I. INTRODUCTION

Here I discuss three important ways to tackle pulse propagation in nonlinear optics. These include methods that both do and do not follow the traditional approach of using pulse envelopes. The description is taken in the 1D limit, but some discussion on including transverse effects is made. The aim is to cover the considerations relevant when modeling wideband fields, a regime not comprehensively treated in many standard texts [1, 2, 3, 4, 5, 6].

The three ways are solving (a) Maxwell’s equations, (b) directional Maxwell’s equations, or the (c) standard second order wave equation. Solving Maxwell’s equations is a well established approach, with a long history (i.e. finite difference time domain (FDTD), see e.g. [7]), although it is computationally intensive and has generally been little used in nonlinear optics (but see e.g. [8, 9, 10]). Practical versions of directional Maxwell’s equations have appeared only recently, such as that of Kolesik et al. [11, 12]; other approaches followed [13, 14, 15]. However the first proposal dates back to Fleck in 1970 [16], although only as something of a remark in passing, rather than a full investigation. The most common approaches nonlinear optics are those based on the standard second order wave equation, particularly with regard to envelope propagation and the celebrated slowly varying envelope approximation (SVEA). The SVEA allows us to convert the second order wave equation into a first order equation that can efficiently propagate narrowband pulses. Recently the SVEA has been relaxed [17, 18, 19], extending the use to moderate bandwidths. However, much better approaches based on factorizing the second order wave equation also exist. An early example can be seen in [2], but also most notably by Blow and Wood [20], and also the recent Ferrando et al. [21] and Genty et al. [22].

We can try to solve any of these equations directly,
without recourse to an envelope and carrier representation. This means ensuring sufficient numerical resolution to integrate each of the field oscillations as it propagates across the simulation window. This approach is the standard one when solving Maxwell’s equations (i.e. FDTD), but generally in nonlinear optics an envelope approach is used. This has a number of advantages: it imposes a direction on the modeled pulse, and it removes the fast oscillations at the centre frequency. In combination with a moving frame, it can turn a pulse of rapidly oscillating fields moving at the speed of light into a smooth, nearly-stationary waveform – with commensurate gains in simulation speed. These benefits usually come with a restriction on the allowed bandwidth of the pulse being modeled.

This paper is organized as follows: in section II I compare field and envelope approaches. In section III I consider Maxwell’s equations in both field and envelope pictures, followed in section IV by the same, but utilizing a directional rewriting of Maxwell’s equations. Then, in section V I consider the role of second order wave equations, in particular using factorization methods. Finally, in section VI I present some conclusions.

Although not directly relevant to the discussion here, it is also worth noting that directional waves moving at the speed of light into a smooth, nearly-stationary waveform – with commensurate gains in simulation speed. These benefits usually come with a restriction on the allowed bandwidth of the pulse being modeled.

II. FIELDS VS ENVELOPES

It is often remarked upon that envelope methods work surprisingly well. However, this surprise seems to be based largely upon the SVEA equation for pulse propagation, which indeed contains many approximations (see [19, 24]). Recently it has been shown by several groups [11, 13, 15, 21] that equations nearly identical to those generated by the SVEA can be found by assuming little more than the lack of backward-going field components. Even when revisiting Blow and Wood [20], we can see that their mathematics contained minimal constraints on the bandwidth of the envelope, although their specific nonlinearity model did contain such restrictions.

A. The definition

For envelope methods, the direction is imposed by the form for the carrier function, and is usually a plane wave traveling in the chosen direction. Thus the typical envelope and carrier representation of some field \( Q \) is

\[
Q(t; z) = A(t; z)e^{i(k_0 z - \omega_0 t)} + A^*(t; z)e^{-i(k_0 z - \omega_0 t)}.
\]

\[
\dot{Q}(\omega; z) = \dot{A}(\omega + \omega_0; z)e^{i k_0 z} + \dot{A}^*(\omega - \omega_0; z)e^{-i k_0 z}.
\]

In some of the following equations, I will shorten the argument of the exponential in the carrier function with \( \Xi = t(k_0 z - \omega_0 t) \). It is worth noting that we are not required to use carrier functions with the usual exponential form [23], e.g. in semiconductor physics, Bloch functions are routinely used as carriers to form a basis for electron (or hole) envelope functions.

Note that it is approximations that restrict the validity of envelope approaches, not the use of them in itself. This is contrary to the impression that might be gained from SVEA approaches, and even their generalizations [17, 19]. The potential benefits of envelopes are not tied to restrictions on the bandwidth of the pulse being modeled.

B. The big advantage

Replacing real fields \( E \) and \( H \) with an envelope-carrier description gives us at least one clear advantage: it removes the dominant contribution to the underlying field oscillations. The resulting smoother envelope is therefore easier, and much less computationally expensive to propagate. It is the rapidity of the fastest time-domain modulation of the field or envelope which constrains our time resolution, and the rapidity of the fastest spatial modulation which constrains the spatial resolution. Note that although we usually hope that our envelope will then have a relatively slowly varying form, the mere replacement of the EM fields by envelope-carrier combinations imposes of itself no approximations whatsoever.

Two processes may act to twist an initially smooth envelope into something more problematic. First, linear dispersion can add chirp, which manifests itself as a nonlinear phase ramp across the pulse. These are usually relatively smooth changes, and cause little problem. Second, there are nonlinear effects. Some, such as self phase modulation (SPM) can be relatively mild, others, such as coupling to backward propagating waves and harmonic generation can impose significant oscillations.

C. Nonlinear polarization terms

As mentioned above, nonlinear processes can generate oscillatory contributions to the envelope. We can see how this occurs by considering an instantaneous third order nonlinearity, which depend on \( E^3 \) and has the form

\[
E^3(t; z) = \left[ A(t; z)e^{i\Xi} + A^*(t; z)e^{-i\Xi} \right]^3 \tag{3}
\]

\[
= A(t; z)^3 e^{+3\Xi} + 3A(t; z)^2 A^*(t; z)e^{+\Xi} + c.c.
\]

Here we see a useful side-effect of the envelope-carrier representation – that nonlinear terms can be separated into convenient components. In this example, the full \( \chi^{(3)} \) nonlinearity splits into a third harmonic generation (THG) term proportional to \( A^3 \), and an SPM term proportional to \( |A|^2 \); along with complex conjugate counterparts (c.c.). Clearly the THG term is non-resonant with the chosen carrier, and keeping such non-resonant nonlinear terms will impose significant oscillations onto our envelope as it propagates. Such oscillations break...
approximations relying on a relatively smooth envelope, which is why in SVEA models they are discarded; however there is no \textit{a priori} requirement to do so. E.g., in the wideband Raman model of Kinsler and New \cite{26,27}, the Stokes and anti-Stokes fields appeared as sidebands on the envelope spectrum.

D. Multiple carriers, wideband envelopes

We can generalize from a single envelope-carrier pair by using multiple envelopes with carriers at different carrier frequencies. However, each added envelope greatly increases the number of individual polarization terms resulting from a nonlinearity, so as a rule it is best to use the minimum number possible. As an exercise, just calculate the number of terms in an eqn. \ref{eq:3} derived from a field defined as $E = A_1 e^{+xi} + A_2 e^{+yi} + c.c$, not $E = A_1 e^{+xi} + c.c$!

Multiple carriers work best when there are multiple narrowband fields which resonantly interact, such as in an optical parametric amplifier \cite{2,3} (check) or for Raman processes \cite{26,27}. In such cases we can ruthlessly discard nonlinear polarization terms which are not perfectly in resonance with processes of our choosing. Another use for multiple carriers is for including both forward and backward propagating fields.

If we use multiple carriers, and also allow wideband envelopes, then it is possible for multiple envelopes to cover the same piece of spectrum. In a continuous mathematical description this overlap will always happen, but in a discrete or numerical implementation it will depend on our parameters.

This overlap is not necessarily a problem, as long as we are careful about assigning polarization terms to whichever envelope equation we choose – we must make sure not to add the same term twice, for example. This can also lead to a non-unique description, in the case where a polarization term could be equally well drive the evolution of one of two (or more) envelopes. Nevertheless, such non-uniqueness does not break our model, it just allows us a choice which we might be able to use to our advantage. In a simulation, we could try to assist our numerics by managing the envelope spectra by generating a total spectrum, and then reassigning components in the overlap region according to some smoothing procedure.

The use of wideband envelopes can raise some interesting issues. For example, if the bandwidth of an envelope is greater than its carrier frequency, then the envelope will extend into negative frequencies. This is not a problem for our physical model, since we still have to reconstruct the field from the envelopes and carriers, and those negative frequency components are matched by complementary positive frequency ones from the complex conjugate of the envelope\textsuperscript{1}. Again, we might consider a spectral management scheme which swaps these unexpected components over, restoring the envelope to pure positive frequency content (and hence its conjugate to pure negative frequency content). However, we then find that at zero-frequency we have introduce a hard cutoff in the envelope spectra, and so induced unwanted oscillations in the time domain version of the envelope.

