial_{\tilde{z}}A]^{(j)}$ into the RHS of Eq. (32). The estimates of the difference $([\partial_{\tilde{z}}A]^{(j+1)} - [\partial_{\tilde{z}}A]^{(j)})$ can be calculated using essentially the same arguments as for the linear case, taking into account the new definition of f. One can also prove that $\lim_{j\to\infty} [\partial_{\tilde{z}}A]^{(j)} = \partial_{\tilde{z}}A$, since $[\partial_{\tilde{z}}A]^{(\infty)}$ satisfies the same equations as $\partial_{\tilde{z}}A$. If we truncate the expansion after the second order in f we find

$$\begin{aligned}\partial_{\tilde{z}}A = \hat{\mathscr{L}}A + \frac{2\pi\chi}{n_0^2}\Bigg\{ &\mathrm{i}|A|^2 A - \mathrm{i}\frac{\pi\chi}{n_0^2}|A|^4 A + \eta\left[\left(\frac{\beta_1 c}{n_0} - 2\right)\partial_{\tilde{t}}(|A|^2 A)\right] \\ &- \mathrm{i}\eta^2\left[\left(\frac{\beta_1 c}{n_0} - 1\right)^2 \partial_{\tilde{t}}^2(|A|^2 A) - \frac{\beta_2 \omega_0 c}{n_0}\left(A|\partial_{\tilde{t}}A|^2 + |A|^2\partial_{\tilde{t}}^2 A + \frac{1}{2}A^*(\partial_{\tilde{t}}A)^2\right)\right] \\ &- \mathrm{i}\epsilon^2\left[A|\partial_{\tilde{x}}A|^2 + |A|^2\partial_{\tilde{x}}^2 A + \frac{1}{2}A^*(\partial_{\tilde{x}}A)^2 + A|\partial_{\tilde{y}}A|^2 + |A|^2\partial_{\tilde{y}}^2 A + \frac{1}{2}A^*(\partial_{\tilde{y}}A)^2\right]\Bigg\}. \end{aligned} \tag{33}$$

4. Vectorial case

In this section we generalize the techniques introduced in Section 3.2 to the full vectorial case. Previously we used two scalar operators $\hat{L}$ and $\hat{N}$ to define recurrence relations (31a) and (32). If we take into account vectorial character of the electric field and include all three components of the vectors, operators $\hat{L}$ and $\hat{N}$ have to be replaced with tensorial operators. Fortunately, in (3.2) we did not use the fact that these operators are scalars and most of the algebra from paragraph (3.2) was universal and can be directly extended to the multi-component case.

First we derive a vectorial analog of Eq. (16). We start the derivation by rewriting Eqs. (1) and (2), repeating the steps in Section 2.2:

$$-\tilde{\nabla}\times\tilde{\nabla}\times\mathbf{A}(\mathbf{r},t)=\tilde{\nabla}^2\mathbf{A}(\mathbf{r},t)-\tilde{\nabla}(\tilde{\nabla}\cdot\mathbf{A}(\mathbf{r},t))=\tilde{\nabla}^2\mathbf{A}-\tilde{\nabla}\left(\tilde{\nabla}\cdot\mathbf{A}\right)=\frac{4\pi}{c^2}\partial_{\tilde{t}}^2\mathbf{R}-\hat{D}^2\mathbf{A}, \tag{34a}$$

$$\tilde{\nabla}\cdot\left(\mathbf{R}+\hat{\varepsilon}(\partial_t)\mathbf{A}\right)=0. \tag{34b}$$

