Unidirectional Optical Pulse Propagation Equation

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A unidirectional optical pulse propagation equation, derived directly from Maxwell's equations, provides a seamless transition between various nonlinear envelope equations in the literature and the full vector Maxwell's equations. The equation is illustrated in the context of supercontinuum generation in air and is compared to a recent scalar model of Brabec and Krausz. Fully vectorial aspects of the model are illustrated in the context of extreme focusing of a femtosecond pulse.

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The higher dimensional nonlinear Schrödinger equation (NLS) is ubiquitous as a remarkably robust description of weakly nonlinear dispersive wave propagation in widely different physical contexts. In optics, it can be derived, with higher order correction terms included, from Maxwell's equations as an asymptotic expansion in a small parameter [1]. Recent experimental developments in extreme femtosecond nonlinear optics have led to situations where the validity of the NLS model, even with correction terms included, comes into question. Several recent studies have focused on studying or deriving various improved, corrected equations that extend beyond the basic quasimonochromatic, slowly varying NLS envelope approximation [2–9]. Despite the robustness of the NLS in describing extreme nonlinear behavior well beyond its expected range of validity, there exists no means of gauging the accuracy of various correction terms beyond directly integrating Maxwell's equations themselves. In the present Letter, we derive a unidirectional pulse propagation equation (UPPE) that provides a seamless transition from Maxwell's equations to the various envelope-based models. A key is to express the resulting equation in the spectral domain. The UPPE captures the true dielectric (linear and nonlinear) response of real materials over the physically relevant frequency bandwidth. Moreover, unlike earlier approaches, extreme linear and nonlinear focusing events approaching scales of the order of the wavelength of light in the material are correctly described. In addition, known envelope equations can be obtained in a physically transparent manner from it. The UPPE equation can be implemented numerically in an efficient manner, and the effects of turning on and off various correction terms in the envelope approximations can be evaluated. We derive the UPPE from Maxwell's equations and elucidate its relation to envelope equations by deriving the nonlinear envelope equation (NEE) introduced previously by Brabec and Krausz [2]. Finally, we present numerical simulation of supercontinuum generation in air to demonstrate different levels of approximations, from UPPE, to NEE. We also show how terms, not included in scalar propagation equations, affect extreme self-focusing behavior.

We suppose a homogeneous, isotropic, dispersive, and nonmagnetic medium characterized by its linear relative permittivity $\epsilon(\omega)$. Besides the linear permittivity, the medium exhibits a nonlinear response with an arbitrary functional form. Our goal is to derive a unidirectional, first-order equation that describes nonlinear pulse propagation in this medium. For concreteness, we call the positive z axis the forward direction, while the negative z axis points in the backward direction.

Let us consider, for a moment, only a linear "background" medium. In general, it is possible to split an arbitrary radiation field into forward- and backward-propagating parts. For a homogeneous medium we have an explicit expression, in the spectral representation, for a pair of the corresponding projection operators

$$\mathcal{P}^{\pm}\begin{pmatrix}\vec{D}(\vec{k})\\ \vec{H}(\vec{k})\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\vec{D}(\vec{k}) \mp \mathrm{sgn}(k_z)\frac{1}{\omega(k)}\vec{k}\times\vec{H}(\vec{k})\\ \vec{H}(\vec{k}) \pm \mathrm{sgn}(k_z)\frac{\omega(k)}{k^2}\vec{k}\times\vec{D}(\vec{k})\end{pmatrix}. \quad (1)$$

Here, the argument $\vec{k}$ denotes the corresponding plane-wave (Fourier) component of the vector field, and the angular frequency $\omega(k)$ and the wave-vector amplitude k are related through the linear dispersion relation $\omega(k)^2\epsilon(\omega(k)) = c^2k^2$. It is straightforward to check that $\mathcal{P}^{\pm}$ leaves invariant any forward (backward) propagating plane-wave solution of Maxwell's equations, while it annihilates all plane waves going in the opposite direction. The projection properties for general fields then follow from linearity and completeness of plane-wave functions.

