Nonlinear optical pulse propagation simulation: From Maxwell's to unidirectional equations

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Spatial- and time-domain versions of the unidirectional pulse propagation equation (UPPE) are derived and compared from the point of view of their practical application in simulations of nonlinear optical pulse dynamics. A modification of the UPPE suitable for ultrathin optical waveguides, such as submicron silica wires, is also presented. We show in detail how various, previously published propagation equations follow from the UPPE in a unified way that clearly elucidates their underlying approximations and areas of applicability.

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I. INTRODUCTION

Propagation equations have been important computational tools in many different areas of optics, especially in nonlinear optics. On one side of the spectrum we have numerical Maxwell's equations solvers (see, e.g., [1]) that capture the light-propagation physics very accurately, but require large-scale computational resources for most problems. The numerical difficulty of the direct Maxwell's equations simulation severely restricts the set of problems that can be tackled. On the other side of the spectrum we have the workhorse of the nonlinear optics, the nonlinear Schrödinger equation (NLS) (see [2] for applications in optics), that considerably reduces the computational effort and works extremely well for certain propagation problems. However, its computational simplicity comes at the price of several approximations that restrict the applicability of the equation. As a consequence, although the NLS often works far beyond what one would naively expect [1,3], it generally fails for ultrashort pulses [4–10].

Considerable effort has been devoted to designing propagation equations that would share the advantages of both the "raw" Maxwell's solvers and the "simple" NLS [11–14]. Several types of equations with "correction terms" were derived extending the region of validity of the NLS, while preserving its computational simplicity. In most cases, the basic idea was to maintain the unidirectional character of the NLS equation, and relax the quasimonochromatic and slow-evolution requirements. Most authors concentrated on real-space representations [11,12,14], but parallel efforts were made in the spectral [15] and mixed [13] representations as well. Issues of the time-domain dispersion [16–19], vectorial character of light [20,21], and nonparaxial propagation were addressed [6,21,22].

All non-Maxwell pulse propagation equations exploit, in one way or another, the assumed localization properties of pulsed solutions that propagate in a nearly z-invariant way. The propagation equation then describes the evolution "on top" of this self-replicating translation. However, different equations required different approximations to be invoked for their derivation, and the physical significance of the neglected terms is not always evident. Moreover, for equations that are derived as perturbation expansions [20,23] in terms of some small parameters, the question arises about the correct way to truncate the perturbation series such that a consistent model is obtained.

The goal of this paper is threefold. First, we want to expand the development we started in Ref. [24], this article being sort of a long version of the latter. In [24], the unidirectional pulse propagation equation (UPPE) was introduced that is solved in the time domain, based on initial data given in the whole [three-dimensional (3D)] space. Here, we add to this picture the complementary approach, namely a UPPE version solved in the spatial domain, starting from initial data given in two spatial and one temporal dimensions, as it is most usual in optics.

Our second goal is to provide a unifying framework for all unidirectional optical propagation equations. We show in detail how various equations can be derived starting from the UPPE and employing *the same procedure* that clearly elucidates the physical meaning of all underlying approximations, and also reveals relations between different equations.

Last, but not least, our third goal is to provide a brief but usable reference for practitioners of numerical nonlinear optics simulations. We identify problems suitable for the time- and spatial-domain UPPE equations. We also show that the UPPE can be implemented in an equally straightforward way as, say, the NLS equation. We emphasize that the wider applicability of the UPPE does not come with any substantial computational penalty in comparison with some other, more restricted equations. Thus, the UPPE should provide a robust, widely applicable computational tool. Although we do not discuss technicalities, this paper is also intended as a guide for implementing practical solvers based on the various versions of the UPPE.

The rest of the paper is organized as follows. In the Sec. II, we specify the types of media for which we derive our propagation equations. Then, for the sake of concreteness, we outline a generic model for ultrashort, high-power pulse propagation in gases and condensed media in Sec. III. Although most equations do not rely on any specific features of the model, we feel it is useful to provide the reader with a concrete example. In Sec. IV, the general coupled-mode equation is derived and serves as a starting point for the bulk-media UPPEs, and can be used for fiber-like structured media as well. Section V A shows the derivation of the z-propagated UPPE in detail. Section V B follows with a description of its time-domain UPPE counterpart, and Sec.

V C continues with a discussion of some practical computational issues. In Sec. V D, we present a UPPE that extends the generalized NLS, and is suitable for very thin, high-contrast optical waveguides, such as submicron silica tapers or silica "wires." Section VI is devoted to the systematic derivation of several previously introduced propagation equations. Here we draw a consistent, unified picture that connects different equations into a hierarchy, based on their underlying physical restrictions. Finally, we conclude in Sec. VII with a brief discussion and a summary.

II. MODEL MEDIUM PROPERTIES

A. Linear medium properties

Our goal is to systematically derive a hierarchy of electromagnetic field propagation equations suitable for numerical simulations of optical pulse propagation. We are interested in approximating localized (in time and space) solutions to Maxwell's equations. Such pulse solutions usually propagate in a well-defined direction which we choose as the positive z-coordinate axis direction. Therefore, we restrict ourselves to a medium with no sharp optical interfaces crossing the z-coordinate axis, and consider a nonmagnetic, dispersive medium with relative permitivity ϵ that is a function of the transverse coordinates x,y, and of the angular frequency ω,

$$\epsilon = \epsilon(\omega,x,y), \quad \mu = \mu_0. \tag{1}$$

This medium specification includes any dispersive homogeneous medium, such as air or water, as well as structured fiberlike media, such as photonic, microstructured, and tapered optical fibers.

B. Nonlinear material response

Nonlinearity, and other effects beyond the linear chromatic dispersion will be lumped in the polarization P in the material constitutive relation,

$$\vec{D} = \epsilon_0 \epsilon * \vec{E} + \vec{P}. \tag{2}$$

The asterisk in this formula stands for the temporal convolution integral, with ϵ being the memory function corresponding to $\epsilon(\omega,x,y)$. The (nonlinear) polarization is an "arbitrary" function of the electric field $\vec{P}=\vec{P}(\vec{E})$. We will also include a current density that is nonlinearly driven by the optical field

$$\vec{j} = \vec{j}(\vec{E}), \tag{3}$$

for capturing interactions with dilute plasma generated by the high-intensity optical pulse.

While the derivation of various propagation equations does not depend on the concrete form of various nonlinear responses, we next give an example of a generic model that includes the optical Kerr and stimulated Raman effects, free-electron generation, defocusing by the generated plasma, and losses caused by avalanche and multiphoton ionization (MPI). Such a model, with minor modifications, can be used for the description of ultrashort optical pulses propagation in gases [25–41], condensed bulk media [42–46], and in conventional, microstructured, and tapered fibers [47–49], as well as in ultrathin silica "wires" [50].