Here we used the fact that $\mathbf{A}$ and $\mathbf{R}$ satisfy similar equations as $\mathbf{E}$ and $\mathbf{P}$ provided we make the substitutions given by (7a), as we pointed it out in Section 2.2. We introduced a new operator $\hat{\varepsilon}(\partial_t)$,

$$\hat{\varepsilon}(\partial_t)\mathbf{A}(\mathbf{r},t)\equiv\int_{-\infty}^{+\infty}\mathrm{d}\omega\,\mathrm{e}^{-\mathrm{i}\omega t}\,\varepsilon(\omega+\omega_0)\tilde{\mathbf{A}}(\mathbf{k},\omega), \tag{35a}$$

$$=\left(\sum_{j=0}\frac{1}{j!}\frac{\partial^j\varepsilon(\omega)}{\partial\omega^j}\bigg|_{\omega=\omega_0}(\mathrm{i}\partial_t)^j\right)\mathbf{A}(\mathbf{r},t). \tag{35b}$$

$\hat{\varepsilon}(\partial_t)$ is related to the operator $\hat{D}$

$$\hat{D}^2=\frac{(\mathrm{i}\partial_t+\omega_0)^2\hat{\varepsilon}(\partial_t)}{c^2}. \tag{36}$$

Relation (36) is simply a Fourier transform of the relation, $k^2(\omega)=\varepsilon(\omega)\omega^2/c^2(=n^2(\omega)\omega^2/c^2)$, written in operator form. Furthermore, using Eq. (34b) we can write

$$\tilde{\nabla}\cdot\mathbf{A}=-\tilde{\nabla}\cdot\hat{\varepsilon}^{-1}(\partial_t)\mathbf{R}, \tag{37}$$

where $\hat{\varepsilon}^{-1}$ is defined by the relation

$$\hat{\varepsilon}^{-1}(\partial_t)\mathbf{R}(\mathbf{r},t)=\left(\sum_{j=0}\frac{1}{j!}\frac{\partial^j}{\partial\omega^j}\left[\frac{1}{\varepsilon(\omega)}\right]\bigg|_{\omega=\omega_0}(\mathrm{i}\partial_t)^j\right)\mathbf{R}(\mathbf{r},t). \tag{38}$$

Upon substituting Eq. (37) into (34a), expanding and reorganizing terms we obtain

$$2\mathrm{i}k_0\partial_z\mathbf{A}=k_0^2\mathbf{A}-\partial_z^2\mathbf{A}-\nabla_{\perp}^2\mathbf{A}-\tilde{\nabla}\left(\tilde{\nabla}\cdot\hat{\varepsilon}^{-1}(\partial_t)\mathbf{R}\right)-\hat{D}^2\mathbf{A}+\frac{4\pi}{c^2}\partial_{\tilde{t}}^2\mathbf{R}. \tag{39}$$

We can express Eq. (39) in dimensionless units, just as we did in the scalar case of Section 3.1

$$\partial_{\tilde{z}}\mathbf{A}=\frac{\mathrm{i}}{2}\partial_{\tilde{z}}^2\mathbf{A}+\underbrace{\frac{\mathrm{i}}{2}\left(\frac{\hat{D}^2(\omega_0\eta\partial_{\tilde{t}})}{k_0^2}-1-\epsilon^2\nabla_{\tilde{\perp}}^2\right)}_{\hat{\mathbf{L}}}\mathbf{A}$$
$$+\underbrace{\left[-\frac{2\pi\mathrm{i}}{n_0^2}(\eta\partial_{\tilde{t}}-\mathrm{i})^2+\frac{\mathrm{i}}{2}\hat{\varepsilon}^{-1}(\omega_0\eta\partial_{\tilde{t}})\begin{pmatrix}\epsilon^2\partial_{\tilde{x}}^2 & \epsilon^2\partial_{\tilde{x}}\partial_{\tilde{y}} & \epsilon\partial_{\tilde{x}}(\partial_{\tilde{z}}+\mathrm{i})\\ \epsilon^2\partial_{\tilde{x}}\partial_{\tilde{y}} & \epsilon^2\partial_{\tilde{y}}^2 & \epsilon\partial_{\tilde{y}}(\partial_{\tilde{z}}+\mathrm{i})\\ \epsilon\partial_{\tilde{x}}(\partial_{\tilde{z}}+\mathrm{i}) & \epsilon\partial_{\tilde{y}}(\partial_{\tilde{z}}+\mathrm{i}) & (\partial_{\tilde{z}}+\mathrm{i})^2\end{pmatrix}\right]}_{\hat{\mathbf{N}}}\mathbf{R}. \tag{40}$$