We now return to our original, nonlinear problem. The optical field modifies the background medium through a nonlinear response that is characterized by the constitutive relation connecting the electric field and electric induction. Usually, the constitutive equation expresses $\vec{D}$ as a functional of $\vec{E}$, $\vec{D} = \epsilon_o\epsilon * \vec{E} + \vec{P}_{\mathrm{NL}}(\vec{E})$. Here, we use it in the reverse direction to express $\vec{E}$ as a functional of $\vec{D}$ in order to split the electric field into a "background-medium contribution" and a nonlinear part:

$$\vec{E}(\vec{D}) \equiv \vec{E}_{\mathrm{L}}(\vec{D}) + \vec{E}_{\mathrm{NL}}(\vec{D}). \quad (2)$$

Here, the left-hand side is the solution to the complete constitutive equation, while the first term is the solution to the linearized constitutive equation. The last term represents the nonlinear response of the medium to the optical field, and Eq. (2) is used to define it. In terms of nonlinear polarization, $\vec{P}_{\rm NL}$, $\vec{E}_{\rm NL}(\vec{D})$ can be expressed in the spectral representation as

$$\epsilon_0 \epsilon(\omega(k)) \vec{E}_{\rm NL}(\vec{D}, \vec{k}) + \vec{P}_{\rm NL}(\vec{D}, \vec{k}) = 0. \quad (3)$$

Because we are interested in a unidirectional equation, we are by definition restricted to a situation where the light backscattered from the pulse is weak relative to the pulse itself, and second, it cannot significantly contribute to the nonlinear response of the medium. These approximations are inherent to all unidirectional envelope propagation equations.

Expressed mathematically, the first condition reads

$$\begin{pmatrix} \vec{D} \\ \vec{H} \end{pmatrix}_{\rm PULSE} \approx \mathcal{P}^{+} \begin{pmatrix} \vec{D} \\ \vec{H} \end{pmatrix} \equiv \begin{pmatrix} \vec{D}_{\rm f} \\ \vec{H}_{\rm f} \end{pmatrix}. \quad (4)$$

In other words, the pulse optical field has to be almost invariant under the forward-projection action. The second condition can be stated as

$$\vec{P}_{\rm NL}(\vec{D}) \approx \vec{P}_{\rm NL}(\vec{D}_{\rm f}), \quad (5)$$

which means that the nonlinear response is mainly due to the forward-propagating part of the field.

Having introduced the physical motivation, we are now in a position to derive the propagation equation. In fact, Eq. (4) suggests the procedure. One needs to write down an equation for the forward-projected field $\vec{D}_{\rm f}$. To this end, we start from Maxwell's equations and use the formal splitting (2) of the electric field into "linear" and "nonlinear" parts and express the system in operator form

$$\partial_t \begin{pmatrix} \vec{D} \\ \vec{H} \end{pmatrix} = \begin{pmatrix} \nabla \times \vec{H} \\ \frac{-1}{\mu_0} \nabla \times \vec{E}_{\rm L}(\vec{D}) \end{pmatrix} - \begin{pmatrix} 0 \\ \frac{1}{\mu_0} \nabla \times \vec{E}_{\rm NL} \end{pmatrix}. \quad (6)$$

Acting with $\mathcal{P}^{+}$ from the left on this equation we obtain the desired projection. Since $\mathcal{P}^{\pm}$ are time independent and because they commute with the right-hand side of the linear Maxwell's equations, the projector "passes through" the linear part and projects out the forward fields. To evaluate the nonlinear part, we then transform the projected equations into the spectral domain in which both the linear propagation generator as well as the projectors $\mathcal{P}^{\pm}$ are diagonal. Using Eqs. (1) and (3), a straightforward calculation leads to a propagation equation in the spectral domain restricted to $k_z > 0$

$$\partial_t \vec{D}_{\rm f}(\vec{k}) = -i\omega(k)\vec{D}_{\rm f}(\vec{k}) + \frac{i}{2}\omega(k)\left[\vec{P}_{\rm NL}(\vec{D}, \vec{k}) - \frac{1}{k^2}\vec{k}\vec{k}\cdot\vec{P}_{\rm NL}(\vec{D}, \vec{k})\right]. \quad (7)$$

This is our central result, a UPPE. We emphasize that this is an exact equation with an arbitrary functional form of $\vec{P}_{\rm NL}$ that can represent instantaneous or delayed nonlinear response of the medium. The only approximation necessary for practical calculations is to use Eq. (5) in the nonlinear term. Then, if Eq. (4) also holds, the solution can be interpreted as a propagating pulse field.