The optical Kerr and stimulated Raman effects can be described in terms of local modification of the optical susceptibility,

$$\vec{P} = \epsilon_0 \Delta\chi \vec{E}, \tag{4}$$

that responds to the history of the light intensity I,

$$\Delta\chi = 2n_b n_2 \left[(1-f)I + f\int_0^\infty \mathcal{R}(\tau) I(t-\tau) \mathrm{d}\tau \right]. \tag{5}$$

Here, f stands for the fraction of the delayed nonlinear response and $\mathcal{R}$ represents a memory function that describes the stimulated Raman effect. Often, parametrization in the form $\mathcal{R}(\tau) \sim \sin(\Omega\tau)e^{-\Gamma\tau}$ is sufficient for ultrashort pulses [51]. The advantage of this approach lies in that its easy implementation does not require calculation of the convolution integral in the Fourier domain. The convolution approach must be used in case the memory function is measured and parametrized in a complicated way, e.g., in silica [52].

Note that the above expressions neglect the chromatic dispersion of the Kerr effect. Although $\Delta\chi$ may exhibit a finite memory, it acts on the instantaneous value of $\vec{E}$ only. This fact greatly simplifies practical calculations. Moreover, there is only rather limited data available on frequency dependence of the nonlinear coefficients n_2 (see Ref. [53] for silica). Therefore, the "background" index of refraction n_b is taken to be constant, too, usually at the central frequency of the initial pulse.

Often, it is necessary to account for the response of the optical field to the presence of a dilute plasma. Because of the extremely short times scales implied by the pulse duration, plasma diffusion and ion motion can be safely neglected in most cases. Thus, the free-electron density ρ is usually obtained as a solution to an equation of the following type [35,36,51]:

$$\partial_t \rho = aI\rho + b(I) - c\rho^2. \tag{6}$$

The first term represents the avalanche free-electron generation, with I being the light intensity, the second term is the MPI, which is a highly nonlinear function of the intensity, and the last term describes plasma recombination.

One usually assumes that the collective electron velocity $\vec{v}$ responds to the optical field and, consequently, the total current density is governed by the following simple equation (see, e.g., Ref. [54]):

$$\frac{d}{dt}\vec{j}(t) = \frac{e^2}{m_e}\rho(t)\vec{E}(t) - \vec{j}(t)/\tau_c, \tag{7}$$

where τ_c is the electron collision time.This equation can be solved together with (6) to capture the effects of the plasma on the propagation of the optical field, namely defocusing due to plasma and plasma-induced losses. This approach also captures the linear chromatic dispersion caused by the plasma.

Alternatively, one can treat the plasma-induced effects as a susceptibility modification and lump them with the rest of $\vec{P}$, which simplifies numerical calculations. The price for this is that one must neglect the chromatic dispersion induced by the free electrons. Then, $\partial_t \vec{P} = \vec{j}$ is interpreted as a component of the nonlinear polarization time derivative and $\vec{P}$ is approximated by

$$\vec{P} = \epsilon_0 \Delta\chi_{\mathrm{pla}}(\rho)\vec{E} = \rho \frac{ie^2}{m_e \omega_{\mathrm{R}}(1/\tau_c - i\omega_{\mathrm{R}})}\vec{E}, \tag{8}$$

with ω_{R} being a chosen reference angular frequency. It needs to be emphasized that this approximation not only completely neglects the plasma induced chromatic dispersion, but also modifies the "correction terms" that we discuss in the following.

We also treat losses due to multiphoton ionization as nondispersive effects. Either an equivalent current (see, e.g., [12,54]) or imaginary susceptibility contributions are included that correspond to the local rate of free-electron generation. Note that this is a universally utilized approximation in the femtosecond pulse propagation area, but if the pulse spectrum broadens in such a way that new frequencies carry a significant portion of its energy, the absorption losses (as well as MPI generation rate) should be frequency selective.

III. INITIAL DATA AND MODAL EXPANSIONS

Most often, the initial data for optical pulse propagation are given (or approximated) in the x,y,t domain and the corresponding "initial value problem" is solved in the z direction. We refer to such equations as z-propagated propagation equations. If, on the other hand, the initial data is known in the x,y,z domain, equations are solved in the time domain, and we term them t-propagated equations. From a practical point of view, the z- and t-propagated equations are pretty much equivalent, but the z-propagated versions are much more popular in the literature. We will therefore present detailed calculations for the z-propagated equations and show their t-propagated counterparts only for the most important case.

Thus, let our initial data be given in the x,y,t domain. Then, the x,y components of the electromagnetic field of a pulse propagating along the z-axis can be expressed as a superposition of the electromagnetic modal fields

$$\begin{matrix}\vec{E}(x,y,z,t) \\ \vec{H}(x,y,z,t)\end{matrix} = \sum_{m,\omega} A_m(\omega,z) \times \left\{ \begin{matrix}\vec{\mathcal{E}}_m(\omega,x,y) \\ \vec{\mathcal{H}}_m(\omega,x,y)\end{matrix} \right\} \times e^{i\beta_{\mathrm{m}}(\omega)z - i\omega t}, \tag{9}$$

where $A_m(\omega, z=0)$ are known from a given initial condition. The sum runs over all transverse modes and over a discrete set of angular frequencies, the latter corresponding to a finite, large normalization "volume" T in the time domain. In what follows, we use the notation

$$\int \mathrm{d}t \equiv \frac{1}{T}\int_{-T/2}^{+T/2} dt \tag{10}$$

for all time-domain integrations, unless integration bounds are shown explicitly.

The transverse mode index m is a shorthand notation for whatever a unique identification of the transverse mode requires. For example, in a homogeneous medium, it includes two transverse components of the plane-wave's wave vector and an index that specifies the polarization.

To keep the notation short, we also use the convention that if modal fields appear without explicitly showing their arguments, the time-dependent and propagation phase factors are understood to be absorbed into modal fields,

$$\vec{\mathcal{E}}_m \equiv \vec{\mathcal{E}}_m(\omega,x,y)e^{i\beta_{\mathrm{m}}(\omega)z - i\omega t},$$

$$\vec{\mathcal{H}}_m \equiv \vec{\mathcal{H}}_m(\omega,x,y)e^{i\beta_{\mathrm{m}}(\omega)z - i\omega t}. \tag{11}$$

The general orthogonality relation

$$\int \vec{z}\cdot[\vec{\mathcal{E}}_m \times \vec{\mathcal{H}}_n^* - \vec{\mathcal{H}}_m \times \vec{\mathcal{E}}_n^*]\mathrm{d}x\mathrm{d}y = 2\delta_{m,n}N_m(\omega) \tag{12}$$

will be used below.