Eq. (40) is an analog of Eq. (16). In principle we can again use procedures developed in Section 3.2 to obtain an expression for $\partial_{\tilde{z}}\mathbf{A}$. After replacing $\hat{L}$ with $\hat{\mathbf{L}}$, $\hat{N}$ with $\hat{\mathbf{N}}$, A with $\mathbf{A}$ and R with $\mathbf{R}$ (operators $\hat{\mathbf{L}}$ and $\hat{\mathbf{N}}$ are defined in Eq. (40)), we can construct recurrence relations Eqs. (31a)–(32). Thus we obtain a series of successive approximations for $\partial_{\tilde{z}}\mathbf{A}$ for the vectorial field case.

Again, we consider the specific example of a Kerr medium and define $\mathbf{R}$ appropriate for the vectorial case. In general, the nonlinear polarization is related to the $\mathbf{E}$-field by the tensor susceptibility $\hat{\chi}$. Here however, in order to obtain a compact final result, we assume that the medium is isotropic and we take $\mathbf{R}$ in the form

$$\mathbf{R} = \chi\Big\{(\mathbf{A}\cdot\mathbf{A}^*)\mathbf{A} + \frac{\gamma}{2}(\mathbf{A}\cdot\mathbf{A})\mathbf{A}^*\Big\}, \tag{41}$$

where χ is the third order nonlinear susceptibility, $\gamma = 0$ for electrostriction, $\gamma = 1$ for nonresonant electronic nonlinearities and $\gamma = 6$ for molecular orientation [16,17].

We can now write a three-dimensional version of Eq. (33), and directly solve the vectorial version of recurrence relations (32). We notice, however, that we can introduce further simplification, namely it is possible to eliminate A_z from the set of final coupled equations. To achieve this we replace the equation for $\partial_{\tilde{z}}A_z$ in the set of equations (40) with an equation for A_z obtained from (37)

$$A_z = \mathrm{i}\begin{pmatrix}\epsilon\partial_{\tilde{x}}\\ \epsilon\partial_{\tilde{y}}\\ \partial_{\tilde{z}}\end{pmatrix}\cdot\mathbf{A} + \mathrm{i}\begin{pmatrix}\epsilon\partial_{\tilde{x}}\\ \epsilon\partial_{\tilde{y}}\\ \partial_{\tilde{z}}+\mathrm{i}\end{pmatrix}\cdot\hat{\varepsilon}^{-1}(\omega_0\eta\partial_{\tilde{t}})\mathbf{R}. \tag{42}$$

Thus, instead of finding a recurrence relation for $(\partial_{\tilde{z}}A_x, \partial_{\tilde{z}}A_y, \partial_{\tilde{z}}A_z)$ we switch to a recurrence relation for $(\partial_{\tilde{z}}A_x, \partial_{\tilde{z}}A_y, A_z)$ which takes the following form:

$$[\partial_{\tilde{z}}A_x]^{(1)} = (\hat{\mathbf{L}}\mathbf{A} + \hat{\mathbf{N}}\mathbf{R})_x, \tag{43a}$$

$$[\partial_{\tilde{z}}A_y]^{(1)} = (\hat{\mathbf{L}}\mathbf{A} + \hat{\mathbf{N}}\mathbf{R})_y, \tag{43b}$$

$$A_z^{(1)} = \mathrm{i}\begin{pmatrix}\epsilon\partial_{\tilde{x}}\\ \epsilon\partial_{\tilde{y}}\\ 0\end{pmatrix}\cdot\mathbf{A} + \mathrm{i}\begin{pmatrix}\epsilon\partial_{\tilde{x}}\\ \epsilon\partial_{\tilde{y}}\\ \mathrm{i}\end{pmatrix}\cdot\varepsilon^{-1}(\omega_0\eta\partial_{\tilde{t}})\mathbf{R}. \tag{43c}$$