However, while such spectral management might seem to offer advantages, in practice it makes little difference, and adds needless complication to simulation code. I would consider it only if some unexpected interaction was generating significant spectral content near the band edge of an envelope, at a position where it would be well within the spectral range of some other envelope; and even then it might be easier to simply increase the envelope bandwidth.

E. Directionality

A carrier imposes a direction of propagation, and most carrier-based models silently neglect even the possibility of backward propagating fields, even though there is a coupling between them. However, Casperson \cite{28} used both forward and backward carriers to construct an envelope model with a separation of the forward and backward field components and interactions. The more recent paper of Sanborn et al. \cite{29} used the same approach.

Backward traveling components, if forced onto a forward traveling envelope, will appear as non-resonant terms. If identified correctly, these can then be discarded.

See also section \ref{sec:VI} for a discussion of the coupling between forward and backward waves which is induced by a nonlinearity.

F. Moving frames

In combination with a suitable moving frame, an envelope representation can turn a pulse of rapidly oscillating fields moving at the speed of light into a smooth, nearly-stationary waveform – with commensurate gains in simulation speed.

However, we need to guarantee that all contributions from backward traveling components are removed, otherwise the envelope will contain oscillatory components moving at approximately twice the frame speed.

A typical moving frame is defined by for a frame speed $v$ as $t' = t - z/v$. Thus the spatial derivatives in propagation equations are altered using

$$\partial_z = \partial_{z'} - v \partial_t$$

\textsuperscript{1} That is, they \textit{should} be so matched. If they aren’t, you’ve done something wrong.
G. Estimating the computational cost

Consider a wideband pulse, with a bandwidth of the order of its centre frequency $\omega_0$. In a full-field approach, this will have the fastest modulations of the field being of the order $2\omega_0$. In comparison, an envelope approach results in the fastest modulations on the envelope being of the order $\omega_0$. Simplistically we might then hope that the envelope approach allows us to halve our time and space resolutions whilst still retaining numerical accuracy. For narrow band fields the advantage is much clearer – a bandwidth of $\omega_0/100$ might allow resolutions to be coarsened by a factor of 100. For fields of a wider bandwidth, we gain little advantage, unless we shift our carrier frequency $\omega_0$ to the centre of the spectrum, even if that is not co-incident with the dominant frequency component. A more comprehensive examination of the effects of numerical resolution has been given for the nonlinear Schrödinger equation by Sinkin et al. [30].

Note that since the linear response (dispersion) of the medium can be done exactly in the frequency domain, regardless of step-size, it might seem more appropriate to focus more on the role of the nonlinear response when estimating the necessary temporal and spatial resolutions. However the accuracy of a propagation method cannot be easily evaluated whilst ignoring the dispersive propagation, because both dispersive and nonlinear effects occur simultaneously. Even if a split step method is used, they are interleaved, and their effects cannot be disentangled.

H. Disadvantages

The slight disadvantage of using envelopes is that real valued time dependent fields are replaced by complex valued envelopes. This doubles the amount of storage used during computations, and also requires the use of complex Fourier transforms rather than the faster real valued ones; although of course the spectra of the fields are complex in any case. In practice, the computational cost is small, although the complexity of the simulation code is increased.

III. MAXWELL’S EQUATIONS

When propagating fields in free space, we use the time-like Maxwell’s equations. To simplify the description we transform their time-like behaviour into frequency space. This enables us to write the convolutions required to model the linear time-response of the medium (e.g. dispersion) as multiplications. However, since the form of the nonlinear response is not simplified by this process, a convolution in frequency space appears. In frequency space, time derivatives convert to factors of $-i\omega$, so the equations are

$$\partial_z \tilde{E}_x(\omega) = -i\omega\tilde{\epsilon}(\omega') \ast \tilde{H}_y(\omega; z),$$  \hspace{1cm} (7)

The “\ast ” denotes a convolution,

$$Q(\tau) \ast P(t) = \int Q(\tau)P(t-\tau)d\tau = \mathcal{F}^{-1}\left[\tilde{Q}(\omega)\tilde{P}(\omega)\right]$$ \hspace{1cm} (8)

A rather nice way to scale these equations is to define suitable $\epsilon_n$ and $\mu_n$ corresponding to a suitably chosen refractive index, hence $\mu_n$ will usually be $\mu_0$. This means $\epsilon_n = 1/\epsilon_n \mu_n$, $k = \omega/\epsilon_n$, $\tilde{\epsilon}_n = \tilde{\epsilon}(\omega')/\epsilon_n \mu_n = \tilde{\mu}(\omega')/\mu_n$.

We then define $e = \sqrt{\epsilon_n}E$ and $h = \sqrt{\mu_n}H$, which ensures $e$ and $h$ are of comparable sizes. This gives us the scaled Maxwell’s equations

$$\partial_z \tilde{h}_y(\omega; z) = -ik\tilde{\epsilon}_n(\omega') \ast \tilde{e}_x(\omega; z),$$ \hspace{1cm} (9)

$$\partial_z \tilde{e}_x(\omega) = -ik\tilde{\mu}_n(\omega') \ast \tilde{h}_y(\omega; z).$$ \hspace{1cm} (10)

It is worthwhile comparing this scaling with that from the directional fields approach in section IV with the correspondences $\sqrt{\epsilon_n} \rightarrow \alpha_r$ and $\sqrt{\mu_n} \rightarrow \beta_r$.

For our purposes, there are two main ways to solve Maxwell’s equations: either FDTD [31] or Pseudo-Spectral Spatial Domain (PSSD) [11]. In FDTD we propagate forward in time, holding the fields $E(z), H(z)$ as a function of space. However, in nonlinear optics, it is more convenient to use PSSD, where we propagate forward in space, holding the fields $E(t), H(t)$ as a function of time.

Under PSSD derivatives are calculated pseudospectrally [31]. However, its most important feature is that the entire time-history (and therefore frequency content) of the pulse is known at any point in space, so applying even arbitrary dispersion incurs no extra computational penalty. In contrast, FDTD (or other temporally propagated methods) must use convolutions or time-response models for dispersion. Although spatially propagated simulations (e.g. PSSD) make it difficult to incorporate reflections properly, this is not a significant constraint as most such simulations are only interested in uni-directional propagation anyway.

For example, in a 1D medium with linear dispersive properties defined by $\epsilon_r, \mu_r$, containing a third order $\chi^{(3)}$ nonlinearity defined by $\epsilon_n$, the equations are

$$\partial_z H_y(\omega; z) = -i\omega\tilde{\epsilon}_r(\omega') \ast \tilde{E}_x(\omega; z)$$ \hspace{1cm}  \hspace{1cm} (11)

$$\partial_z \tilde{E}_x(\omega; z) = -i\omega\tilde{\mu}_r(\omega') \ast \tilde{H}_y(\omega; z),$$ \hspace{1cm} (12)

where $\mathcal{F}[Q(t)](\omega)$ denotes the Fourier transform of some function $Q(t)$. This model allows for the time-response of the nonlinearity, and is thus applicable to (weakly coupled) Raman systems as well. Note that the terms dependent on $\epsilon_r$ and $\mu_r$ are simple products. The linear dispersion combined with a time-dependent third order nonlinearity gives a permittivity function which would be written

$$\epsilon(\tau, t) = \epsilon_r(\tau) + \epsilon_n(\tau) \ast E(t)^2$$ \hspace{1cm} (13)

$$\epsilon(\tau, t) \ast E(t) = \epsilon_r(\tau) \ast E(t) + \{\epsilon_n(\tau) \ast E^2(t)\} E(\tau)$$ \hspace{1cm} (14)
\[\begin{align*}
\tilde{E}(\omega') \ast \tilde{E}(\omega) & = \tilde{e}_{r}(\omega) \tilde{E}(\omega) + \{ \tilde{e}_{c}(\omega') \mathcal{F}[E^2(t)](\omega') \} \ast \tilde{E}(\omega) \tag{15}\end{align*}\]

In the case of instantaneous nonlinearity, \(\tilde{E} = \tilde{e}_{r} \tilde{E} + \epsilon_{c} \mathcal{F}[E^3]\).

A simple and efficient way to propagate these equations is using staggered \(E\) and \(H\) fields, which allow us to use an Euler-like integration for each field, but achieves second-order accuracy \[32\]. However, while the \(E\) and \(H\) fields necessary for a forward propagating pulse are easy to determine for co-incident \(E\) and \(H\), we need to use staggered initial conditions or else we get a significant backward propagating component. Even with correctly staggered initial conditions, we see a small spurious backward component, the size of which depends on the time step. This backward pulse is hard to get rid of completely, but it can be filtered in the time domain when the two pulses have propagated apart far enough. Another point to consider, particularly when generating the initial conditions for very short pulses, is the zero-force condition \[33\]. This can be easily satisfied by deriving the \(E\) and \(H\) fields for the pulse from a suitable vector potential, rather than simply assuming a form for the \(E\) field.