IV. COUPLED-MODE EQUATIONS

Having fixed the notation, we proceed with the derivation of the z-propagated UPPE. First, we follow a textbook method based on the reciprocity relation that leads to a general form of coupled-mode equation. Then, we specialize the intermediate result for the case of the homogeneous dielectric medium and for the fiberlike geometry. We start from Maxwell's equations,

$$\vec{j} + \partial_t \vec{P} + \epsilon_0 \partial_t \epsilon * \vec{E} = \vec{\nabla} \times \vec{H},$$

$$-\mu_0 \partial_t \vec{H} = \vec{\nabla} \times \vec{E}, \tag{13}$$

which we scalar multiply by the complex conjugate modal fields, including their time and z-dependent phase factors $e^{+i\omega t - i\beta_m(\omega)z}$,

$$\vec{\mathcal{E}}_m^* \cdot (\vec{j} + \partial_t \vec{P}) + \epsilon_0 \vec{\mathcal{E}}_m^* \cdot \partial_t \epsilon * \vec{E} = \vec{\mathcal{E}}_m^* \cdot \vec{\nabla} \times \vec{H},$$

$$-\mu_0 \vec{\mathcal{H}}_m^* \cdot \partial_t \vec{\mathcal{H}} = \vec{H}_m^* \cdot \vec{\nabla} \times \vec{E}. \tag{14}$$

Let us rearrange both right-hand sides as follows:

$$\vec{\mathcal{E}}_m^* \cdot (\vec{j} + \partial_t \vec{P}) + \epsilon_0 \vec{\mathcal{E}}_m^* \cdot \partial_t \epsilon * \vec{E} = \vec{\nabla} \cdot [\vec{H} \times \vec{\mathcal{E}}_m^*] + \vec{H} \cdot [\vec{\nabla} \times \vec{E}_m^*],$$

$$-\mu_0 \vec{\mathcal{H}}_m^* \cdot \partial_t \vec{H} = \vec{\nabla} \cdot [\vec{E} \times \vec{\mathcal{H}}_m^*] + \vec{E} \cdot [\vec{\nabla} \times \vec{\mathcal{H}}_m^*], \tag{15}$$

and use Maxwell's equations for the complex-conjugate modes that appear in the last terms,

$$\vec{\mathcal{E}}_m^* \cdot (\vec{j} + \partial_t \vec{P}) + \epsilon_0 \vec{\mathcal{E}}_m^* \cdot \partial_t \epsilon * \vec{E} = \vec{\nabla} \cdot [\vec{H} \times \vec{\mathcal{E}}_m^*] - \mu_0 \vec{H} \cdot \partial_t \vec{\mathcal{H}}_m^*,$$

$$-\mu_0\vec{\mathcal{H}}_m^*\cdot\partial_t\vec{H}=\vec{\nabla}\cdot[\vec{E}\times\vec{\mathcal{H}}_m^*]+\epsilon_0\vec{E}\cdot\partial_t\epsilon*\vec{\mathcal{E}}_m^*. \quad (16)$$

Next, we subtract the two equations and integrate over the whole xyt domain, using the fact that fields vanish at infinity,

$$\int\vec{\mathcal{E}}_m^*\cdot(\vec{j}+\partial_t\vec{P})dxdydt=\partial_z\int\vec{z}\cdot[\vec{H}\times\vec{\mathcal{E}}_m^*]dxdydt-\partial_z\int\vec{z}\cdot[\vec{E}\times\vec{\mathcal{H}}_m^*]dxdydt. \quad (17)$$

Note that only the x,y components of the pulse field appear in this equation. Thus, keeping in mind the implicit z,t dependence of the modal field, we insert the modal expansion (9) and use the orthogonality relation (12) to obtain the evolution equation for the expansion coefficients,

$$\partial_z A_m(\omega,z)=-\frac{1}{2N_m(\omega)}\int e^{-i\beta_m(\omega)z+i\omega t}\vec{\mathcal{E}}_m^*(\omega,x,y)\cdot[\vec{j}(x,y,t)+\partial_t\vec{P}(x,y,t)]dxdydt. \quad (18)$$

V. UNIDIRECTIONAL PULSE PROPAGATION EQUATION (UPPE)

A. The z-propagated version

The above equation can serve as a starting point for the derivation of various propagation equations in many systems, including optical fibers, hollow waveguides, microstructured and tapered fibers, and ultrathin silica wires. Here we specialize it to the case of a homogeneous, dispersive medium. The eigenmodes are specified by their transverse wave numbers, polarization index $s=1,2$, and a propagation-direction sign $\pm$,

$$m\equiv k_x,k_y,s,\pm. \quad (19)$$

The modal fields are the plane waves

$$\vec{\mathcal{E}}_{k_x,k_y,s,\pm}=\vec{e}_s\,\exp[ik_x x+ik_y y\pm ik_z(\omega,k_x,k_y)], \quad (20)$$

$$\vec{\mathcal{H}}_{k_x,k_y,s,\pm}=\frac{1}{\mu_0\omega}\vec{k}\times\vec{\mathcal{E}}_{k_x,k_y,\omega,s,\pm}, \quad (21)$$

where $\vec{e}_{s=1,2}$ are unit polarization vectors normal to the wave vector

$$\vec{k}=\{k_x,k_y,k_z\equiv\sqrt{\omega^2\epsilon(\omega)/c^2-k_x^2-k_y^2}\}. \quad (22)$$

These formulas allow us to calculate the modal normalization constants $N_{k_x,k_y,s,\pm}(\omega)$ [see Eq. (12)]. To make the contact with the numerical solver implementation closer, we choose to normalize the plane-wave modal fields to a large, finite volume $L_x\times L_y\times T$. The normalization constant $N_m(\omega)$ then reads

$$N_{k_x,k_y,s,\pm}(\omega)=\pm\frac{k_z(\omega,k_x,k_z)}{\mu_0\omega}L_xL_y, \quad (23)$$

and the evolution equations for the two polarization components propagating in the positive z direction are

$$\partial_z A_{k_x,k_y,s,+}(\omega,z)=-\frac{\omega\mu_0}{2k_z}e^{-ik_z z}\times\int\frac{dxdydt}{L_xL_yT}e^{i(\omega t-k_x x-k_y y)}\times\vec{e}_s\cdot[\vec{j}(x,y,z,t)+\partial_t\vec{P}(x,y,z,t)]. \quad (24)$$

Performing the temporal and spatial Fourier transforms leads to

$$\partial_z A_{k_x,k_y,s,+}(\omega,z)=\frac{\omega}{2ck_z}e^{-ik_z z}\vec{e}_s\cdot\left[\frac{i\omega}{\epsilon_0 c}\vec{P}_{k_x,k_y}(\omega,z)-\frac{1}{\epsilon_0 c}\vec{j}_{k_x,k_y}(\omega,z)\right]. \quad (25)$$

This system of equations determines the evolution of the two transverse components of the electric field, which can be obtained as $\vec{E}^{\perp}_{k_x,k_y,+}(\omega,z)=\Sigma_{s=1,2}\,\vec{e}_s^{\perp}\vec{A}_{k_x,k_y,s,+}(\omega,z)e^{ik_z(k_x,k_y,\omega)z}$. We thus arrive at the homogeneous-medium UPPE,

$$\partial_z\vec{E}^{\perp}_{k_x,k_y,+}(\omega,z)=ik_z\vec{E}^{\perp}_{k_x,k_y,+}(\omega,z)+\sum_{s=1,2}\vec{e}_s^{\perp}\vec{e}_s\cdot\left[\frac{i\omega^2}{2\epsilon_0c^2k_z}\vec{P}_{k_x,k_y}(\omega,z)-\frac{\omega}{2\epsilon_0c^2k_z}\vec{j}_{k_x,k_y}(\omega,z)\right]. \quad (26)$$

Here, $k_z=\sqrt{\omega^2\epsilon(\omega)/c^2-k_x^2-k_y^2}$, and one has to keep in mind that the polarization vectors $\vec{e}_s$ also implicitly depend on the wave vector. Although this equation describes the transverse field components only, the z-component of the field can be obtained from the known transverse components [55] if it is needed for the calculation of the nonlinear polarization $\vec{P}$ and of the current density $\vec{j}$.