For the general case we have:

$$[\partial_{\tilde{z}}A_x]^{(j+1)} = (\hat{\mathbf{L}}\mathbf{A} + \hat{\mathbf{N}}\mathbf{R})_x + \frac{\mathrm{i}}{2}\partial_{\tilde{z}}[\partial_{\tilde{z}}A_x]^{(j)}, \tag{44a}$$

$$[\partial_{\tilde{z}}A_y]^{(j+1)} = (\hat{\mathbf{L}}\mathbf{A} + \hat{\mathbf{N}}\mathbf{R})_y + \frac{\mathrm{i}}{2}\partial_{\tilde{z}}[\partial_{\tilde{z}}A_y]^{(j)}, \tag{44b}$$

$$A_z^{(j+1)} = \mathrm{i}\begin{pmatrix}\epsilon\partial_{\tilde{x}}\\ \epsilon\partial_{\tilde{y}}\\ 0\end{pmatrix}\cdot\mathbf{A} + \mathrm{i}\partial_{\tilde{z}}A_z^{(j)} + \mathrm{i}\begin{pmatrix}\epsilon\partial_{\tilde{x}}\\ \epsilon\partial_{\tilde{y}}\\ \partial_{\tilde{z}}+\mathrm{i}\end{pmatrix}\cdot\varepsilon^{-1}(\omega_0\eta\partial_{\tilde{t}})\mathbf{R}. \tag{44c}$$

Recall that here, in a manner similar to what we did in the linear and nonlinear scalar cases, when we evaluate right-hand side of Eq. (44a) we substitute $\partial_{\tilde{z}}A_x$, $\partial_{\tilde{z}}A_y$ and A_z with the jth approximation. We can obtain expressions for $\partial_{\tilde{z}}A_x$ and $\partial_{\tilde{z}}A_y$ accurate to any given order. Upon assuming that $A_y(z=0) = A_z(z=0) = 0$, the expression second order accurate in $\max(\eta,\epsilon)$ does not contain A_y

$$\begin{aligned}\partial_{\tilde{z}}A_x = {} & \hat{\mathscr{L}}A_x + \frac{2\pi(1+\gamma/2)\chi}{n_0^2}\Big\{\mathrm{i}|A_x|^2A_x - \mathrm{i}\frac{\pi(1+\gamma/2)\chi}{n_0^2}|A_x|^4A_x + \eta\Big[\Big(\frac{\beta_1 c}{n_0}-2\Big)\partial_{\tilde{t}}(|A_x|^2A_x)\Big]\\ & - \mathrm{i}\eta^2\Big[\Big(\frac{\beta_1 c}{n_0}-1\Big)^2\partial_{\tilde{t}}^2(|A_x|^2A_x) - \frac{\beta_2\omega_0 c}{n_0}\Big(A_x|\partial_{\tilde{t}}A_x|^2 + |A_x|^2\partial_{\tilde{t}}^2A_x + \frac{1}{2}A_x^*(\partial_{\tilde{t}}A_x)^2\Big)\Big]\\ & - \mathrm{i}\epsilon^2\Big[\Big(\frac{2}{1+\gamma/2}-5\Big)A_x|\partial_{\tilde{x}}A_x|^2 + \Big(\frac{1}{1+\gamma/2}-1\Big)|A_x|^2\partial_{\tilde{x}}^2A_x + \Big(\frac{1}{1+\gamma/2}-2\Big)A_x^2\partial_{\tilde{x}}^2A_x^*\\ & - \frac{1}{2}A_x^*(\partial_{\tilde{x}}A_x)^2 + A_x|\partial_{\tilde{y}}A_x|^2 + |A_x|^2\partial_{\tilde{y}}^2A_x + \frac{1}{2}A_x^*(\partial_{\tilde{y}}A_x)^2\Big]\Big\} + \ldots\end{aligned} \tag{45}$$

Eq. (45) determines A_x to second order in η and ϵ.

