Quantifying the limits of unidirectional ultrashort optical pulse propagation

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In this paper we explore the limits of the unidirectional pulse propagation equation (UPPE) in general nonlinear media. Our main aim is to investigate under which physical conditions two-way propagation becomes significant, and leads to a breakdown of the unidirectional approximation. Using a spectral constraint appearing in the derivation of UPPE we derive a first correction which renormalizes the forward-propagating amplitude. This correction is the main result of our paper and we investigate its effects through numerical simulations.

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I. INTRODUCTION

In numerical simulation of ultrashort, high-power optical pulses propagating in dispersive nonlinear media, it is not feasible to solve Maxwell equations directly. Instead, they are replaced by a pulse-propagation equation which is designed to take advantage of the well-defined direction of propagation in a laser pulse. There is a number of different pulse evolution equations published in the literature (see, e.g., Ref. [1], and references therein), and they differ from each other in the specific assumptions and approximations adopted in each derivation. However, there is one approximation which pertains to *all* equations which treat the optical field as propagating in one direction. It is the assumption that the nonlinear response of the medium, say polarization P_{NL}, can be approximated by the response calculated from the forward-propagating portion of the optical field, i.e.,

$$P_{\mathrm{NL}}(E_{\mathrm{total}}) \approx P_{\mathrm{NL}}(E_{\mathrm{forward}}). \quad (1)$$

It is obvious that every method which does not account for the electromagnetic field in its entirety, but only models the portion which propagates "forward," is relying on this assumption whether it is stated explicitly or not. Replacement (1) is what we call the unidirectional approximation. The first derivation to invoke this explicitly was the unidirectional pulse propagation equation (UPPE) [2,3]. In fact, (1) is the only approximation necessary to reduce Maxwell equations to a single UPPE.

Relatively little attention was devoted to clarifying when it is actually possible to assume that a given situation can be treated within the unidirectional approximation. Notable exceptions are the works by Kinsler [4] and Baruch, Fibich, and Tsynkov [5]. Baruch *et al.* demonstrated that nonparaxiality and backscattering can arrest a self-focusing collapse in the monochromatic Helmholtz equation. Kinsler explored the limits to unidirectional propagation in a one-dimensional model, and showed that the existence of the backward-propagating wave "renormalizes" the nonlinear response in the forward-going wave component. Applicability of the unidirectional approximation was shown to depend on the nonlinearity and field strengths [4].

So far there is no universally applicable tool to assess the degree to which unidirectionality is satisfied in practically important situations involving ultrashort pulses which undergo complex spatiotemporal reshaping. Various pulse-propagation equations have been used for years with a silent assumption that the backward-propagating field is negligible. While we may base this belief on the lack of experimental evidence to the contrary, the assumption is in fact stronger than one may think. It is because the possibility alone of the backward-propagating wave gives rise to a correction of the forward-going wave. This correction, while formally belonging to the backward wave is dragged together with the forward wave [6]. One could say that it behaves as a forced oscillator driven far off-resonance: it will obey, and follow the driving frequency (which is the analog of the forward wave number in an optical pulse) but it will do so with a correspondingly small amplitude. Thus, using one-way pulse-propagation equations in reality requires one to assume that not only the backward-scattered field can be neglected, but also that this renormalization of the forward amplitude is small.

The main result of this paper is a derivation of a correction to the unidirectional pulse evolution equations, which originates in the existence of backward-propagating modes, and renormalizes the forward-propagating wave amplitude. We also describe how this modification can be straightforwardly adopted in an arbitrary solver. Our results represent a practical tool to answer the long-standing question of applicability of the unidirectional approximation in arbitrary situations. We show that, as expected, the unidirectional approximation is very accurate for naturally occurring femtosecond filaments in gases [7]. In condensed media, the interaction with the backward-propagating waves gives rise to small modifications of the forward-propagated wave forms, but these are still too weak to be of any concern when comparing simulation results with experiments. However, the explicit form of the correction makes it evident that it becomes important for sufficiently long wavelengths. For example, it suggests that the unidirectional approximation may not be applicable at all in the terahertz regime.