We will refer to Eq. (26) as the full, z-propagated UPPE. Its derivation is formally exact and, naturally, a similar equation holds for the backward-propagating portion of the field. However, to close the system of equations for practical calculations, one needs to calculate the nonlinear responses given by $\vec{P}$ and $\vec{j}$, which in turn requires knowledge of the *complete* field. Since the whole purpose of unidirectional equations is to eliminate the need for knowledge of the "backward-propagating" portion of the field, we have to adopt an approximation at this point. Instead of calculating $\vec{P}(\vec{E}),\vec{j}(\vec{E})$ from the complete field, we approximate these quantities by their counterparts obtained from the simulated forward-propagating field $\vec{E}_f$,

$$\vec{P}(\vec{E}),\vec{j}(\vec{E})\rightarrow\vec{P}(\vec{E}_f),\vec{j}(\vec{E}_f). \quad (27)$$

Put in words, this approximation requires that the field "reflected" in the backward direction is weak from the point of view of generating the nonlinear response. Naturally, the necessary condition for that is that the nonlinear response is itself a small perturbation on the background of the linear medium.

In many practical applications, the z components of the field and of the nonlinear response are negligible in comparison with the transverse ones. In such a regime, the equation can be further simplified to a two-component or scalar form. To this end, the sum over the polarization vectors $\Sigma_{s=1,2}\,\vec{e}_s^{\perp}\vec{e}_s$ is replaced by an identity operator in the transverse (paraxial) vector subspace. This is a fair approximation, since this projector acts on the nonlinear term, which itself must be a small perturbation in view of (27). The scalar form of the equation then reads,

$$\partial_z E_{k_x,k_y}(\omega,z) = ik_z E_{k_x,k_y}(\omega,z) + \frac{i\omega^2}{2\epsilon_0 c^2 k_z} P_{k_x,k_y}(\omega,z) - \frac{\omega}{2\epsilon_0 c^2 k_z} j_{k_x,k_y}(\omega,z),$$

$$k_z = \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2}. \tag{28}$$

We will refer to this equation simply as the z-propagated UPPE, since it is actually its most useful form.

B. The *t*-propagated version

The UPPE solved in the time domain was derived in Ref. [24]. It is nothing but a projection of Maxwell's equations onto forward-propagating half of the plane-wave space, and in contrast to (26), it describes the spectral amplitudes of the electric induction vector,

$$\partial_t \vec{D}_{\vec{k}}(t) = i\omega(\vec{k})\vec{D}_{\vec{k}}(t) + \left[1 - \frac{\vec{k}\vec{k}}{k^2}\right]\cdot\left[\frac{i\omega(\vec{k})}{2}\vec{P}_{\vec{k}}(t)\right]. \tag{29}$$

Here, $\vec{k}$ is a 3D wave vector labeling the spectral amplitudes $\vec{D}_{\vec{k}}(t)$ that evolve in time. The "free-plane-wave" angular frequencies $\omega(\vec{k})$ satisfy the dispersion relation of the given (homogeneous) dielectric medium,

$$\omega^2\epsilon(\omega)/c^2 = k^2. \tag{30}$$

Hence, the first term of the equation is the exact linear propagator written in the spectral representation where it is diagonal. The second term on the right-hand side represents the nonlinear interactions expressed in terms of the polarization. We have factored out the transverse projection operator $[1 - \vec{k}\vec{k}/k^2]$ to make it evident that the "initial condition" $\nabla\cdot\vec{D} = 0$ remains preserved during the evolution, as it should.

Note that the structure of the equation is the same as that of the z-propagated version: The right-hand side consists of the linear propagator and of the nonlinear response term that acts as a perturbation to the former. However, here we have an equation that holds for all three components of $\vec{D}$. For practical purposes, one solves the equation for two components and only calculates the z component from the divergence equation when needed for calculation of the nonlinear response $\vec{P}$.

Just as in the z-propagated case, the equation is formally exact. Together with its backward-propagating counterpart they are equivalent to Maxwell's equations. In practice, and in complete analogy with the z-propagated version, we close the system of equations by calculating the nonlinear responses $\vec{P}$ from the forward-propagating field only, thus approximating

$$\vec{P}(\vec{D}), \vec{j}(\vec{D}) \to \vec{P}(\vec{D}_f), \vec{j}(\vec{D}_f). \tag{31}$$

Note that, unlike in the z-propagated case, we solve the nonlinear material constitutive equation for a given vector field $\vec{D}$ and express the polarization $\vec{P}$ as its functional. This is in the spirit of most numerical Maxwell's equations solvers where $\vec{E}$, needed for the time-derivative evaluation, is calculated from $\vec{D}$.

One can see that the physical nature of the underlying approximation, expressed in Eqs. (27) and (36), is the same in both the z and t-propagated versions of the UPPE. That makes these equations essentially equivalent from the point of view of how accurately they capture the pulse propagation physics. There are, however, practical issues that make one or the other equation better suited for a given purpose. We briefly discuss these computational aspects in the next section.

C. *t*-propagated versus *z*-propagated equation: Computational issues

For most practical purposes, especially when one introduces additional approximations (e.g., scalar field, axial symmetry, etc.) the two approaches are practically equivalent. Both are very large systems of coupled, nonlinear ordinary differential equations (ODE's) with highly oscillatory solutions. Available ODE solver libraries can be used, although such "canned" routines are often written with relatively small systems of equations in mind, and may use more memory space than is actually necessary. We have not noticed a big difference between numerical efforts required for the two UPPE versions, at least in the "paraxial situations."

The difference between the two becomes more appreciable in a regime of extreme focusing and/or when the vector effects are not negligible. The z-propagated version only gives us the transverse fields and though the longitudinal component can be calculated from these, this is more complicated than in the t-propagated version. Thus, in such a regime, the t-propagated equation is more straightforward to implement.