The structure of the UPPE is similar to that of other nonlinear propagation equations with the linear and nonlinear "propagators" separated. Here, however, we have a vector equation that correctly reflects the fact that $\nabla \cdot \vec{E} \neq 0$ in general. This is expressed by the last term which becomes important for tightly focused pulses and that has a profound effect on the self-focusing behavior.

We now show how this equation reduces to the NEE model of Brabec and Krausz [2]. Other envelope equations follow from NEE [9] through further approximations or they are closely related to it [7]. As a first step, the last term on the right-hand side of Eq. (7), which reflects $\nabla \cdot \vec{E} \neq 0$ due to nonlinear response gradients, is neglected. Next, to reduce UPPE to an envelope equation, one replaces $\omega(k)$ by a suitably approximated expression, both in the linear propagator and in the nonlinear response part. Finally, the resulting equation is transformed to real space.

To this end, we write the exact dispersion relation

$$\frac{\omega}{c}\sqrt{\epsilon(\omega)} = \sqrt{k_z^2 + k_\perp^2}, \quad (8)$$

and Taylor expand it around a reference frequency $\omega_{\rm R}$, formally up to infinite order, and in $k_\perp$ up to second order:

$$k_{\rm R} + \frac{(\omega - \omega_{\rm R})}{v_g} + \sum_{n=2} \frac{\beta^{(n)}(\omega - \omega_{\rm R})^n}{n!} = k_z + \frac{k_\perp^2}{2k_z}, \quad (9)$$

where $k_{\rm R} = \omega_{\rm R} n_b / c$ is the reference wave vector, and expansion coefficients $\beta^{(n)}$ are complex in general. Rearranging this expression and approximating $1/k_z \approx c/(n_b \omega) = c/n_b(\omega_{\rm R} + \omega - \omega_{\rm R})^{-1}$, one gets

$$\frac{\omega}{v_g} = \frac{\omega_{\rm R}}{v_g} + (k_z - k_{\rm R}) - \sum_{n=2} \frac{\beta^{(n)}(\omega - \omega_{\rm R})^n}{n!} + \left(1 + \frac{\omega - \omega_{\rm R}}{\omega_{\rm R}}\right)^{-1} \frac{c k_\perp^2}{2 n_b \omega_{\rm R}}. \quad (10)$$

This approximation to $\omega(k)$ is used in the linear part of Eq. (7). Physically, it corresponds to the linear dispersion relation of the NEE equation. In the corresponding nonlinear term, $\omega(k)$ is rewritten equivalently as

$$\omega(k) = \omega_{\rm R} + (\omega - \omega_{\rm R}). \quad (11)$$

These expressions are now inserted into Eq. (7), and the forward complex amplitude is expressed in terms of an envelope A as $D_{\rm f} = A \exp[i k_{\rm R} z - i\omega_{\rm R} t]$. The spectral-domain operators $(k_z - k_{\rm R})$ and $(\omega - \omega_{\rm R})$, which act on $D_{\rm f}$, then transform in the real-space domain into $-i\partial_z$

and $i\partial_t$, respectively, which act on the envelope A only:

$$(k_z - k_R)D_f \to -i\partial_z A \exp[ik_R z - i\omega_R t], \\ (\omega - \omega_R)D_f \to +i\partial_t A \exp[ik_R z - i\omega_R t]. \quad (12)$$

As a result, we obtain the well-known NEE equation of Brabec and Krausz [2]

$$\partial_\xi A = \frac{i}{2k_R}\left(1 + \frac{i\partial_t}{\omega_R}\right)^{-1}\Delta_\perp A + i\mathcal{D}A + \frac{ik_R}{2}\left(1 + \frac{i\partial_t}{\omega_R}\right)P_{NL}, \quad (13)$$

where $\mathcal{D} = \sum_{n=2}^{\infty} \beta^{(n)}/n!(i\partial_t)^n$ is the dispersion operator, $\partial_\xi = v_g^{-1}\partial_t + \partial_z$, and P_{NL} stands now for the nonlinear polarization envelope.