II. THE MODIFIED UPPE PROPAGATION MODEL

Our basic model equations in this paper are the Maxwell equation including a general linear dispersion and an additional nonlinear polarization response. We introduce the usual beam propagation geometry with the z axis pointing in the propagation direction. Having in mind applications to filamentation, where spot sizes are much larger than wavelength, we will work with the notationally simpler scalar case. Nevertheless, the main result can be straightforwardly generalized to the full vectorial case. We start from the wave equation

$$\partial_{zz} E = -\nabla_\perp^2 E + \frac{1}{c^2}\partial_{tt}(1+L)E + \mu_0 \partial_{tt} P_{\rm NL} \qquad (2)$$

where we have introduced the dispersion operator $L = \int_{-\infty}^{t} dt'\, \chi(t-t')$. We will now rewrite this system in the spectral domain. From this formulation the UPPE approximation is easily described and corrections to the UPPE can be derived in a natural way. The key step here is to find all the modes of the linearized system

$$\partial_{zz} E = -\nabla_\perp^2 E + \frac{1}{c^2}\partial_{tt}(1+L)E.$$

This is easy to do since the system is homogeneous in space and time. We find the two types of modes $e^{\pm i\beta(\omega,\xi)z} e^{i(\xi\cdot\mathbf{x}-\omega t)}$, where $\mathbf{x} = (x,y)$, $\beta(\omega,\xi) = \sqrt{\omega^2 n^2(\omega)/c^2 - \xi^2}$ is the propagation constant, and where ξ is the transverse wave number. For positive frequencies $\omega > 0$, these are left and right traveling modes, respectively.

Because of completeness, any function and, in particular, any solution to the wave equation (2), can be expanded in terms of the modes of the linearized system

$$E(z,t,\mathbf{x}) = \frac{1}{8\pi^3}\int d\omega\, d\xi \{A_+(z,\omega,\xi) e^{i\beta(\omega,\xi)z} + A_-(z,\omega,\xi) e^{-i\beta(\omega,\xi)z}\} e^{i(\xi\cdot\mathbf{x}-\omega t)}.$$

In order to ensure reality of the electric field we must pose the condition $A_-(z,\omega,\xi) = A_+^*(z,-\omega,-\xi)$. In other words, spectral amplitudes at $\omega < 0$ are determined by those at positive frequencies. We can thus restrict the ω integration above to $\omega > 0$, and take the real part of the integral, which then represents what is called the analytic signal of the electric field. Next, it is important to realize that by allowing $A_\pm$ to vary with z, we represent a single function as a combination of two functions. Also note that the variation of $A_\pm$ could be so fast that it completely overrides the exponential factors $e^{\pm i\beta(\omega,\xi)z}$ that accompany them. In effect, we have introduced artificial degrees of freedom and doubled the number of variables needed to represent the electric field. We take advantage of this redundancy to simplify our equations.

We are now going to insert the mode expansion into the wave equation (2), and we can simplify resulting expressions considerably by imposing the constraint

$$\partial_z A_+ e^{i\beta z} + \partial_z A_- e^{-i\beta z} = 0. \qquad (3)$$

Note that this relation arises automatically in the original derivation of UPPE equations [3]. Here we have chosen a different approach to emphasize that our result is not specific to the UPPE, but applies to all pulse-propagation solvers which neglect backward-propagating waves. This relation is also completely analogous to the variation-of-constants method for ODEs: Indeed, observe that because of the constraints (3) the expressions for $\partial_{zz} E$ contain only first derivatives of the amplitudes with respect to z. Inserting this expression for E and its derivative into the wave equation (2) gives after some manipulations the system

$$\partial_z A_+(z,\omega,\xi) = +\frac{e^{-i\beta z}}{2i\beta}\widehat{\rm NL}(z,\omega,\xi), \qquad (4)$$

$$\partial_z A_-(z,\omega,\xi) = -\frac{e^{+i\beta z}}{2i\beta}\widehat{\rm NL}^*(z,-\omega,-\xi) \qquad (5)$$

for the spectral amplitudes (of course, this is nothing but a pair of coupled UPPEs [3]). In these equations, because of the condition $A_-(z,\omega,\xi) = A_+^*(z,-\omega,-\xi)$, we can restrict to $\omega > 0$. The nonlinear term is defined by ${\rm NL} = \mu_0 \partial_{tt} P_{\rm NL}$, and the hat denotes the Fourier transform.