5. Normal-incidence boundary matching

In this section we set up the boundary matching of the field across an interface for normal incidence from vacuum onto a nonlinear medium. For simplicity we analyze the scalar case, but our considerations are general and may be extended to the vectorial case. The normal incidence boundary matching can be simply performed using our method because both the value of the WPE and its derivative with respect to the coordinate normal to the surface are known at the interface within the nonlinear medium. This is an important advantage of our method over other possible propagation methods.

We consider a field incident from the left onto a nonlinear medium whose interface is located at $z = 0$. The field in vacuum to the left of the nonlinear medium is given by $E(\mathbf{r}, t) = (B(\mathbf{r}, t)\mathrm{e}^{\mathrm{i}kz} + C(\mathbf{r}, t)\mathrm{e}^{-\mathrm{i}kz})\mathrm{e}^{-\mathrm{i}\omega_0 t}$, where $k = \omega_0/c$ is the central wavevector in vacuum, the amplitude $B(\mathbf{r}, t)$ is given as an initial condition, and the reflected amplitude $C(x, y, t)$ is to be determined, together with the amplitude $A(\mathbf{r}, t)$ of the field inside the nonlinear medium, $E(\mathbf{r}, t) = A(\mathbf{r}, t)\mathrm{e}^{\mathrm{i}k_0 z - \mathrm{i}\omega_0 t}$. The boundary matching conditions are given by:

$$A(\mathbf{r}, t)|_{z=0} = B(\mathbf{r}, t)|_{z=0} + C(\mathbf{r}, t)|_{z=0}, \tag{46}$$

$$\mathrm{i}k_0 A(\mathbf{r}, t)|_{z=0} + k_0 \partial_{\tilde{z}} A(\mathbf{r}, t)|_{z=0} = \mathrm{i}k(B(\mathbf{r}, t)|_{z=0} - C(\mathbf{r}, t)|_{z=0}) + k(\partial_{\tilde{z}} B(\mathbf{r}, t)|_{z=0} + \partial_{\tilde{z}} C(\mathbf{r}, t)|_{z=0}). \tag{47}$$

The terms involving $\tilde{z}$ derivatives in Eq. (47) can be evaluated using the RHS of Eq. (22) for the linear (vacuum) side and (33) for nonlinear side of the interface. Hence, Eq. (47) only involves derivatives with respect to x, y and t. Eqs. (46) and (47) can be Fourier transformed with respect to x, y and t and this yields a set of algebraic equations that can then be solved for $A(k_x, k_y, \omega)$ and $C(k_x, k_y, \omega)$ in terms of $B(k_x, k_y, \omega)$.

If the nonlinear terms are negligibly small, the standard linear boundary matching conditions apply [15]. If higher order diffraction and dispersion terms are kept, boundary matching can be accurately applied even for tight focusing and short pulse conditions. For the nonlinear problem, the resulting algebraic equations will be nonlinear.

6. Comparison with other methods

For very long pulses and beams our final result of the expansion may be simplified by setting all the terms with time derivatives equal to zero. Several attempts has been already made to derive in the rigorous way the parabolic propagation equation for optical beams and our result should be related to them. Our propagation equation for beams is identical to that of Fibich and Ilan [12]. Approach presented here is a direct generalization of their method for time dependent pulse case. Few other authors [11,13] developed another calculational scheme for the same problem. The comparison in this case is a bit more subtle and requires more careful discussion, since the final propagation equation obtained by Ciattoni et al. [11] and de la Fuente et al. [13] differs from the one presented above. Since both groups get mutually consistent results we will explain the difference between our and theirs results using paper of de la Fuente et al. [13] as an example. Authors of [13] use the concept of decomposition of the electric field vector E into E_+ and E_-, which they identify as forward and backward moving waves. In one dimension it can be illustrated upon taking Fourier transform of equation