When considering the solution of these three Maxwell’s equations, it is useful to partly calculate the time derivative of eqn.\[14\]. For dispersion and a time response \(\chi^{(3)}\) this gives us three terms,

\[\begin{align*}
\partial_{t}(e(\tau, t) \ast E(t)) & = \partial_{t}e_{r}(\tau) \ast E(t) \\
& + \{\partial_{t} \{ e_{c}(\tau) \ast E^2(t) \} \} E(t) \\
& + \{ e_{c}(\tau) \ast E^2(t) \} (\partial_{t} E(t)) \tag{16}\end{align*}\]

Thus we see that to solve the equations, we will need to calculate the derivatives of three terms: the usual dispersive term, the time response term, and the field. We will also need to retain the value of the time response term as well. Since the time response term contains a convolution, it is best calculated in the frequency domain, which is particularly convenient when using pseudospectral derivatives. We will need two FFT’s to transform \(E\) and \(E^2\) into frequency space. There we construct the dispersion term and the time response term by simple multiplications, and set up arrays for the derivatives by multiplying by \(-\omega\). We then need four back transforms for a total of six in all: one more for the time response, and three for the time derivatives of the dispersion, time response, and field. For an instantaneous nonlinearity, we need only three FFT’s: two forward transforms (for \(E\) and \(E^3\)), and one back transform for the combined derivative. In addition to these six (or three) FFT’s needed to solve the \(\partial_{t}H\) equation, the \(\partial_{t}E\) equation requires another two, for a total of eight (or five).

A. Envelopes

Although it is not often done, we can represent Maxwell’s equations using an envelope and carrier representation. We express the fields \(E\) and \(H\) using

\[\begin{align*}
E_{x}(t; z) & = A(t; z)e^{i(k_{0}z - \omega_{0}t)} + A^{*}(t; z)e^{-i(k_{0}z - \omega_{0}t)} \tag{17} \\
H_{y}(t; z) & = F(t; z)e^{i(k_{0}z - \omega_{0}t)} + F^{*}(t; z)e^{-i(k_{0}z - \omega_{0}t)} \tag{18}\end{align*}\]

We insert these into the Maxwell’s equations above, separate out the normal and complex conjugate (c.c.) parts, cancel the carrier exponentials present on both sides of the equations, and rearrange to leave only \(\partial_{z}\) terms on the RHS,

\[\begin{align*}
\partial_{z}\tilde{F}(\omega; z) & = -i\omega\tilde{e}(\omega') \ast \tilde{A}(\omega; z) - i k_{0}\tilde{F}(\omega; z), \tag{19} \\
\partial_{z}\tilde{A}(\omega; t) & = -i\omega\tilde{e}(\omega') \ast \tilde{F}(\omega; t) - i k_{0}\tilde{A}(\omega; t). \tag{20}\end{align*}\]

Of course there is still much detail hidden in the permittivity \(\tilde{e}\), since it contains the nonlinearity. Consequently, I do not apply this envelope definition to a general equation of motion because how \(\tilde{e}\) is expressed usually depends on the field and therefore on those envelopes. Starting with eqn.\[14\], and expanding \(e\) with terms for both (linear) dispersion \(e_{r}\) and a time dependent \(\chi^{(3)}\) nonlinearity \(\epsilon_{c}\) gives

\[\begin{align*}
\epsilon(\tau, t) \ast A(t)e^{+\Xi} & + c.c. \\
& = e_{r}(\tau) \ast \{ A(t)e^{+\Xi} + A^{*}(t)e^{-\Xi} \} \\
& + \{ e_{c}(\tau) \ast \{ A(t)^{2}e^{+2\Xi} \\
& + A(t)A^{*}(t)e^{-2\Xi} \} \} \\
& \times \{ A(t)e^{+\Xi} + A^{*}(t)e^{-\Xi} \} \tag{21}\end{align*}\]

\[\begin{align*}
\epsilon(\tau, t) \ast A(t)e^{+\Xi} & = e_{r}(\tau) \ast A(t)e^{+\Xi} \\
& + 2 \{ e_{c}(\tau) \ast |A(t)|^{2} \} A(t)e^{+\Xi} \\
& + \{ e_{c}(\tau) \ast A(t)^{2} \} A(t)e^{+\Xi} \\
& + \{ e_{c}(\tau) \ast A^{*}(t)^{2} \} A(t)e^{+\Xi} \tag{22}\end{align*}\]

\[\begin{align*}
\tilde{e}(\omega + \omega_{0})\tilde{A}(\omega) & = \tilde{e}_{r}(\omega' + \omega_{0}) \ast \tilde{A}(\omega) \\
& + 2 \{ \tilde{e}_{c}(\omega' + \omega_{0}) \mathcal{F}[|A(t)|^{2}] \ast \tilde{A}(\omega) \} \\
& \times \tilde{A}(\omega) \\
& + \{ \tilde{e}_{c}(\omega' + 3\omega_{0}) \mathcal{F}[|A(t)|^{2}] \ast \tilde{A}(\omega) \} \ast \tilde{A}(\omega). \tag{23}\end{align*}\]

We can see in eqn.\[23\] that the first three of the terms (one dispersion and two SPM-like) are resonant with the chosen envelope, but the last (third harmonic generation) is not, and it modulates the envelope at \(2\omega_{0}\), (and subsequently the propagation by \(\sim 2k_{0}\)). Note the form of the second SPM-like term, which needs contributions from two \(A(t)^{2}\)‘s and one \(A(t)^{*}\) have to have the correct frequency dependence, but the convolution is with the \(A(t)^{*}\) and not an \(A(t)\) as might be expected.
Note that in the case of instantaneous $\chi^{(3)}$, the third RHS term reduces to $\epsilon_\epsilon |A(t)|^2 A(t)$, giving

$$\epsilon(\tau) * A(t)e^{+\Xi} = \epsilon_\epsilon(\tau) * A(t)e^{+\Xi} + 3\epsilon_\epsilon |A(t)|^2 A(t)e^{+\Xi}$$

$$+ \epsilon_\epsilon A(t)^3 e^{+3\Xi}, \quad (24)$$

$$\tilde{\epsilon}(\omega + \omega_0) * \tilde{A}(\omega) = \tilde{\epsilon}_\epsilon(\omega + \omega_0)\tilde{A}(\omega)$$

$$+ 3\epsilon_\epsilon \mathcal{F} \left[ |A(t)|^2 A(t) \right] (\omega)$$

$$+ \epsilon_\epsilon \mathcal{F} \left[ A(t)^3 \right] (\omega). \quad (25)$$

This expression can then be substituted directly into eqns. \textcolor{red}{19-20}

In this formulation, we have made no “slowly varying” approximation like those in traditional approaches \textcolor{red}{1-2, 3, 11-16}, or in the variously corrected extensions \textcolor{red}{17-19}. The price we pay is having two envelopes instead of one, since now the magnetic field is explicitly retained. Also, the model still contains backward propagating components; which, with the chosen carrier functions, will impress oscillations at $2\omega_0$ on the envelope, and oscillations of $2k_0$ on the propagation, placing greater demands on our numerics. Unfortunately there is no way to filter these out at any point in the simulation, because their backward propagating nature can only be established by linking the time-like behaviour and space-like propagation of both $E$ and $H$ fields. We cannot always rely on only time-like behaviour to filter them out, because, e.g., both backward propagating terms (at $+k_0$ and $-\omega_0$) and third harmonic generation (at $+3k_0$ and $2\omega_0$) are equally detuned from the carrier (at $+k_0$ and $\omega_0$); although we could do so if we were in a regime where third harmonic generation were negligible.

At the start of this subsection, we hoped that dividing out the carrier oscillations would give us a slowly varying pulse envelope, which would then enable us to coarsen our numerical resolution, and speed simulations. This is true, up to a point – but remember the most likely reason we are using a Maxwell solver is that we want to model a wideband situation. It is the rapidity of the fastest time-domain modulation of the field or envelope which constrains our time resolution, and the rapidity of the fastest spatial modulation which constrains the spatial resolution.

We can do better than these Maxwell equations approaches without having to use second order wave equations and their complicated approximations by using directional Maxwell’s equations, as described in the next section.

### B. Transverse effects

There are two main transverse effect likely to be of interest in pulse propagation models: mode averaging, and diffraction or off-axis propagation.

Mode averaging is easy to incorporate if you assume some known transverse profile for the mode: e.g. for an optical fibre or some other waveguide. The transverse derivatives vanish, and the material properties are evaluated as an integral over the transverse dimensions, weighted by the mode function.

Diffraction and off-axis propagation they result from a coupling between the vector components of the $E$ and $H$ fields – including those along the propagation direction. Thus they are much harder to understand, as compared to a paraxial model based on (e.g.) the second order wave equation, although they can be simulated easily enough in a full 4D FDTD code. This is because they result from a coupling between the vector components of the $E$ and $H$ fields – including those along the propagation direction.