Several other envelope equations can be derived from NEE (or directly from UPPE). For example, an equation in which the space-time focusing operator $(1 + i\omega_R^{-1}\partial_t)^{-1}$ [see Eq. (13)] is replaced by its first-order expansion $(1 - i\omega_R^{-1}\partial_t)$ has been used [5,6,9]. We show elsewhere that this kind of truncated approximation is restricted to relatively narrow-bandwidth pulses. Examples of equations that go beyond the envelope approach (but retain the paraxial approximation) are the so-called first-order propagation equation by Geissler *et al.* [7] and reduced Maxwell's equation [10]. Both can be derived from UPPE along the same lines as above.

Thus, instead of Maxwell equations we have a general unidirectional equation that is easier to solve numerically, it is still essentially exact, and it preserves the vectorial character. Instead of just a Taylor expanded susceptibility, the linear response that can include absorption lines and arbitrary chromatic dispersion is used. Moreover, UPPE enables us to derive all the known approximations in a physically transparent way by simply replacing the exact dispersion relation by a suitable approximation. This makes it possible to use a UPPE numerical solver to mimic solutions of these equations and, thus, assess their validity within realistic physical settings. We demonstrate this in the following part of this Letter.

We consider a 25-femtosecond (0.1 mm waist) pulse with a carrier wavelength of 775 nm and power of 8 GW propagating in air. The pulse duration is chosen very short to highlight propagation effects that are absent in the NLS approach, namely, space-time focusing and the frequency dependent nonlinear response (shock formation). We compare supercontinuum generation in three models. First, we use UPPE with full chromatic dispersion of dry air taken into account in the wavelength region from 1200 to 200 nm [11]. The other two models, emulated by our UPPE solver, will be the NEE equation in which the dispersion operator $\mathcal{D} = \sum_{k=2}^{L} \beta^{(k)}/k!(i\partial_t)^k$ [Eq. (13)] is expanded up to the second ($L = 2$) and/or third ($L = 3$) order with $\beta^{(k)}$ being purely real in this case. For notational purposes, we term these approximations ad2NEE and ad3NEE, respectively (standing for NEE with approximate dispersion). In all cases, we assume an instantaneous optical Kerr effect with $n_2 = 5 \times 10^{-23}$ m^2/W and plasma generation by multiphoton ionization. The reader is referred to Ref. [12] for a physical description of the model.

Figure 1 shows the pulse spectrum after the self-focusing collapse is arrested by plasma generation. In all cases, a broad high-frequency component is generated on the steepened trailing edge of the pulse as described previously in Ref. [8]. However, we see that the details of the spectra are rather different. Here, the UPPE solution describes the correct propagation properties of all wavelengths that contribute to the spectral range shown. The difference between the UPPE and ad2(3)NEE solutions can be traced to a difference in the susceptibility they model. It happens that the group velocity dispersion is rather small around 800 nm and the approximated susceptibility rapidly deviates from the actual susceptibility at higher frequencies. Including the third-order dispersion substantially improves the agreement with the UPPE solution. The remaining discrepancy is then restricted to the high-frequency range in which the supercontinuum spectral intensity falls off. This demonstrates that in the NEE the dispersion operator should be treated exactly in the spectral domain or care should be exercised in approximating chromatic dispersion by an expansion. When the dispersion is handled properly, NEE is an excellent approximation. It can be shown that the error it introduces is of fourth order in the transverse wave number. Thus, NEE is accurate in most situations, with the exception of extremely nonparaxial propagation.