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\mathbf{E}(z) + k_0^2\mathbf{E}(z) = -\frac{4\pi}{c^2}\omega_0^2\mathbf{P}(z), \tag{48}$$

where $k_0 = (n(\omega_0)\omega_0)/c$, ω_0 is beam frequency and $\mathbf{P}(z)$ is nonlinear polarization. In Fourier domain the analog of equation (48) takes the form

$$(k^2 - k_0^2)\tilde{\mathbf{E}}(k) = \frac{4\pi}{c^2}\omega_0^2\tilde{\mathbf{P}}(k). \quad (49)$$

This equation can be treated as a sum of two equations involving functions $\tilde{\mathbf{E}}_\pm$ defined as

$$\tilde{\mathbf{E}}_\pm = \pm\frac{4\pi\omega_0^2}{2k_0c^2}\frac{\tilde{\mathbf{P}}(k)}{k \mp k_0}. \quad (50)$$

Similar decomposition is possible in three-dimensional case; after some algebra, one obtains

$$\tilde{\mathbf{E}}_\pm = \frac{\pm 4\pi}{2\beta n_0^2}\left[\frac{k_0^2\tilde{\mathbf{P}}_t(\mathbf{k}) - \mathbf{k}_t(\mathbf{k}_\pm \cdot \tilde{\mathbf{P}}(\mathbf{k}))}{k_z \pm \beta}\right], \quad (51)$$

where $\tilde{\mathbf{P}}_t(\mathbf{k})$ is a transverse part of polarization, $\mathbf{k}_t$-transverse (perpendicular to $\hat{z}$ direction) part of wave vector, $\beta = \sqrt{k_0^2 - \mathbf{k}_t^2}$ and $\mathbf{k}_\pm = \mathbf{k}_t \pm \beta\hat{z}$. Further simplification is obtained upon assuming that $\tilde{\mathbf{E}}(\mathbf{k})$ is nonnegligible only for $\mathbf{k}$ in the neighborhood of $(0, 0, k_z)$ and ignoring $\tilde{\mathbf{E}}_-$ in the nonlinear polarization. This assumption allows for solving the equation for $\tilde{\mathbf{E}}_+$ only. One can find that

$$k_z\tilde{\mathbf{E}}_+(\mathbf{k}) = \beta\tilde{\mathbf{E}}_+(\mathbf{k}) + 4\pi\frac{k_0^2\tilde{\mathbf{P}}_t(\mathbf{k}) - \mathbf{k}_t(\mathbf{k}_\pm \cdot \tilde{\mathbf{P}}(\mathbf{k}))}{2\beta n_0^2}, \quad (52)$$

and authors of [13] (upon taking backward Fourier transform and expanding β) derive a nonparaxial propagation equation for the envelope of electric field vector. We derived an equation for the quantity $\tilde{\mathbf{E}} = \tilde{\mathbf{E}}_+ + \tilde{\mathbf{E}}_-$ by taking a sum of Eq. (52) with an analogous equation for $\tilde{\mathbf{E}}_-$. It turns out that the form of our new equation for $\tilde{\mathbf{E}}$ is almost the same as the mathematical form of the equation for $\tilde{\mathbf{E}}_+$ (Eq. (52)), but we have a few additional terms that are of the second order in the nonparaxiality parameter f, defined above. When all of the additional terms are included, after some algebra, we obtain an equation that is exactly identical with (45).