### IV. DIRECTIONAL MAXWELL’S EQUATIONS

To my knowledge, the earliest rewriting of Maxwell’s equations in a directional form was by Fleck \textcolor{red}{10}, who treated a dispersionless medium and plane polarized wave. However, the idea was not used beyond its brief appearance there. Fleck constructed his directional fields by combining the sum and difference of the $E$ and $H$ fields, weighted by the square roots of the permittivity $\epsilon$ and permeability $\mu$ respectively. The new combined fields represent the forward and backward traveling components of the total field, and we can derive first-order wave equations for these new fields.

In the mid 1990’s, the concept was rediscovered and used to evaluate the properties of grating structures by de Sterke, Sipe, and co-workers \textcolor{red}{34, 35}, but not applied to pulse propagation. The work considered materials with a spatially varying refractive index, but did not incorporate material dispersion or nonlinearity.

This concept of using directional fields for pulse propagation was not revisited until the work of Kolesik et al. \textcolor{red}{11-12}. After selecting a preferred direction, they then projected out the forward-like and backward-like parts of the propagating fields. This procedure resulted in first order wave equations for the propagation of the forward and backward field components. Subsequent work by Kinsler et al. \textcolor{red}{13-14}, presented a directional rewriting of Maxwell’s equations using a generalized form of Fleck’s construction. It is also worth noting the independent work of Mizuta et al. \textcolor{red}{15}, published at the same time. All of these methods use the same basic concept – use the right combination of $E$ and $H$ fields so as to create a pair of forward and backward-like fields.

Here I follow the formulation of Kinsler et al. \textcolor{red}{13-14}, which handles the electric and magnetic properties of the propagation medium on an equal footing, incorporates the dispersive properties of the medium in a very general way, and retains all the vectorial behaviour of the fields. The result is paired first-order equations for the plane-polarized directional fields $G^\pm$ (and a longitudinal component $G^z$). Although complicated in the general case, these simplify greatly in the usual case(s) of transverse...
and/or paraxial propagation regimes. The cost of using these directional fields is that while we can efficiently remove backward propagating contributions, computing the nonlinear terms is more demanding. In contrast, the work of Kolesik et al. and Mizuta et al. is distinguished by a greater emphasis on the practical applications of directional fields.

Because these new $G^\pm$ fields are directional, we can efficiently separate out the forward-going part of the field, and neglect the backward. This is an important step, because the standard Maxwell equations based approaches treated in the previous section could not easily remove the backward parts of the field, and these can cause inconvenience in numerical simulations. For example, the spurious backward component caused by imperfect initial conditions should no longer occur.

The definitions of the $G^\pm$ fields, describing the transverse properties of a plane polarized EM field, in the frequency domain are

$$
\dot{G}^\pm_x(\omega) = \bar{\alpha}_r(\omega)\dot{E}_x(\omega) \pm \bar{\beta}_r(\omega)\dot{H}_y(\omega),
$$

(26)

The $\bar{\alpha}_r$ and $\bar{\beta}_r$ “reference” parameters are best chosen to closely match the medium, whilst ignoring nonlinear effects, so that $\bar{\alpha}_r(\omega)\bar{\beta}_r(\omega) = 1/c(\omega)$. That is, relevant (linear) dispersive properties of the medium are included in the reference parameters, i.e. that $\bar{\alpha}_r(\omega) = \epsilon_r(\omega)^{1/2}$. They have the definitions

$$
\begin{align*}
\bar{\epsilon} &= \epsilon_r(\omega) + \bar{\epsilon}_c(\omega) = \bar{\alpha}_c^2(\omega) + \bar{\alpha}_r(\omega)\bar{\alpha}_c(\omega), \\
\bar{\mu} &= \bar{\mu}_c(\omega) + \bar{\mu}_r(\omega) = \bar{\beta}_c^2(\omega) + \bar{\beta}_r(\omega)\bar{\beta}_c(\omega),
\end{align*}
$$

(27)

(28)

where the correction parameters $\bar{\epsilon}_c$ and $\bar{\mu}_c$ represent the discrepancy between the true values and the reference. These correction terms will usually just be the nonlinearity. More generally, the smaller these correction terms are, the better the match, and the more likely it is that a description involving only $G^+$ will suffice. Note also that there are alternative ways of constructing directional $G^\pm$-like fields.

In the widely used moving frame defined by $v = 1/\alpha_f/\beta_f$, where $\partial_z Q = \partial_z Q - \alpha_f/\beta_f\partial_t Q$, using these $G^\pm$ fields gives the (non-magnetic case) propagation equation

$$
-\partial_z \dot{G}^\pm_x = \pm i\omega\bar{\alpha}_r\dot{\bar{\beta}}_r(1 \mp \xi) G^\pm + \frac{\omega_0\bar{\alpha}_r\dot{\bar{\beta}}_r}{2} * \left[G^+_x + \dot{G}^-_x\right],
$$

(29)

where $\xi = \alpha_f/\beta_f/\bar{\alpha}_r\bar{\beta}_r$. Although this moving frame has no sensible limit as the frame speed tends to zero, the stationary frame case can be recovered by setting $\xi = 0$ and replacing $\dot{z}'$ by $z$. $G^\pm$ field simulations usually assume $G^-_z = 0$, and treat only the forward traveling components of the EM field.

Correctly writing down the form of nonlinear terms for eqn. (29) requires some care, and consideration of the specific nonlinearity involved. Fortunately the task is simplified because it is simply a rewriting of the (electric) nonlinear term from Maxwell’s equations with the appropriate scaling factors relating $\alpha_c$ to $\epsilon$, and $G^\pm_x$ to $E$.

Wave equations with a more familiar appearance can be obtained using

$$
\dot{E}^\pm(\omega) = \tilde{G}^\pm_x(\omega)/2\bar{\alpha}_r(\omega).
$$

(30)

These have the units of an electric field (i.e. V/m), but actually incorporate information about the magnetic field as well. If we take this step, we can transform back into forward propagating “electric fields” $E^\pm$, and get

$$
-\partial_z \dot{E}^\pm = \mp i\omega\bar{\alpha}_r\bar{\beta}_r(1 \mp \xi) \dot{E}^\pm + \frac{\omega_0\bar{\alpha}_r\bar{\beta}_r}{2} * \left[E^+_x + \dot{E}^-_x\right].
$$

(31)

An approximate forward-only wave equation can be found by setting $E^- = 0$ in eqn. (31) (or $G^- = 0$ in eqn. (29)). For a time response $\chi^{(3)}$ nonlinearity, this is

$$
-\partial_z \dot{E}^+(\omega) = -i\omega\bar{\alpha}_r\bar{\beta}_r(1 - \xi) \dot{E}^+(\omega) + i\omega\{\bar{\beta}_r\bar{\epsilon}_c(\omega)\cdot \mathcal{F}\left[E^+_x(t)^2\right](\omega)\} * \dot{E}^+(\omega)
$$

(32)

Notice the similarity to eqn. (11), but that the field is propagated in a single first order equation, rather than two (i.e. both eqn. (11) and (12)). The cost is that it only propagates forwards, but this is what we wanted. Further, the method can be implemented using fewer Fourier transforms than are required for a full Maxwell equation solver. The gain is that of not solving for $\partial_t E$ (eqn. (12)), which requires a pair of FFT’s if done pseudospectrally. Solving for pulse propagating in a medium with dispersion and a time dependent (or instantaneous) third order nonlinearity therefore requires only six (or three) FFT’s, as compared to eight (or five) for solving Maxwell’s equations.

However, in practice the speed gain can be less clear cut. A PSSD solver moves forward one full step $dz$ in two staggered steps, one integrating for the magnetic field, and integrating for the electric field; and only the magnetic field integration needs to calculate the nonlinearity. This staggered scheme is second order accurate even though each stagger-step is only integrated using an Euler method. We can achieve nearly the same level of accuracy for the directional fields by employing a leapfrog algorithm. If we wish to use more accurate (and so more complicated) numerical integration algorithms (e.g. a Runga-Kutta scheme), then we can only outperform the staggered (or leapfrog) PSSD schemes if the propagation step size is (greater than) twice that of the staggered PSSD. To complicate matters further, for reasons of numerical stability, we often need to tie the propagation step $dz$ to the time grid step $dt$. This means that if there are bandwidth constraints limiting our $dt$, we may not have as much much freedom to adjust $dz$ as we might like.
1. Special case: $\chi^{(2)}$

In the case of a $\chi^{(2)}$ nonlinearity, two different field polarizations are coupled together, and the equations given above tend to obscure the final form the nonlinear term will take. In this case, the time-domain displacement fields $D$ in the two polarizations are

\[
D_y = \epsilon_y \times E_y + 2\epsilon_0 \chi^{(2)} E_x E_y = \epsilon_y \times E_y + N_y^{(2)}.
\]

If we assume that all of the linear response of the material (denoted above by $\epsilon_x, \epsilon_y$) is absorbed into the reference parameters $\tilde{\alpha}_r, \tilde{\beta}_r$, we need only consider the nonlinear part. Note in particular that for the $D_y$ field (i.e. $N_y^{(2)}$) this does not depend on $E_y$, meaning that the forms of the wave equations given above (aimed largely at a $\chi^{(3)}$ system) are not very useful.