The unidirectional approximation consists in assuming that the positive frequency content of the amplitude A_- is exactly zero at $z = z_0$ corresponding to the assumption that there are only right traveling waves at $z = z_0$ and any positive frequency spectral content of A_- that might be generated during the numerical propagation of the amplitudes is disregarded. The success of the unidirectional approximation depends on whether or not the positive frequency content in A_- that is generated by the actual system is small compared to the positive frequency content of A_+. In order to get a handle on this we can use the constraint (3). Integrating between two points $w < z$ we get

$$A_-(z,\omega,\xi) = A_-(w,\omega,\xi) - \int_w^z dz'\, \partial_z A_+(z',\omega,\xi) e^{2i\beta z'}. \qquad (6)$$

Unless the amplitude $\partial_z A_+(z,\omega,\xi)$ varies on the same scale as the phase factor $e^{2i\beta z}$, we can integrate (6) once by parts and truncate the remainder. This gives the expression

$$A_-(z,\omega,\xi) - A_-(w,\omega,\xi) = \frac{1}{2i\beta}\partial_z A_+(w,\omega,\xi) e^{2i\beta w} - \frac{1}{2i\beta}\partial_z A_+(z,\omega,\xi) e^{2i\beta z},$$

which is correct to $O(\frac{1}{\beta^2})$. This identity holds for all z and w and is in fact an equation for the unknown amplitude $A_-(z,\omega,\xi)$. The following expression solves this equation:

$$A_-(z,\omega,\xi) = -\frac{1}{2i\beta}\partial_z A_+(z,\omega,\xi) e^{2i\beta z}. \qquad (7)$$

Thus, the corrected UPPE will have the same form as before, namely (to keep notation simple, we use the same generic name for the spectral amplitudes A_+ of approximate solutions),

$$\partial_z A_+(z,\omega,\xi) = \frac{e^{-i\beta z}}{2i\beta}\widehat{\rm NL}(z,\omega,\xi),$$

but the nonlinear terms should be evaluated using the following approximation to the mode expansion:

$$E(z,t,\mathbf{x}) = \frac{1}{8\pi^3}\int d\omega\, d\xi \left\{A_+ - \frac{1}{2i\beta}\partial_z A_+\right\} e^{i\beta z} e^{i(\xi\cdot\mathbf{x}-\omega t)}. \qquad (8)$$

$\partial_z A_+$ in this formula is actually the right-hand side of the conventional UPPE and thus the very quantity which a pulse-propagation solver requires to advance a solution along the z axis. So, as written, this correction is of little use because it is implicit. Fortunately, the following iterative procedure works well: As a first step we evaluate $\partial_z A_+$ as usual. Then we correct the spectral amplitude as in Eq. (8), $A_+ \to A_+ + i/2\beta\partial_z A_+$, and from it we calculate a corrected value of $\partial_z A_+$. This is repeated until convergence is achieved, which usually happens after only one or two iterations. It is obvious that this method can be applied in any pulse-propagation solver.

It is evident from the mode expansion for the electric field (8) that at this level of approximation E has no actual left propagation component. The fact that the approximation (7) to the spectral amplitude A_- is nonzero is not a contradiction to this because the interpretation of A_- as the amplitude of left propagating waves actually depends on an assumption that A_- vary slowly on the scale $1/i\beta$ and this is not the case here.

III. DISCUSSION

In this section we discuss the magnitude of the correction to unidirectionality. First, note that if we require that the correction is small, i.e., $|A_+(z,\omega,\xi)| \gg |\partial_z A_+(z,\omega,\xi)|/2\beta$, we ask for the spectral amplitude to change little on the length scale of the wavelength (for all relevant ω!). This condition is also known as the slowly evolving wave approximation (SEWA) [8]. We thus see that our correction can only become significant once SEWA starts to break, which in turn means that pulse reshaping occurs over very short distances.

One can apply the above inequality to a naturally occurring femtosecond filament in a gaseous medium to see that this correction is most likely unimportant. Indeed, we know, both from simulations and experiments, that a typical longitudinal propagation scale for nonlinear reshaping of the optical pulse is centimeters and longer. Compared to the micron-scale wavelength content of the pulse, this implies rather slow evolution, and the relative strength of the correction is typically of the order of 10^{-4}. To confirm this, we have compared simulations with and without the correction in several typical single-filamentation scenarios in air. Not surprisingly, we found that the correction is virtually undetectable on the background of the simulated solution.

The situation changes in condensed media, where the characteristic length over which the self-focusing collapse occurs is only hundreds of microns or less. Then the relative correction strength can be of the order of 10^{-2}. In a favorable situation (i.e., combination of power and focusing geometry), the resulting deviations can accumulate during the propagation and result in a detectable effect. This is illustrated next.

Long wavelengths have attracted more and more interest recently (see, e.g., Ref. [9]), and it motivates our illustrative example. We have simulated a 35-fs duration pulse with a wavelength of 3 μm, collimated at the facet of an yttrium aluminum garnet sample. The latter is characterized in our model by the nonlinear index $n_2 = 7.0 \times 10^{-20}$ W/m^2 [10], and by a multiphoton ionization rate calculated from a Keldysh formula for condensed media given in Ref. [11]. The chromatic dispersion was based on the refractive index data for YAG obtained from Ref. [12].