However, the most popular optical propagation equations, including the NEE, are still scalar equations derived under the assumption of $\nabla \cdot E = 0$. Because of the spatially inhomogeneous nonlinear response, the correct description must take into account the vectorial nature of light, which manifests itself in the form of the last, polarization scrambling term in Eq. (7). The vectorial effects were studied in [13] for a Helmholtz (cw) equation and were shown to be more important than nonparaxiality. They have even more profound effect on the

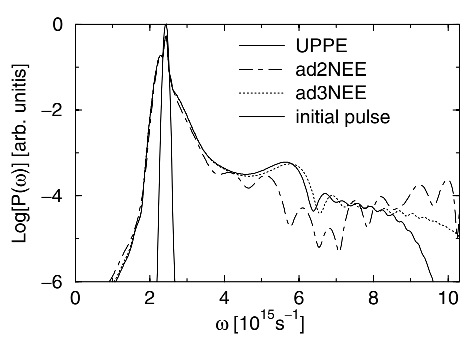

FIG. 1. Supercontinuum generation in a 25-femtosecond pulse in air. Power spectra after the self-focusing collapse, at a propagation distance of ≈ 0.55 m.

self-focusing behavior of ultrashort pulses. While in the cw regime nonparaxiality arrests the self-focusing collapse [14], it is not the case, in general, in the fully time-resolved case. The difference comes from the fact that the high transverse wave numbers do not represent evanescent waves, like in the cw case, but contribute to higher-frequency components of the optical field that continue to participate in the self-focusing process.

To demonstrate the importance of the vectorial nature of the propagation equation, we present below an idealized case study designed to facilitate comparison with a scalar approach. Let us consider an initially tightly collimated (waist of 1 μm, $\lambda = 800$ nm) femtosecond pulse that enters an instantaneous nonlinear Kerr medium. To avoid competing physical effects, we do not consider any other interaction (e.g., multiphoton ionization) and we use a relatively long-duration pulse (170 fs) to minimize other correction effects (e.g., spatiotemporal focusing). To facilitate comparison with scalar equations, we consider the radially symmetric, linearly polarized component of the optical field. We have performed simulations of the full UPPE equation with and without the divergence correction. Figure 2 shows the evolution of the maximal intensity along the propagation distance in the nonlinear medium for a pulse with a supercritical peak power. We see that the noncorrected solution exhibits an NLS-type blowup singularity while the full solution undergoes initial self-focusing that is arrested by the correction effect. Thus, the new term brings a qualitatively new behavior. Although it is relatively small in many circumstances, it plays an important role both in a tightly focused situation and whenever the polarization scrambling effects are significant. We emphasize that this effect is completely omitted in scalar propagation equations and thus far has been treated only in a perturbative fashion in vectorial approaches (see, e.g., Refs. [13,15]). Here we provide a full, self-consistent treatment.

In conclusion, we have derived a robust unidirectional nonlinear pulse propagation equation. It provides a seamless transition between a full vector Maxwell and various envelope approaches discussed earlier. Computationally, it is possible using the UPPE to accurately evolve carrier-resolved high and low power electromagnetic pulses over meter-scale physical distances which is a few orders of magnitude longer than those accessible by vector Maxwell solvers. In addition, extreme self-focusing events with transverse physical scales approaching the wavelength of light in the material can be accurately tracked. An analogous equation to (7) can be written for the backscattered component of the optical field. This, in principle, makes it possible to investigate the properties of the backscattered light. In this Letter we showed that the UPPE model allows us to establish the validity of

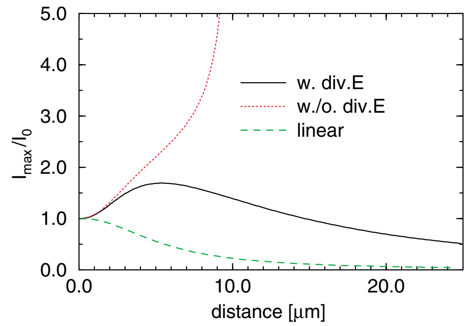

FIG. 2 (color online). Influence of the nonzero $\nabla \cdot E$ correction term for a tightly focused pulse entering a nonlinear Kerr medium. The full line represents a UPPE simulation of the radially symmetric component of the optical field; the dotted line is obtained from the simulation without $\nabla \cdot E$-related corrections, while the dashed line shows a linear case for comparison.

various approximations inherent in various envelope approaches and investigate extreme nonlinear self-focusing of a femtosecond pulse. Full details will appear in a longer publication.

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