First, note that for a $\chi^{(3)}$ nonlinearity

\[
N^{(3)} = \epsilon_0 \chi^{(3)} E^3,
\]

\[
\tilde{N}^{(3)} = \mathcal{F} \left[ \epsilon_0 \chi^{(3)} E^2 \right] \times E
\]

and these give a nonlinear term for the wave equations of

\[
\frac{\omega \tilde{\alpha}_r \tilde{\beta}_r}{2} \times \left[ \tilde{G}_x^+ + \tilde{G}_x^- \right] = \omega \tilde{\beta}_r \tilde{\alpha}_r \tilde{\alpha}_c \times \tilde{E},
\]

By comparing these $\chi^{(3)}$ terms, we can see that in the $\chi^{(2)}$ case, the nonlinear terms in the $\tilde{G}_x^\pm$ and $\tilde{G}_y^\pm$ wave equations (see eqn. [24]) will be rewritten as follows

\[ x : \quad \frac{\omega \tilde{\alpha}_c \tilde{\beta}_r}{2} \times \left[ \tilde{G}_x^+ + \tilde{G}_x^- \right] \Rightarrow \omega \tilde{\beta}_r \mathcal{F} \left[ 2\epsilon_0 \chi^{(2)} E_x E_y \right] \]

\[ y : \quad \frac{\omega \tilde{\alpha}_c \tilde{\beta}_r}{2} \times \left[ \tilde{G}_y^+ + \tilde{G}_y^- \right] \Rightarrow \omega \tilde{\beta}_r \mathcal{F} \left[ \epsilon_0 \chi^{(2)} E_x^2 \right]. \]

These can then be put in a form containing only $\tilde{G}_x^\pm$, $\tilde{G}_y^\pm$ if desired, but it is simplest to reconstruct the $E_x, E_y$ directly before calculating the nonlinear terms. If a more extensive collection of the $\chi^{(2)}$ coefficients needs to be included, this procedure can be reproduced using the appropriate nonlinear field combinations. Further, if the time-response of the nonlinearity is also important, then we can include this by replacing $\chi^{(2)} E_x E_y$ and $\chi^{(2)} E_x^2$ with appropriate convolutions: e.g. $(\chi^{(2)} \ast E_y) E_x$ and $(\chi^{(2)} \ast E_x) E_x$.

For the $\tilde{E}\pm$-like wave eqns. [31] the nonlinear terms are

\[ x : \quad \frac{\omega \tilde{\alpha}_c \tilde{\beta}_r}{2} \times \left[ \tilde{E}_x^+ + \tilde{E}_x^- \right] \Rightarrow \omega \tilde{\beta}_r \mathcal{F} \left[ 2\epsilon_0 \chi^{(2)} E_x E_y \right] \]

\[ y : \quad \frac{\omega \tilde{\alpha}_c \tilde{\beta}_r}{2} \times \left[ \tilde{E}_y^+ + \tilde{E}_y^- \right] \Rightarrow \omega \tilde{\beta}_r \mathcal{F} \left[ \epsilon_0 \chi^{(2)} E_x^2 \right]. \]

Since we will want to apply the nonlinear effects in the time domain, we need to back-transform the terms in eqns. [31] or eqns. [32], requiring a pair of Fourier transforms in addition to those required to get the time-domain fields. If using the $\tilde{G}\pm$ form, there is an additional transform, because we also need the time domain field(s) $E(t)$ with the $\tilde{E}\pm$ form $E(t)$ can be found directly.

Further simplifications can be made: e.g. in a semi-wideband limit around a central frequency $\omega_0$, we can assume the frequency dependence of the $\tilde{\alpha}$ parameters in the nonlinear terms vanishes, so that the transform(s) to convert from $\tilde{G}\pm$ to $E$ is unnecessary. In an SVEA-like narrowband limit all these transforms vanish because (in the nonlinear terms) the frequency dependence of the $\tilde{\alpha}$ parameters vanish and the the factor of $\omega$ simple becomes $\omega_0$.

A. Envelopes

Here I have intentionally simplified the definitions to best match what is most likely to be used in practice: a forward propagating $G^+$ (or $E^+$) only model. A more complete description of $G^\pm$ envelopes, such as that in [12], would include the role of forward and backward traveling envelopes for both of $G^\pm$.

We have seen that in the forward-only approximation, $G^+$ and $E^+$ follow identical equations of motion. The envelope and carrier representation of $E^+$ is

\[ E^+(t; z) = C(t; z) e^{i(k_0 z - \omega_0 t)} + C^*(t; z) e^{-i(k_0 z - \omega_0 t)} \]

I do not apply this envelope definition to the general equation of motion because how $\tilde{\alpha}_c$ is expressed depends on the field and therefore on those envelopes.

We now, for the case of a time response $\chi^{(3)}$ nonlinearity, substitute eqn. [43] into eqn. [42], we then (as usual) split the normal and c.c. parts, cancel exponentials, and rearrange leaving only the $\partial_z$ terms on the left,

\[ -\partial_z \tilde{C}(\omega) = -\omega (1 - \xi) \tilde{\beta}_r \tilde{\alpha}_c \tilde{C}(\omega) + i k_0 \tilde{C}(\omega) \]

\[ -\omega \tilde{\beta}_r \hat{\epsilon}_c (\omega + \omega_0) \mathcal{F} \left[ \frac{1}{2} |C(t)|^2 \right] (\omega) \tilde{C}(\omega) \]

\[ -\omega \tilde{\beta}_r \hat{\epsilon}_c (\omega + \omega_0) \mathcal{F} \left[ |C(t)|^2 \right] (\omega) \tilde{C}(\omega) \]

\[ -\omega \tilde{\beta}_r \hat{\epsilon}_c (\omega + 3\omega_0) \mathcal{F} \left[ |C(t)|^2 \right] (\omega) \tilde{C}(\omega) \]

The first line on the RHS will mostly cancel in the narrowband case, since $\tilde{\beta}_r \tilde{\alpha}_c = 1/c(\omega)$, and $k_0 = \omega_0/c(\omega_0)$, thus with $\delta = \omega - \omega_0$ it becomes

\[ -i \left[ \frac{\omega}{c(\omega)} - k_0 \right] = -i \left[ k(\omega) - k_0 \right] \]

\[ = -i \left[ \frac{\partial k}{\partial \omega} \right] \left[ \delta + \frac{1}{2} \frac{\partial^2 k}{\partial \omega^2} \right] \delta^2 + ... \]
where in the truncated expansion on the second line we can see the expected group velocity and group velocity dispersion terms.

Note that eqn. (44) is directly comparable to one derived from the NEE of Brabec and Krausz [17], but the only approximation I have made is to discard backward propagating fields. Since the NEE makes several additional approximations, eqn. (44) is more accurate and less approximate. Indeed, Brabec and Krausz were fortunate in that their chosen approximations produced a result remarkably similar to that from the less restricted directional fields approach. Note that Kolesik and Moloney [12] also reduced their directional wave equation to a number of special cases, including that of Brabec and Krausz.

B. Transverse effects

As for Maxwell’s equations, there are two main transverse effect likely to be of interest in pulse propagation models: mode averaging, and diffraction or off-axis propagation.

Mode averaging is easy to incorporate if you assume some known transverse profile for the mode: e.g. for an optical fibre or some other waveguide. The transverse derivatives vanish, and the material properties are evaluated as an integral over the transverse dimensions, weighted by the mode function. This is just the same as for Maxwell’s equations, although we now may be averaging slightly different quantities (e.g. $\alpha_r$ rather than $\epsilon$).

The work of Kolesik et al. [11, 12] allows for transverse mode structure, that of Mizuta et al. [15] for transverse averaging over a single mode.

Diffraction and off-axis propagation are again much harder to understand, because (again) they result from a coupling between the vector components of the $E$ and $H$ fields – including those along the propagation direction. However, second order wave equations derived from the first order directional fields equations exhibit a $\nabla_\perp^2$ diffraction term which is the same as that seen in standard second order wave equations (see e.g. eqn. (47), in section V). This means that weakly transverse effects can be accurately incorporated by using a split step scheme alternating between the wave equation and a $\nabla_\perp^2$ diffraction term. Note that Kolesik et al. [12] had wave equations incorporating diffraction (transverse) terms.

V. SECOND ORDER WAVE EQUATIONS

The standard second order wave equation applies to propagation in non-magnetic materials. If we consider the case of small transverse inhomogeneities of the polarization, the three dimensional wave equation in typical notation (e.g. from [17, 19]) is

$$\left(\partial_\tau^2 + \nabla_\perp^2 \right) E(\vec{r}, t) - \frac{1}{c^2} \partial_\tau^2 \left\{ \epsilon_L(\tau) \star E(\vec{r}, t) \right\} = \frac{4\pi}{c^2} \partial_\tau^2 P_{nl}(\vec{r}, t).$$

Here $\nabla_\perp^2$ is the transverse Laplace operator, $\epsilon_L(t) = (2\pi)^{-1} \int_{-\infty}^{\infty} d\omega \epsilon_L(\omega) e^{i\omega t}$, $\epsilon_L(\omega) = 1 + 4\pi \chi(\omega)$, and $\chi(\omega)$ is the linear electric susceptibility. The electric field $E$ propagates along the $z$ direction. Both $E$ and the nonlinear polarization $P_{nl}$ are polarized parallel to the $x$ axis.