It turns out that the iterative procedure to evaluate the corrected nonlinear response of the medium converges almost instantly. In the data presented here, we have only used a single iteration—on the scale of Fig. 1, the differences between results obtained with different numbers of iterations are not discernible.

A comparison of results obtained with uncorrected and corrected propagation is depicted in Fig. 1. It shows filament

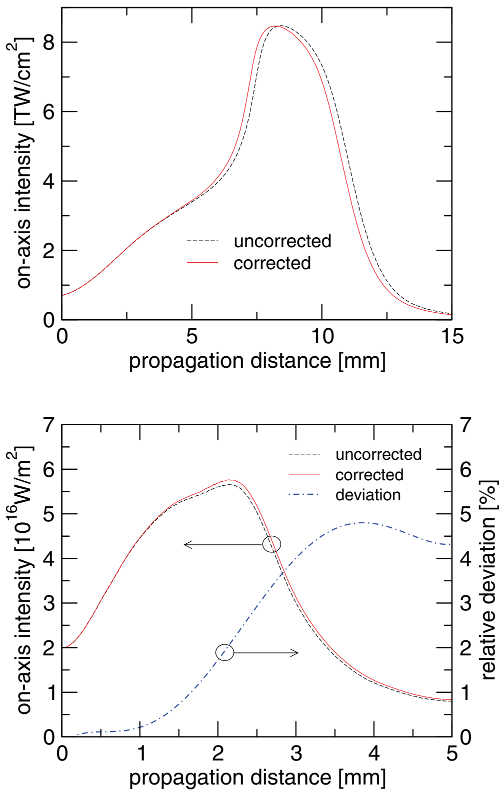

FIG. 1. (Color online) Corrected vs uncorrected pulse-propagation simulations. On-axis intensity evolution is shown for filaments created by a 3-μm wavelength, 35-fs duration pulse in YAG. Upper panel: Beam collimated to 50 μm exhibits correction-induced shift of the collapse-onset distance. Lower panel: Intensity modification for the initial beam size of 25 μm.

formation in a YAG sample with the excitation pulse energy just above the threshold. The correction shows up clearly, and manifests itself as a shift of the filament onset. In other instances, we have seen intensity modifications of up to 5% at this wavelength (an example shown in the lower panel). However, this is still small for all practical purposes; because a truly quantitative comparison with experiments is not yet possible, corrections at this level are difficult to verify experimentally.

We thus come to see that in the filamentation regimes studied to date, it is not necessary to include any corrections beyond the unidirectional approximation. While this is indeed an expected result, we have found that deviations due to the correction to unidirectional propagation increase from utterly negligible at short wavelengths, to clearly observable at mid-infrared wavelengths. This suggests that it may be necessary to account for these effects in future experiments with even longer-wavelength pulses. Moreover, it is evident from the formula in Eq. (8) that the correction to unidirectionality becomes significant at terahertz frequencies generated in the femtosecond filaments: there, the length scale of the second term in Eq. (8) is governed by the length of the filament onset which in turn is controlled by the infrared driver pulse. Thus, the rate of change of the spectral amplitude at terahertz frequency may become comparable to its wavelength. However, it is known that the terahertz radiation is generated in all directions from a filament, and this means that most likely the whole concept of the unidirectional propagation model is not applicable.

IV. SUMMARY

We have analyzed the mutual interaction between forward- and backward-propagating wave components in optical pulses propagating through nonlinear dispersive media. We have identified a contribution to the forward-propagating amplitude which originates in the backward-propagating field modes, but which is dragged in the direction of the main pulse. An approximate local condition was found, which makes it possible to implement a correction to unidirectional propagation regime in any pulse-propagation solver. It is expressed as a correction to the field that enters in the evaluation of the nonlinear response. We have proposed and tested an iterative scheme to evaluate the latter, and implemented the method in our UPPE solver. Computer simulations confirmed that in the normal filamentation regimes, the corrections to unidirectionality are not important. However, they become observable in principle at the wavelength of a few microns, and we expect that they become progressively stronger at yet longer wavelengths. In summary, after years that the nonlinear optics community used various one-way propagation equations in the computer-aided explorations of filamentation and other highly nonlinear effects, we have devised a straightforward, practically applicable method to evaluate the accuracy of the approximation that underpins all these numerical pulse-propagation experiments. Our method makes it possible to use unidirectional techniques even in situations when coupling to back-propagating modes occurs, and this approach is applicable irrespectively of details of a particular pulse-propagation solver.

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