7. Numerical results

We consider a tightly focused beam propagating in silica (SiO_2). The central wavelength is taken to be $\lambda_0 = 800$ nm, the initial spot size $\sigma_p = 1.5\lambda_0$. Fig. 1 shows the on axis value of $|A(x = 0, y = 0, z)|^2$ versus z normalized to the initial value ($A(0, 0, 0) = 1$) for two different powers $P = 2.2P_{CR}$ (solid curve) and $P = 3.5P_{CR}$ (dashed curve). P_{CR} is the critical power for self-focusing and for fused silica it is equal to 2.6 MW. Numerical data was obtained using 2D+1 code, based on explicit two-step leapfrog method [18]. We kept all the new nonparaxial terms. The solid curve corresponds to intensity oscillations in the strong self-focusing regime and the dashed curve corresponds to the case when two oscillations are followed by the breakup into two maxima which eventually are smeared out due to diffraction. These oscillations, due to the competition between self-focusing and diffraction, are only present when we include higher order terms in Eq. (45). Without these terms our numerical simulations lead to catastrophic self-focusing as indicated by the two additional curves in Fig. 1. The dotted curve corresponds to the higher intensity case, and dash–dotted curve corresponds to the lower intensity case. In both cases we included only self-phase-modulation nonlinearity and first order diffraction (we used the usual nonlinear Schrödinger equation). Figs. 2–4 correspond again to the higher intensity case and present full three-dimensional picture of the beam amplitude $|A(x, y, z)|$ for three different values of z; 6.2, 8.5 and 18.8 μm. Fig. 2 shows the beam intensity at the plane of tightest focusing, Fig. 3 correspond to the minimum between two peaks on the dashed curve in Fig. 1 and finally Fig. 4 shows the beam after it broke into two separate beams. At higher intensities and/or stronger focusing one can observe multiple filamentation in the beam dynamics [12]. Evidently initial cylindrical symmetry of the pulse is broken.

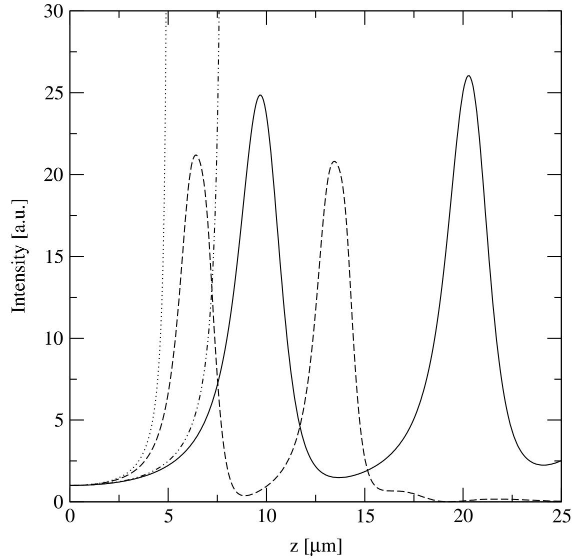

Fig. 1. One-dimensional plot of the on-axis beam intensities versus propagation distance z for two different powers $P = 2.2P_{CR}$ (solid curve) and $P = 3.5P_{CR}$ (dashed curve) calculated with new terms of the propagation equation derived in this paper. Dotted and dot–dashed lines correspond to NLS solutions.

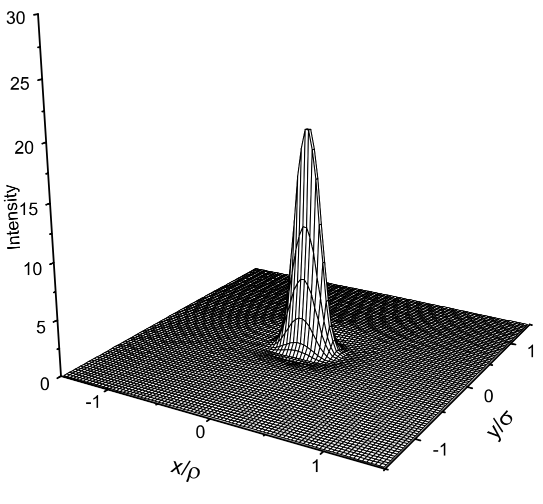

Fig. 2. Three-dimensional plot of the beam intensity at the propagation distance of $z = 6.2$ μm for power $P = 3.5P_{CR}$.