Because of their starting point, methods based on this second order equation are slightly more restricted than those starting from Maxwell’s equations. However, the differences in practice will likely be small, especially in the usual case of non-magnetic propagation media.

Most uses of eqn. (46), notably the slowly varying envelope approximation (SVEA) relies on using an envelope-carrier description for the fields, then expands for weak dispersion, and resonant nonlinear perturbations about this carrier. This approach is discussed below in subsection VA

Alternatively, we can attempt to factorise the equation into a product of two first order parts, as can be done for linear waves (see e.g. [37]). Factorization is considerably more useful than the traditional approach, and is discussed below in subsection VD.

A. Traditional approach

Unlike the other approaches discussed in this paper, the traditional approach assumes the use of an envelope-carrier description of the field.

Kinsler and New [14, 24] presented a comprehensive re-derivation of the envelope propagation equation based on the second order wave equation, which subsumes the SVEA and Brabec and Krausz’s NEE [17] as special cases. Since it is the most general, I use the Kinsler and New calculation, leaving some definitions to their paper rather than repeat them here. Noting that $\xi$ and $\tau$ are scaled space and time variables, that $alpha$ and $beta$ have different meanings from the rest of this paper, and that $D^\prime$ contains the dispersion terms, we have

$$\partial_\xi A(\vec{r}_\perp, \xi, \tau) = \left( -\frac{\alpha_0}{\beta_0} + i \hat{D}^\prime \right) A(\vec{r}_\perp, \xi, \tau) + \frac{i/2}{\beta_0} \nabla_\perp^2 A(\vec{r}_\perp, \xi, \tau) + \frac{2 \pi}{\beta_0} \frac{(1 + i \partial_\tau)^2}{1 + i \sigma \partial_\tau} B(\vec{r}_\perp, \xi, \tau; A) + \frac{T_R}{1 + i \sigma \partial_\tau}, \quad (47)$$

where

$$T_R = \left[ -\frac{\eta^2}{2} \partial_\tau^2 + \frac{1}{2} \left( \frac{\alpha_0}{\beta_0} - i \hat{D}^\prime \right)^2 \right] A(\vec{r}_\perp, \xi, \tau). \quad (48)$$

Eqn. (47) is exact – it contains no more approximations than the starting point eqn. (46) except for the expansion of $\epsilon$ in powers of $\omega$. If we set $T_R = 0$, this gives us a generalized few cycle envelope (GFEA) equation, which contains the SVEA [2]. Brabec and Krausz’s NEE can be recovered from eqn. (47) in the 1D case where phase
and group velocities are the same (i.e. $\sigma = 1$), likewise Porras’s SVEA $[18]$ can be identified in the diffraction term. Of course we cannot just set the $T_R$ term to zero without some justification, but this has already been extensively discussed, not only in both $[10]$, but also the detailed analysis $[24]$.

Now consider the complicated few-cycle correction to the polarization term in eqn. (47), which contains partial derivatives $(1 + \sigma \partial_\tau)$ in the denominators. These will need to be evaluated by Fourier transforming into the conjugate frequency space ($\Omega$). Further, the $T_R$ term is divided by another such term. Clearly these might, in wideband cases, result in denominators close to zero, causing the approximations to fail. This means they put a serious brake on the validity of any such approach, especially if the bandwidth of the pulse approaches the carrier frequency.

Note that the best first order expansion of the few-cycle corrections to the polarization term is more general than that given by Brabec and Krausz, and contains the group to phase velocity ratio $\sigma$, i.e.

$$2\pi \frac{(1 + \sigma \partial_\tau)^2}{n_0^2 (1 + \sigma \partial_x)} B(\xi, \tau; A) \approx \frac{2\pi}{n_0^2} (1 + \sigma \partial_\tau) B(\xi, \tau; A) \tag{49}$$

Unfortunately for the venerable SVEA based on the second order wave equation, and even its most general variant presented here, the directional fields method discussed in the previous section has made it utterly redundant; as, indeed, has the approach in the following subsection $[41]$. There is no reason to use any form of the GFEA or SVEA when we can generate equations like eqns. (31)–(32) by not only using fewer approximations, but much simpler ones than those taken by neglecting $T_R$.

### B. Time propagated direct solution

It is of course possible to solve the second order wave equation by propagating it in time, either with or without the use of an envelope and carrier. This approach has been used with significant success by Scalora and co-workers (e.g. their early work $[33, 32, 40]$). By propagating in time reflections are handled correctly, an important feature when treating structured materials. Generally the solution is achieved retaining the second order spatial derivatives (both in $z$ and transversely in $x, y$), but approximating the time derivatives to first-order. The approximation is made using an envelope with a well-chosen carrier frequency, and gives rise to the SVEAT, or slowly varying envelope approximation in time.

### C. Short pulse equation (SPE)

The second order wave equation can be converted into the SPE by using a multiscale expansion $[41]$. First, specialize to a third-order nonlinearity (strength $\rho$) and only second order (ordinary) dispersion (strength $d$) and then rewrite the second order wave equation as

$$\partial^2_z E(t; z) - \frac{1}{c_1^2} \partial^2_t E(t; z) - d \partial_z E(t; z) - \rho \partial^2_z E(t; z)^3 = 0 \tag{50}$$

We introduce the scaled co-moving frame variables $\tau = (t - z/\epsilon)/\sigma$ so that $\partial_\tau = (1/\epsilon) \partial_t$, and $z_n = \sigma^n z$ so that $\partial_z = - (1/c_1 \sigma) \sigma^n \partial_{z_n}$; hence after simplification eqn. (50) becomes

$$- \frac{2}{c_1} \partial_{\tau} \partial_{z_n} E(t; z) - d_2 E(t; z) - \frac{p}{\sigma^2} \partial^2_z E(t; z)^3 = 0 \tag{51}$$

Now, writing the field in multiscaled form as a power series in components $E_i$, scaled by factors of $\sigma$, we have

$$E(t; z) = \sigma E_0(\tau, z_1, z_2, ...) + \sigma^2 E_1(\tau, z_1, z_2, ...) + \cdots \tag{52}$$

and to leading order, we can write eqn. (51) down as the SPE

$$- \frac{2}{c_1} \partial_{\tau} \partial_{z_n} E_0 - d_2 E_0 - p \partial^2 E_0^2 = 0 \tag{53}$$

This equation has spawned a literature all of its own, because it (like the ordinary nonlinear Schrödinger equation) provides a rich variety of mathematical solutions.

### D. Factorization approach

An alternative to the traditional style of derivation discussed above, we can instead factorise the second order wave equation in a way similar to that done for linear waves (see e.g. $[37]$). This was initially suggested by Shen $[2]$, followed by Blow and Wood $[20]$, and more recently revisited by Ferrando et al. $[21]$ and Genty et al. $[22]$.

First we reduce eqn. (46) to the 1D strictly paraxial limit; then transform into frequency space. Here I re-use the symbol $\beta$ as the propagation wave vector to match the notation of Genty et al. $[22]$, so that $\beta(\omega) = \omega \sqrt{\epsilon_r(\omega)} \mu_0$. The wave equation therefore is

$$\partial^2_t E(t; z) - \frac{1}{c^2_2} \partial^2_z E(t; z) - \mu_0 \partial^2_z P(t; z) = 0 \tag{54}$$

$$\nabla^2 \tilde{E}(\omega; z) + \beta(\omega)^2 \tilde{E}(\omega; z) + \mu_0 \omega^2 \tilde{P}(\omega; z) = 0 \tag{55}$$

$$\partial^2_t \tilde{E}(\omega; z) + \beta^2(\omega) \tilde{E}(\omega; z) + \beta^2(\omega) N \ast \tilde{E}(\omega; z) = 0 \tag{56}$$

where for a third order nonlinearity, with $\epsilon_c = \epsilon_0 \chi^{(3)}$,

$$N = \mu_0 \epsilon_0 \chi^{(3)} \omega^2 E(r, t; z)^2 / \beta(\omega)^2 \tag{57}$$

$$N = \mu_0 \epsilon_0 \omega^2 E(r, t; z)^2 / \beta(\omega)^2 \tag{58}$$

$$= \frac{\chi^{(3)}(r, t; z)^2}{n(\omega)} \tag{59}$$

I now briefly consider three factorization approaches, from the simple method of Blow and Wood $[20]$, an improved version, and finally the most rigorous approach. Although these traditionally involve an envelope-carrier decomposition introduced early in that calculation (see Blow and Wood), the step is in fact unnecessary and I omit it.
1. Simple factorization

Factorization approaches are simple in two situations: a dispersionless medium with an instantaneous nonlinearity, and a dispersive medium with no nonlinearity. In the dispersionless nonlinearity case, we can factorise in the time domain. In the linear dispersive case, we can factorise in the frequency domain. In the dispersive nonlinear case, it is (usually) not possible to analytically factorise the second order wave equation.