Calculation of the nonlinear responses is another aspect in which the z- and t-propagated equations pose different requirements. In both versions, it is computationally convenient to introduce a moving frame of coordinates that follows the center of the pulse, usually with the velocity equal to the group velocity of the initial pulse. (Note that if chromatic dispersion is strong and spectral broadening occurs, preferably on one side of the spectrum, it may be advantageous to adjust the moving frame velocity accordingly.) Very often the evolution of the pulse is relatively slow in the moving frame, and the adaptive integration step Δz can be significantly longer than the temporal length of the computational domain cT (multiplied by the speed of light). This is not a problem in the z-propagated version, since the whole history

of the optical field is available at every z and the nonlinear response is straightforwardly calculated along the t axis of the computational domain. On the other hand, in the t-propagated equation, the response $P(x,y,z,t)$ is normally calculated at each spatial location. If the response exhibits memory, such as the stimulated Raman effect, or plasma generation, previous "time slices" of various quantities that contribute to the response, e.g., the plasma density $\rho(x,y,z,t-\Delta t)$, must be kept in memory. This approach works well as long as the integration step $c\Delta t$ is on the micron scale. However, if the slow evolution of the pulse allows a very long integration step, such that $c\Delta t$ is larger than the size of the computational domain along the z-axis, L_z, nonlinear responses must be calculated differently. This is because in the moving frame the past value of $\rho(x,y,z,t-\Delta t)$ transforms into $\rho(x,y,z-v_g\Delta t,t-\Delta t)$, which may be located outside of the computational domain if $v_g\Delta t$ is sufficiently large. Fortunately, under such circumstances one can safely replace $\rho(x,y,z,t-\Delta t)$ by its current-time value on the same "characteristics" $\rho(x,y,z-v_g\Delta t,t)$, which is always available in the computational domain. This is possible because the long integration step is only achievable when the evolution of the pulse is relatively slow and, consequently, this mapping of the local history onto the spatial profile is by default a good approximation. Then, the calculation of the response proceeds along the z axis and thus becomes essentially the same as in the z-propagated equation.

To summarize the above discussion, the z-propagated UPPE is preferred in most conventional pulse propagation situations. On the other hand, when severe focusing occurs, and when capturing the full vectorial nature of the optical field is required, the t-propagated UPPE is more suitable.

To conclude this section, it may be worthwhile to describe briefly the numerical approaches to solve, say, Eq. (28). As pointed above, these equations represent a large system of ordinary differential equations. Besides the large number of equations, an important feature to consider is that in this case it is especially expensive to evaluate the right-hand side, i.e., the derivatives of the spectral amplitudes $\partial_z E_{k_x,k_y}(\omega,z)$ with respect to the propagation variable (z or t). Namely, to obtain the polarization in Eq. (28), one has to perform the transformations between the spectral representation of the field and the real-space representation of the field. Then, the nonlinear responses, such as Kerr or Raman effects, are calculated at each point of the computational domain in real space and can be "collected" into the polarization or current density. This response calculation step is essentially just an implementation of the medium model described in Sec. I B. Once the responses are known in the real-space representation they are transformed back into the spectral-domain representation, and all propagation derivatives can then be evaluated and passed to the ODE solver.

The volume of computations necessary for the right-hand-side (RHS) evaluations is much larger than that of relatively simple calculations done by the ODE driver. Therefore, we only parallelize the RHS evaluation and use a single-threaded ODE solver. This greatly simplifies the parallel execution synchronization: Roughly speaking, it is sufficient to place synchronization barriers around the spectral transforms.

One of the decisions to make when implementing the solver is to choose a method to control the adaptive ODE solver. We usually employ a conservative approach and compare two solutions obtained with a coarse and finer step size. Less expensive approaches are certainly possible, for example, monitoring maximal intensities and/or plasma densities, which correlate well with the computational effort needed to resolve the solution properly, is one simple way to control adaptive integration step. However, it requires some "tuning" of the step-change decision thresholds and can fail to sufficiently decelerate the solver in some extreme self-focusing situations.

D. Optical waveguide z-propagated UPPE

Recently, very thin tapered fibers and submicron diameter silica wires [50] have attracted much attention. These high-contrast waveguides exhibit very small mode areas that depend strongly on the frequency. Since the frequency dependence of the modal fields is completely neglected in the generalized NLS equation that is commonly used for microstructured-fiber simulation, the new waveguides, such as silica wires, will in certain situations require an improved propagation model. We describe such a model in the following.

Let us restrict the propagated pulse to the fundamental mode of the straight cylindrical waveguide of radius a, and write the electric-field modal expansion in terms of the *normalized* modes $[N_m(\omega)=1]$ as

$$\vec{E}(t,r,\phi,z)=\sum_{\omega} C(\omega,z)\vec{\mathcal{E}}(\omega,r,\phi)e^{-i\omega t+i\beta(\omega)z}. \tag{32}$$

Here, the fundamental mode electric-field components are

$$\mathcal{E}_\alpha=\mathcal{M}_\alpha(r,\omega)f_\alpha(\phi),\quad \alpha=r,\phi,z, \tag{33}$$

where $f_\alpha(\phi)$ stands for cosine and/or sine functions, depending on polarization and components, e.g.,

$$\begin{pmatrix}\mathcal{E}_r\\ \mathcal{E}_\phi\\ \mathcal{E}_z\end{pmatrix}=\begin{pmatrix}\mathcal{M}_r(r,\omega)\cos(\phi)\\ \mathcal{M}_\phi(r,\omega)\sin(\phi)\\ \mathcal{M}_z(r,\omega)\cos(\phi)\end{pmatrix}\exp[-i\omega t+i\beta(\omega)z]. \tag{34}$$

Using a frequency-dependent parametrization for the material index of refraction, one can calculate the modal fields and the corresponding propagation constants exactly over the desired range of frequencies.

For the relatively low intensities typical for supercontinuum generation in microstructured silica fibers, the nonlinear material response is due to the optical Kerr and stimulated Raman effects. They generate the polarization

$$P_\alpha(r,\phi,t,z)=\epsilon_0\Delta\chi(r,\phi,t,z)E_\alpha(r,t,z)f_\alpha(\phi), \tag{35}$$

with

$$\Delta\chi(r,\phi,t,z)=2n_b\bar{n}_2\sum_\alpha f_\alpha^2(\phi)E_\alpha^2(r,t,z)*\mathcal{R}(t) \tag{36}$$

being the local susceptibility modification and $\mathcal{R}(\tau)$ the normalized Kerr and Raman response function.

We insert these expansions into Eq. (18) and perform integration over the azimuthal angle to obtain

$$\partial_z C(\omega,z) = i\omega\epsilon_0 n_b \bar{n}_2 \times \int_0^a r\mathrm{d}r \int \mathrm{d}t e^{+i\omega t - i\beta(\omega)z} \sum_{\alpha\beta} M_\alpha^*(\omega,r) \times E_\alpha(r,t,z) K_{\alpha\beta}[E_\beta^2(r,t,z) * \mathcal{R}(t)], \quad (37)$$

where a is the radius of the waveguide strand and $K_{\alpha\beta} = \int_0^{2\pi} d\phi f_\alpha^2(\phi) f_\beta^2(\phi)$ is the angular overlap integral. This is the z-propagated UPPE specialized for the ultrathin waveguide, such as submicron silica taper or a silica wire. The generalization for two polarization components is obvious: It amounts to two coupled equations of the same type for the expansion amplitudes $C^a(\omega,z), a=1,2$, with the coupling through the angular overlap integrals $K_{\alpha\beta}^{ab}$. Of course, one can include the higher-order modes the same way.