The effects of the new terms including derivatives of the nonlinearity with respect to time become important for short pulses. The most important modification introduced by our expansion is the modification of the coefficient in front of the self-steepening term $\partial_t(|A|^2A)$. The coefficient obtained from the Kerr nonlinearity (2 in our dimensionless units) is replaced by $(c\beta_1/n - 2)$ in Eq. (33), hence corrections are of the same order as original coefficient. In conclusion, our expansion method introduces noticeable corrections leading both temporal and spatial modification of the pulse shape and phase.

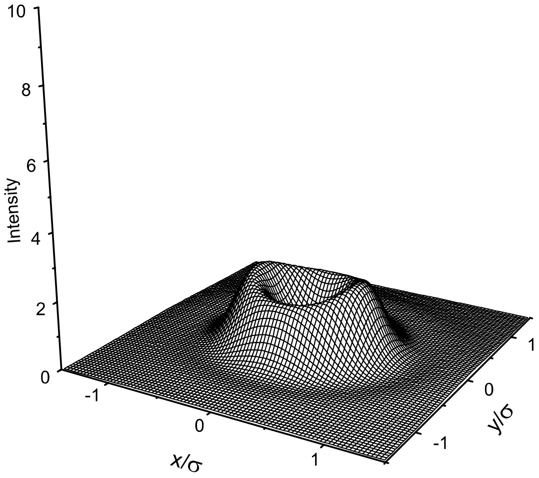

Fig. 3. Three-dimensional plot of the beam amplitude at the propagation distance $z = 8.5$ μm for power $P = 3.5P_{CR}$.

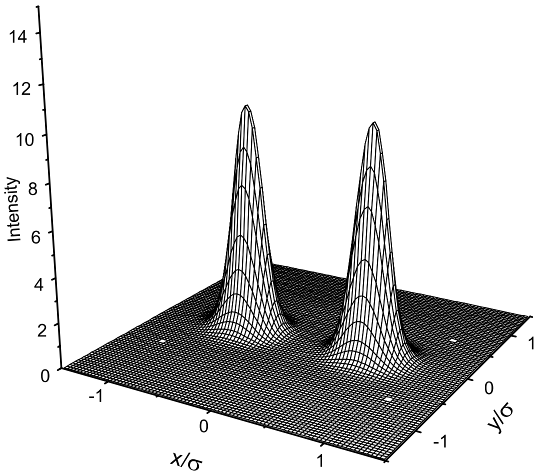

Fig. 4. Three-dimensional plot of the beam amplitude at the propagation distance $z = 18.8$ μm for power $P = 3.5P_{CR}$.

8. Summary and conclusion

The concept of the wave packet envelope (slowly varying envelope) has been extended to the regime of extremely tightly focused and extremely short duration optical pulses. We derived a propagation equation for the wave packet envelope in an isotropic nonlinear dispersive media that is valid to all orders in diffraction and dispersion. The vectorial character of the electromagnetic field was fully taken into account; the vector character generates corrections of the same order as the scalar nonparaxial ones. We self-consistently introduce both types of corrections. Final results were given for a Kerr-type nonlinearity in the form of a truncated nonlinear differential polynomial. Surprisingly, even in the vectorial case, the second order expansion can be reduced to the equation for only one component of the field. This enormously simplifies numerical simulations of optical pulse propagation.

The boundary matching of the electromagnetic wave as it enters the nonlinear medium can be simply performed for normal-incidence using our method because both the value of the wave packet envelope and its derivative with respect to the coordinate normal to the surface are known. The normal-incidence scalar case was explicitly considered; a generalization to the vectorial case is straightforward.

Finally we notice that our method is able to treat propagation in the anisotropic media. In this case operators $\hat{\varepsilon}$ and $\hat{D}$ will no longer be diagonal in the vector field components, which makes the algebra more sophisticated. Furthermore, we can easily treat other types of nonlinear polarization, e.g., including Raman scattering, a saturated nonlinearity and even a coupled set of equations as in the case of third harmonic generation, as long as the pulse spectral width is narrow in comparison with the central frequency.

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