Regardless of mathematical difficulties, Blow and Wood [20] used a simple factorization procedure which ignored the details of nonlinearity and dispersion. Remembering that \( \beta = \beta(\omega) \), and without their envelope-carrier decomposition, they had

\[
\left[ \partial_z + i \beta \sqrt{1 + \tilde{N} E(\omega)} \right] \left[ \partial_z - i \beta \sqrt{1 + \tilde{N} E(\omega)} \right] \tilde{E} = 0. \tag{60}
\]

They then separated out the forward propagating term. The envelope equivalent of this was then expanded using a “weak nonlinearity” assumption with a binomial expansion, keeping only the first order corrections.

2. Improved factorization

The approach of Blow and Wood ignores the mathematical difficulties due to the use of the square root in combination with the frequency-domain convolutions between the nonlinear term \( N \) and the field spectrum \( \tilde{E} \).

Fortunately, we can instead “complete the square” (e.g. \( 1 + N \simeq 1 + N + N^2/4 = (1 + N/2)^2 \)), enabling us to preserve the convolutions correctly. This requires us to make a weak nonlinearity approximation, but it is one nearly identical to that used when expanding the square root in the Blow and Wood calculation. So, with a the weak nonlinearity constraint

\[
\frac{1}{2} \tilde{N} \ast \tilde{E} \ll 1, \tag{61}
\]

we get

\[
\left[ \partial_z + i \beta \left( 1 + \tilde{N} E(\omega) \right) \right] \left[ \partial_z - i \beta \left( 1 + \tilde{N} E(\omega) \right) \right] \tilde{E} = 0. \tag{62}
\]

By assuming the forward-like and backward-like terms in square brackets factorise,

\[
\left[ \partial_z \pm i \beta \left( 1 + \tilde{N} E(\omega) \right) \right] \tilde{E} = 0. \tag{63}
\]

\[
\partial_z \tilde{E} = \pm i \beta \tilde{E} \pm \tilde{N} E(\omega), \tag{64}
\]

While this equation can give excellent results, it is restricted to weak nonlinearity: as we see below, it lacks the nonlinear coupling term between the forward and backward propagating fields.

3. Linear factorization

Ferrando et al. [21] treat this approach in detail, separating this second order equation into two first order equations using a Greens function approach. More recently, Genty et al. [22] have used it to generate a nonlinear envelope equation, and specialised it to the case of nonlinear waveguides. First we move the nonlinear term from eqn. (56) to the RHS and Fourier transform \( z \) into \( k \)-space, so that the \( \partial_z \) becomes \(-ik\),

\[
[-k^2 + \beta^2] \tilde{E} = -\beta^2 \tilde{N} \ast \tilde{E} \tag{65}
\]

\[
\tilde{E} = \frac{\beta^2}{k^2 - \beta^2} \tilde{N} \ast \tilde{E} \tag{66}
\]

\[
= \frac{\beta^2}{(k + \beta)(k - \beta)} \tilde{N} \ast \tilde{E} \tag{67}
\]

\[
\tilde{E}_+ + \tilde{E}_- = -\frac{\beta^2}{2}\left[ \frac{1}{k + \beta} - \frac{1}{k - \beta} \right] \tilde{N} \ast \left[ \tilde{E}_+ + \tilde{E}_- \right] \tag{68}
\]

where I’ve taken \( E \) to be a sum of both forward and backward propagating parts \( \tilde{E} = \tilde{E}_+ + \tilde{E}_- \). I now split eqn. (68) into a sum of two parts, where each half represents the propagation of the forward field \( \tilde{E}_+ \) or the backward field \( \tilde{E}_- \), and rearrange,

\[
\tilde{E}_\pm = \pm \frac{\beta/2}{k \mp \beta} \tilde{N} \ast \left[ \tilde{E}_+ + \tilde{E}_- \right] \tag{69}
\]

\[
[k \mp \beta] \tilde{E}_\pm = \pm \frac{\beta}{2} \tilde{N} \ast [ \tilde{E}_+ + \tilde{E}_- ]. \tag{70}
\]

Now I transform back from \( k \)-space into \( z \), so that

\[
[-i \partial_z + \beta] \tilde{E}_\pm = \pm \frac{\beta}{2} \tilde{N} \ast [ \tilde{E}_+ + \tilde{E}_- ] \tag{71}
\]

\[
\partial_z \tilde{E}_\pm = \pm i \beta \tilde{E}_\pm \pm \frac{i \beta}{2} \tilde{N} \ast [ \tilde{E}_+ + \tilde{E}_- ]. \tag{72}
\]

If we compare this result (i.e. eqn. (72)) with the comparable equations for the directional fields \( G \), in particular with the electric field form given in eqn. (83); we see that they are essentially identical: since \( \omega_0 \beta_r = \omega/c_r \leftrightarrow \beta \).

A similar procedure can be applied to eqn. (62) if desired. Eqn. (72) is almost the same as the (more approximate) eqn. (63). Since the RHS nonlinear term is a function of \( (E_+ + E_-) \), it provides a route for coupling between the forward and backward waves; its form can be obtained from the nonlinear part of (e.g.) eqn (11). A specific example for the case of a time-response \( \chi^{(3)} \) nonlinearity has been given in [22], but in my notation it is identical to that for the rescaled directional \( G \) fields (i.e. \( E \)), i.e. eqn. (82).

4. Special case: \( \chi^{(2)} \)

In the case of a \( \chi^{(2)} \) nonlinearity, two different field polarizations are coupled together, and the equations
given above tend to obscure the final form of the nonlinear term will take. First, note that the factorisation process changes the nonlinear term from \( \beta^2 \omega^2 \tilde{N} \ast \tilde{E} \) into \( \tilde{N} \ast \tilde{E}^2 \). This means that the term itself is multiplied by a factor of just \( \sqrt{2} \beta \), and this transforming factor is what we need to use in the general case.

For a \( \chi^{(2)} \) nonlinearity, the time-domain displacement fields \( D \) in the two polarizations are

\[
D_x = \epsilon_x \ast E_x + 2\epsilon_0 \chi^{(2)} E_x E_y, \quad (73)
\]

\[
D_y = \epsilon_y \ast E_y + \epsilon_0 \chi^{(2)} E_x^2. \quad (74)
\]

Note in particular that the nonlinear part of the \( D_y \) field does not depend on \( E_y \), making the wave eqn. (74) (aimed largely at a \( \chi^{(3)} \) system) inappropriate.

In any case, the \( x \) nonlinear term is just \( 2\epsilon_0 \chi^{(2)} E_x E_y \), and the \( y \) term \( \epsilon_0 \chi^{(2)} E_x^2 \) so that in the pair of frequency domain wave equations (cf eqn. (85)), the nonlinear terms are

\[
x : \quad \beta^2 \omega^2 \tilde{N} \ast \tilde{E} \Leftrightarrow 2\mu_0 \epsilon_0 \omega^2 \mathcal{F} \left[ \chi^{(2)} E_x E_y \right] \quad (75)
\]

\[
y : \quad \beta^2 \omega^2 \tilde{N} \ast \tilde{E} \Leftrightarrow \mu_0 \epsilon_0 \omega^2 \mathcal{F} \left[ \chi^{(2)} E_x^2 \right], \quad (76)
\]

and in the factorised equations these become

\[
x : \quad \mathcal{F}^{-1} \left[ \mu_0 \epsilon_0 \frac{\omega^2}{\beta(\omega)} \mathcal{F} \left[ \chi^{(2)} E_x E_y \right] \right] \quad (77)
\]

\[
y : \quad \mathcal{F}^{-1} \left[ \mu_0 \epsilon_0 \frac{\omega^2}{\beta(\omega)} \mathcal{F} \left[ \chi^{(2)} E_x^2 \right] \right]. \quad (78)
\]

Since we will want to apply the nonlinear effects in the time domain, we need to back-transform these nonlinear terms:

\[
x : \quad \mathcal{F}^{-1} \left[ \mu_0 \epsilon_0 \frac{\omega^2}{\beta(\omega)} \mathcal{F} \left[ \chi^{(2)} E_x E_y \right] \right] \quad (79)
\]

\[
y : \quad \mathcal{F}^{-1} \left[ \mu_0 \epsilon_0 \frac{\omega^2}{\beta(\omega)} \mathcal{F} \left[ \chi^{(2)} E_x^2 \right] \right]. \quad (80)
\]

So we see that a true wideband approach to the nonlinearity requires a pair of Fourier transforms. In a semi-wideband limit around a central frequency \( \omega_0 \) we can probably assume the factor \( \omega^2 / \beta(\omega) \) becomes \( c \omega_0 / \omega_0(\omega_0) \). In an SVEA-like narrowband limit it would become \( \omega_0^2 / \beta(\omega_0) = c \omega_0 / \omega_0(\omega_0) \), and the need for Fourier transforms vanishes.