The most important difference from the generalized NLS is that this equation takes into account the full frequency dependence of the modal fields. The NLS is obtained readily when one elects to replace the frequency-dependent modal fields by a fixed radial profile at a chosen reference frequency Ω: $\vec{\mathcal{M}}(\omega,r) \to \vec{\mathcal{M}}(\Omega,r)$. Then, the radial integration can be factored out, resulting in the nonlinear coefficient

$$\gamma = \epsilon_0 n_b \bar{n}_2 \int_0^a r\mathrm{d}r \sum_{\alpha\beta} K_{\alpha\beta} |\mathcal{M}_\alpha^*(\Omega,r)|^2 |\mathcal{M}_\beta(\Omega,r))|^2, \quad (38)$$

and the equation reduces to the NLS in the spectral representation.

We have studied the regimes of pulse propagation in ultrathin silica wires and tapered fibers when the deviations between the generalized NLS solutions and solutions obtained from the above improved equation become significant. These issues will be discussed in a separate work. Here, we only want to point out some computational issues, important for the practical implementation of a solver based on Eq. (37).

From a numerical simulation point of view, the radial integration is the main complication, because it cannot be performed before the spectral transformations of the response are calculated as functions of radius. Indeed, the resulting simulator is roughly an order of magnitude slower than its generalized NLS counterpart. Fortunately, since the modal fields within the core are rather smooth functions of radius, a very simple integration scheme that employs relatively few sampling points turns out to be sufficient. A Gaussian integration scheme with eight radial samples works well. Thus, the nonlinear response is calculated in the same way as for the NLS for each radial sampling point, and the corresponding responses are then "collected" during the radial integration. It is therefore quite straightforward to upgrade the conventional (spectral domain) NLS solver to the z-propagated thin-waveguide UPPE equation.

VI. DERIVATION OF OTHER EQUATIONS FROM UPPE

There are several types of unidirectional propagation equation widely used in the nonlinear optics literature. The most prominent examples are those of the nonlinear Schrödinger (NLS) equation [2], nonlinear envelope equation [11] (NEE), first-order propagation equation [12] (FOP), forward Maxwell's equation [13] (FME), and several other equations that are closely related to these. The derivations found in the literature differ from equation to equation, and in some cases the physical meaning of the required approximations becomes hazy in the multitude of neglected terms. In the following section, we show that all previous propagation equations are in fact special cases of the UPPE, easily obtained using the same, uniform procedure that clearly identifies what physical effects get neglected in the process of derivation.

A. General procedure

First, we adopt a scalar approximation and write Eq. (28) in the form

$$\partial_z E_{k_x,k_y}(\omega,z) = iKE_{k_x,k_y}(\omega,z) + iQP_{k_x,k_y}(\omega,z), \quad (39)$$

where

$$K(k_x,k_y,\omega) = \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2} \quad (40)$$

and

$$Q(k_x,k_y,\omega) = \frac{\omega^2}{2\epsilon_0 c^2 \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2}} \quad (41)$$

are the plane-wave propagation constant and nonlinear coupling coefficient, respectively. For envelope equations, we express the field in terms of an envelope by factoring out the carrier wave at a chosen reference angular frequency ω_R with the corresponding wave-vector $k_\mathrm{R} = K(0,0,\omega_\mathrm{R})$,

$$E(x,y,z,t) = A(x,y,z,t)e^{i(k_\mathrm{R}z - \omega_\mathrm{R}t)}, \quad (42)$$

and similarly for the nonlinear polarization. Then, as a first step, we replace K and Q by suitable approximations. These approximations are usually Taylor expansions in frequency and transverse wave numbers. At that stage, one can easily identify the additional approximations required for the given equation. In the second step, we transform the new equation into the real-space representation, which is formally done by replacing the spectral variables of K and Q by differential operators acting on the envelope,

$$(\omega - \omega_\mathrm{R}) \to i\partial_t \quad ik_x \to \partial_x \quad ik_y \to \partial_y. \quad (43)$$

Also, the z derivative in the envelope representation goes to

$$\partial_z \to ik(\omega_\mathrm{R}) + \partial_z. \quad (44)$$

Finally, we transform to the frame comoving with the group velocity of the pulse to obtain the desired equation. Thus, different equations are obtained from different approximations of the linear propagator K and of the nonlinear coupling Q. Apart from factoring out the carrier wave, the procedure is the same for a nonenvelope equation.

At this stage we can see the approximations that are common to all UPPE. They are those that were needed to obtain Eq. (28).

First, the optical field generated in the backward direction has to be so weak that the nonlinear response calculated from the forward-propagating field is an accurate approximation of the actual response. The obvious problem with this approximation is, of course, that it is not *a priori* clear in a concrete situation whether it holds or not.

Second, we essentially work with scalar equations, even in the case of equations that couple two transverse components. Namely, unless the z components of the field and of the nonlinear response are completely included, the divergence condition in Maxwell's equations is not properly reflected in a unidirectional propagation equation [21]. In some cases this becomes evident already at the first step, when an equation is derived starting from the wave equation and the $\vec{\nabla}\vec{\nabla}\cdot\vec{E}$ term is already neglected [56].

B. Nonlinear Schrödinger equation

This is the simplest case in which we choose a reference angular frequency ω_R and the corresponding reference wave number $k_R = k(\omega_R)$, and take

$$K \approx k_R + v_g^{-1}(\omega - \omega_R) + \frac{k''}{2}(\omega - \omega_R) - \frac{1}{2k_R}(k_x^2 + k_y^2). \tag{45}$$

This is a second-order Taylor expansion in ω and k_x, k_y around ω_R and $(0,0)$. In the nonlinear coupling coefficient, we neglect all variable dependencies and take its value at the reference frequency,

$$Q \approx \frac{\omega_R}{2\epsilon_0 n(\omega_R)c}. \tag{46}$$

For simplicity, in the NLS we only account for the instantaneous optical Kerr effect, and write the nonlinear polarization envelope as

$$\mathcal{P} = 2\epsilon_0 n(\omega_R) n_2 I \mathcal{A}. \tag{47}$$

Inserting the above expression into (39) and (42) we obtain

$$\partial_z \mathcal{A} + ik_R \mathcal{A} = ik_R \mathcal{A} + iv_g^{-1}(\omega - \omega_R)\mathcal{A} + \frac{ik''}{2}(\omega - \omega_R)^2 \mathcal{A} - \frac{i}{2k_R}(k_x^2 + k_y^2)\mathcal{A} + \frac{i\omega_R}{c} n_2 I \mathcal{A}. \tag{48}$$

It is customary to normalize the envelope amplitude such that $|\mathcal{A}|^2 = I$. Using rules (43) we finally obtain the NLS equation,

$$(\partial_z + v_g^{-1}\partial_t)\mathcal{A} = \frac{i}{2k_R}\Delta_\perp \mathcal{A} - \frac{ik''}{2}\partial_{tt}\mathcal{A} + \frac{i\omega_R}{c} n_2 |\mathcal{A}|^2 \mathcal{A}. \tag{49}$$

The above derivation procedure made very explicit what approximations, beyond that specified in (27) and discussed in the previous subsection, need to be implemented to obtain the NLS: Approximating K to second order in frequency and transverse wave number amounts to the paraxial, and quasimonochromatic approximations for the linear wave propagation. The approximation in the nonlinear coupling Q also requires a narrow spectrum. The slow variation of the envelope, usually invoked in the NLS derivation, appears here only as an implicit consequence of the narrowness of the spatiotemporal spectrum.

C. Nonlinear envelope equation

As in the case of the NLS equation, the NEE is paraxial. However, in the temporal domain, the NEE goes far beyond the NLS equation. Formally, the NEE requires very little additional approximation in the temporal domain, and it appears to be extremely close to the paraxial version of UPPE.

Indeed, we take

$$K \approx + k(\omega) - \frac{c}{2\omega n_b(\omega_R)}(k_x^2 + k_y^2), \tag{50}$$

so that the only approximation apart from paraxial is the constant index of refraction $n_b(\omega) \to n_b(\omega_R)$ in the denominator of the diffraction term.

Further, the first term in the above approximation is reexpressed as a sum of its two lowest-order Taylor expansion terms plus the rest,

$$k(\omega) = k(\omega_R) + v_g^{-1}(\omega - \omega_R) + D(\omega - \omega_R), \tag{51}$$

where

$$D(\omega - \omega_R) = \sum_{n=2}^{\infty} \left(\frac{\partial^n k}{\partial \omega^n}\right)_{\omega=\omega_R} \frac{(\omega - \omega_R)^n}{n!}. \tag{52}$$

For the nonlinear coupling term, we preserve the frequency dependence, but neglect the transverse wave-number dependence completely,

$$Q \approx \frac{(\omega - \omega_R) + \omega_R}{2\epsilon_0 c n(\omega_R)}. \tag{53}$$

Here, as in the free-propagation term, we neglect the chromatic dispersion of the background index of refraction. The spectral representation of the equation then reads,

$$\partial_z \mathcal{A} + ik_R \mathcal{A} = ik_R \mathcal{A} + iv_g^{-1}(\omega - \omega_R)\mathcal{A} + iD(\omega - \omega_R)\mathcal{A} - \frac{ic}{2\omega_R n(\omega_R)}\left(1 + \frac{\omega - \omega_R}{\omega_R}\right)^{-1}(k_x^2 + k_y^2)\mathcal{A} + \frac{i\omega_R}{2\epsilon_0 c n(\omega_R)}\left(1 + \frac{\omega - \omega_R}{\omega_R}\right)\mathcal{P}. \tag{54}$$

After transforming into the real-space representation, we obtain the NEE,

$$\partial_z \mathcal{A} + v_g^{-1}\partial_t \mathcal{A} = iD(i\partial_t)\mathcal{A} + \frac{i}{2k_R}\left(1 + \frac{i}{\omega_R}\partial_t\right)^{-1}\Delta_\perp \mathcal{A} + \frac{ik_R}{2\epsilon_0 n_b^2(\omega_R)}\left(1 + \frac{i}{\omega_R}\partial_t\right)\mathcal{P}. \tag{55}$$

To summarize, the additional approximation needed in this

case is paraxiality both in the free propagator and in the nonlinear coupling, and a small error in the chromatic dispersion introduced when the background index of refraction is replaced by a constant, frequency-independent value in both the spatiotemporal correction term and in the nonlinear coupling term. Note that the latter approximation is nothing to worry about: It is such a small effect that in practice there will almost certainly be other, much weaker aspects of the model, such as the plasma equation, neglected nonlinear dispersion, and uncertain MPI parameters, to name a few.

D. Partially corrected NLS

The partially corrected NLS (PC-NLS) equation is similar to the NEE. It is obtained from the UPPE in the same way, with the only difference being the approximation adopted in the spatiotemporal focusing term. Namely, the correction term of the free propagator in Eq. (54) is replaced by its first-order expansion,

$$\left(1+\frac{\omega-\omega_{\mathrm{R}}}{\omega_{\mathrm{R}}}\right)^{-1}\approx\left(1-\frac{\omega-\omega_{\mathrm{R}}}{\omega_{\mathrm{R}}}\right), \tag{56}$$

which leads to the equation

$$\partial_z\mathcal{A}+v_g^{-1}\partial_t\mathcal{A}=iD(i\partial_t)\mathcal{A}+\frac{i}{2k_{\mathrm{R}}}\left(1-\frac{i}{\omega_{\mathrm{R}}}\partial_t\right)\Delta_\perp\mathcal{A}+\frac{ik_{\mathrm{R}}}{2\epsilon_0 n_b^2(\omega_{\mathrm{R}})}\left(1+\frac{i}{\omega_{\mathrm{R}}}\partial_t\right)\mathcal{P}. \tag{57}$$

Thus, it may seem that the PC-NLS is quite close to the NEE, but that is not the case. The dispersion properties of their respective plane-wave solutions are quite different. While the PC-NLS provides better-than-NLS approximation around the reference frequency ω_R, its dispersion properties become rather pathological around $\omega\approx 2\omega_R$, where its diffraction term changes sign as a consequence of the truncated correction factor. As a consequence, PC-NLS should only be used when the pulse spectrum remains narrow. If the spectrum broadens too much, artifacts in the angular distribution of the spectrum occur around and beyond $\omega\approx 2\omega_{\mathrm{R}}$.

E. First-order propagation equation

Unlike the above examples, the (FOP) equation, introduced by Geissler *et al.*, [12], is not an envelope equation. It is, however, equivalent to the NEE from the point of view of the approximations required for its derivation, as we shall see shortly. Though it is not at all necessary, we neglect the linear chromatic dispersion to obtain the same equation as Geissler *et al.*

In Eq. (28), we approximate

$$K\approx\frac{\omega}{c}-\frac{c}{2\omega}(k_x^2+k_y^2)\quad\text{and}\quad Q\approx\frac{\omega}{2\epsilon_0 c}, \tag{58}$$

which is the same approximation as the one in the NEE, only with vacuum in the role of the linear medium. Thus, Eq. (28) becomes

$$\partial_z E_{k_x,k_y,\omega}=\frac{i\omega}{c}E_{k_x,k_y,\omega}-\frac{ic}{2\omega}(k_x^2+k_y^2)E_{k_x,k_y,\omega}+\frac{i\omega}{2\epsilon_0 c}P_{k_x,k_y,\omega}, \tag{59}$$

which is equivalent to Eq. (2) of Ref. [12]. After transforming into the real-space domain, we arrive at the FOP equation,

$$\left(\partial_z+\frac{1}{c}\partial_t\right)E(r_\perp,t)=\frac{c}{2}\Delta_\perp\int_{-\infty}^{t}d\tau E(r_\perp,\tau)-\frac{1}{2\epsilon_0 c}\partial_t P(r_\perp,t). \tag{60}$$

It is clear from the above calculations of the NEE and FOP equation that, despite the rather different ways they were originally derived, these two equations become equivalent if one chooses to treat the dispersion properties of the medium on the same level.

F. Forward Maxwell equation

The FME, introduced by Husakou and Herrmann [13], is another nonenvelope equation that is therefore free of any reference frequency. It was derived in an intuitive way from the wave equation with a neglected $\nabla\vec{\nabla}\cdot\vec{E}$ term, though it was written in a vector form. We therefore start its clean derivation from the full z-propagated UPPE. However, the "zeroth" step is to discard the projector $\Sigma_s\,\vec{e}_s^{\perp}\vec{e}_s$, which gives us essentially the same starting point as for the equations discussed above, only that we have a (coupled) z-propagated UPPE for each component. This tells us that the resulting equation will still be essentially a scalar one, meaning that the vector nature of light is not captured completely correctly, and the reason for this is traced back to the neglected $\nabla\vec{\nabla}\cdot\vec{E}$. This "drawback," however, becomes "justified" in the next step, where we approximate K and Q by its paraxial, and zero-order expansions, respectively,

$$K\approx k(\omega)-\frac{c}{2\omega n_b(\omega)}(k_x^2+k_y^2)\quad Q\approx\frac{\omega}{2\epsilon_0 c n_b(\omega)}. \tag{61}$$

In this paraxial formulation, the equation is limited to the regime in which the polarization scrambling term $\nabla\vec{\nabla}\cdot\vec{E}$ does not play any important role.

Note that the above approximations for K and Q are extremely similar to those for the NEE. Here, the chromatic dispersion of the index of refraction is (correctly) preserved. The resulting equation is then obtained by transforming to real space in the transverse coordinate only, keeping the spectral frequency-time representation,

$$\partial_z E(x,y,\omega,z)=ik(\omega)E(x,y,\omega,z)+\frac{i}{2k(\omega)}\Delta_\perp E(x,y,\omega,z)+\frac{i\mu_0\omega c}{2n_b(\omega)}P(x,y,\omega,z). \tag{62}$$

This equation is equivalent to the FME Eq. (2) of Ref. [13]. The only difference is that we have not changed to the moving frame coordinates $\xi=z$, $\eta=t-z/c$, because in the dispersive medium it is computationally more convenient to use

the frame that moves with a suitable *group* velocity, an important detail in strongly dispersive medium.

Thus, formulas (50), (53), and (61) show that there is very little difference between the FME and NEE. Actually, the most convenient way to solve the NEE is in the spectral domain, where the correct frequency dependence of the background index of refraction can be taken into account—that way the NEE becomes equivalent to the FME.

G. Correction terms and reference frequency

To conclude this section, we would like to point out the relation between what are sometimes called "correction terms" and the reference frequency and reference wave vector that appear in envelope equations. In the present context, the correction terms are understood as "deviation" of a propagation equation from the NLS. Spatiotemporal focusing terms [16] and self-steepening terms [18] are most common examples that appear in the equations discussed above, but there are also perturbation approaches found in the literature that sometimes lead to numerous correction terms.

In all envelope equations a reference frequency and a reference wave number appear, and are mostly chosen equal to the central frequency and wave number of the input pulse. These quantities are artificial and to a certain degree arbitrary "gauge" parameters that, of course, do not appear in the Maxwell's equations. Therefore, any resulting solutions should not depend on how the reference is chosen. This may not be the case if the reference is selected too far from the central frequency of the pulse, or when the spectrum becomes too broad due to nonlinear interactions. The correction terms were introduced into equations to achieve a broader a applicability of the resulting equation. One way to view such corrections is that the additional terms partially restore the equation's invariance with respect to the choice of the reference frequency. For example, the spatiotemporal focusing correction term (operator) $\omega_R^{-1}[1+1/\omega_R\partial_t]^{-1}$ that appears in the NEE equation and modifies the diffraction term seems to depend on the reference ω_R, but it is in fact proportional to the "gauge-independent" ω^{-1}, provided it is properly implemented in the spectral domain.

This observation hints at a simple but rarely performed check of numerical simulations based on envelope equations: A comparative simulation run performed with a shifted reference frequency (i.e., sufficiently different from the pulse carrier frequency) will readily reveal what part of the simulated spectra can be trusted.

VII. CONCLUSION

We have presented several versions of the UPPE. The time-domain UPPE, originally proposed in Ref. [24], is suited to situations when extreme (self-) focusing occurs, and when the longitudinal field and nonlinear response components are not negligible. This equations bridges the gap between the numerical Maxwell's equation solvers on one side, and a family of unidirectional propagation equations, on the other.

The *z*-propagated UPPE is the propagation equation of choice for most situations occurring in high-power femtosecond pulse propagation in bulk condensed and gaseous media, when the typical transverse filament size is sufficiently larger than the wavelength.

We have also presented a *z*-propagated UPPE suitable for strandlike waveguides with transverse dimensions comparable to the wavelength, in which the modal field profiles strongly depend on the frequency.

Many propagation equations previously published can be derived from the UPPE. The derivation follows the same procedure independently of the given equation type. Namely, various equations are obtained by selecting appropriate additional approximations in the UPPE. That way, the propagation equations can be categorized based on the captured *physics*, rather a on the way they are originally derived. This approach readily reveals in what situations one should expect the equation to work well or to fail. It also reveals that some equations published originally in different representations are actually equivalent under certain conditions.

Moreover, viewing the variety of propagation equations from the same point of view, with the UPPE as their origination point, also shows a previously unrecognized meaning of various "beyond the NLS correction terms." Such terms, designed to improve the NLS equation and extend its validity into the realm of ultrafast pulses and of extreme spectral broadening, can be understood as corrections that "repair" the NLS's dependence on the choice of the reference frequency. For example, the NEE equation, though it explicitly contains ω_R, turns out to be almost reference independent, which is indicative of a "good equation." On the other hand, when corrections are treated as series expansions, the desired "gauge invariance" with respect to. ω_R can be badly broken even at frequencies not far from ω_R.

Finally, we note that the *z*-propagated UPPE can be solved with the same ease (or difficulty) as, say, the NEE or even the NLS, in the spectral domain. Ordinary differential equation solvers can be utilized and work well with this equation. The numerical solver can be easily implemented for fibers, radially symmetric geometries or full $3+1$ dimensional simulations. Since the UPPE can be viewed as the "minimal approximation" unidirectional equation, it presents itself as a robust, universal simulation tool.

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