If a more extensive collection of the \( \chi^{(2)} \) coefficients needs to be included, this procedure can be reproduced using the appropriate nonlinear field combinations. If the time-response of the nonlinearity is also important, then we can include this by replacing \( \chi^{(2)} E_x E_y \) and \( \chi^{(2)} E_x^2 \) with appropriate convolutions: i.e. \( \chi^{(2)} * E_y E_x \) and \( \chi^{(2)} * E_x E_x \).

5. Factorization and envelopes

Taking only the forward part of eqn (72), we replace \( \tilde{E}_+ (\omega) = \tilde{A}_+ (\omega + \omega_0) + \tilde{A}_0^+ (\omega - \omega_0) \). Since this the equation is linear in the derivatives, when split into \( \tilde{A}_+ \) and \( \tilde{A}_0^+ \) parts it looks very similar, being

\[
\partial_x \tilde{A}_+ = \pm i \beta \tilde{A}_+ \pm \frac{i \beta}{2} \tilde{N} \ast \left[ \tilde{A}_+ + \tilde{A}_0^+ \right]. \quad (81)
\]

For the case of a time-response \( \chi^{(3)} \) nonlinearity, the equation will be identical to that for the envelope version of the directional \( G^\pm \) fields, i.e. eqn. (43).

6. Factorized fields

An important feature of this approach is that we see that any contribution (whether linear or not) that is included in the source term will couple the forward and backward fields together. Consider two differing factorisations of the same systems; e.g. one with the loss included in \( \beta \), and one with it in the source term. The one with the extra source contribution will see a corresponding extra forward backward coupling term, apparently conflicting with the fact that the two factorisations are of the same system. The resolution of this conundrum is simply that the forward and backward fields of the first factorisations \( (E_{1+}) \) are not the same as those for the second \( (E_{2+}) \); the meaning of “forward field” or “backward field” differs between the two implementations. This is perhaps clearer in the \( G^\pm \) formulation (see section IV), where the different factorisations would correspond to different choices of the reference parameters \( \alpha_r, \beta_r \). If no further approximations have been made, when the real electric and magnetic fields are reconstructed from any factorised \( E_{1+} \), the answers should be in agreement.

E. Transverse effects

In common with most pulse propagation, we can restrict ourselves to paraxial beams and incorporated transverse effects by using a split step scheme alternating between the wave equation and the \( \nabla^2_x \) diffraction term. This is equally applicable to either the traditional or factorization approaches. However, in the factorization approach we can treat the \( \nabla^2_x E \) diffraction term as a “source” term, and, like the nonlinearity, move it to the RHS before factorising. Thus eqn. (72) could be rewritten to include diffraction as

\[
\partial_x \tilde{E}_+ = \pm i \beta \tilde{E}_x \pm \frac{i \beta}{2} \tilde{N} \ast \left[ \tilde{E}_+ + \tilde{E}_- \right] \pm \frac{i}{2 \beta} \nabla^2_x \left[ \tilde{E}_+ + \tilde{E}_- \right]. \quad (82)
\]

VI. FORWARD-BACKWARD COUPLING

We can see in eqns. (29, 31, 72) that we simplify into a forward-only picture by dropping the part of the nonlinear polarization term due to the backward field. In situations where there is no pre-existing backward field, and...
where there are no interfaces to cause reflection, this is an excellent approximation that holds true in the regime of weak nonlinearity. It is only an approximation, because the nonlinear polarization drives both the forward and backward fields, so in strongly nonlinear systems, a backward wave can be generated directly by the forward wave. The important “weak nonlinearity” criteria for perturbative nonlinearities to guarantee the validity of a forward-only model is

\[
\frac{1}{n_0} \sum_{m>1} m \chi^{(m)} E^{m-1} \ll 1. \tag{83}
\]

On the subject of reflections from interfaces, it is worth noting that “nonlinear” reflections can occur even if the linear dispersion on both sides is identical – as long as the nonlinearity changes, as in e.g. periodic poling, where its sign changes.

Note that since nonlinearities are in practice very weak (e.g. \(\chi^{(3)} E^3 \sim 0.06\) at the damage threshold of fused silica), uni-directional propagation models perform very well, and the role of nonlinear reflections is generally negligible.

VII. CONCLUSIONS

I have described three forms for the spatial propagation of optical fields: Maxwell’s equations, directional fields, and second order wave equations. These forms have been described in both standard and envelope-carrier pictures. While solving Maxwell’s equations remains the “gold standard” and most exact procedure, it is computationally demanding, and it can be difficult to set up initial conditions. These difficulties are avoided by using a directional fields approach, where we can propagate more efficiently in the usual forward-only cases. Further, envelope theories based on forward-only directional fields give equations of motion similar in form to the traditional SVEA ones based on the second order wave equation, but without requiring complicated approximations.

When comparing the various approaches taken to directional fields, a number of important points stand out.

1. The first successful attempt at deriving useful directional versions of Maxwell’s equations was by Kolesik et al. \[11, 12\].

2. The most flexible and complete formulation is the directional \(G^\pm\) fields of Kinsler et al. \[13\], relying only on simple combinations of Maxwell’s equations to achieve a directional form. It is applicable to propagation media with any frequency-dependent electric or magnetic properties, and variant forms \[14\] can be used if required.

3. The factorization style approach \[20, 21, 22\] gives propagation equations for the electric field that can be simply expressed and solved for without the construction of the somewhat opaque \(G^\pm\) fields used by Kinsler et al.

It is encouraging that these three approaches discussed in this paper (Maxwell’s equations, directional \(G^\pm\) fields, and factorized second order wave equations) all give essentially identical results in the case of uni-directional propagation in non-magnetic media.

VIII. ACKNOWLEDGMENTS

I acknowledge a wide variety of useful discussions with G.H.C. New, S.B.P. Radnor, J.M. Dudley, and G. Genty. I also thank N. Broderick for bringing refs. [34, 35] to my attention; and to M. Scalora for refs. [33, 39, 40].

[1] G. P. Agrawal, *Nonlinear Fiber Optics* (Academic Press, San Diego, 1995), 4th ed.
[2] Y. R. Shen, *Principles of nonlinear optics* (Wiley, New York, 1984), see Chapter 3 for the factorization approach.
[3] R. W. Boyd, *Nonlinear Optics* (Academic Press, New York, 1994).
[4] A. Yariv, *Quantum Electronics* (John Wiley & Sons, New York, 1989), 3rd ed.
[5] H. A. Haus, *Waves and Fields in Optoelectronics* (Prentice-Hall, Englewood Cliffs, New Jersey, 1984).
[6] A. E. Siegman, *Lasers* (University Science Books, Mill Valley, California, 1986).
[7] L. Gilles, S. C. Hagness, and L. Vázquez, J. Comp. Phys. 161, 379 (2000).
[8] R. G. Flesch, A. Pushkarev, and J. V. Moloney, Phys. Rev. Lett. 76, 2488 (1996).
[9] L. Gilles, J. V. Moloney, and L. Vazquez, Phys. Rev. E 60, 1051 (1999).
[10] J. C. A. Tyrrell, P. Kinsler, and G. H. C. New, J. Mod. Opt. 52, 973 (2005), URL http://journals.cambridge.org/ doi/10.1017/S0950034005006375.
[11] M. Kolesik, J. Moloney, and M. Mlejnık, Phys. Rev. Lett. 89, 283902 (2002), URL http://link.aps.org/abstract/PRL/v89/p283902.
[12] M. Kolesik, J. Moloney, M. Kolesik, and J. V. Moloney, Phys. Rev. E 70, 036604 (2004), URL http://link.aps.org/abstract/PRE/v70/p036604.
[13] P. Kinsler, S. B. P. Radnor, and G. H. C. New, Phys. Rev. A 72, 063807 (2005), note that in this reference, the convolution symbol between the \(\alpha, \beta\) coefficients and the \(G^\pm\) terms in square brackets in the frequency-domain propagation equations was inadvertently omitted. Also, physics/0611215v1, URL http://arxiv.org/abs/physics/0611215.
[14] P. Kinsler (2006), physics/0611216, URL http://arxiv.org/abs/physics/0611216.
[15] Y. Mizuta, M. Nagasawa, M. Ohtani, and M. Yamashita, Phys. Rev. A 72, 063802 (2005), URL http://link.aps.org/abstract/PRA/v72/e063802
[16] J. A. Fleck, Phys. Rev. B 1, 84 (1970), note that I use an alternative notation to avoid possible confusion with the electric field variables $E$ (since Fleck used $E^\pm$, not $G^\pm$), URL http://link.aps.org/abstract/PRB/v1/p84
[17] T. Brabec and F. Krausz, Phys. Rev. Lett. 78, 3282 (1997), URL http://link.aps.org/abstract/PRL/v78/p3282
[18] M. A. Porras, Phys. Rev. A 60, 5069 (1999), URL http://link.aps.org/abstract/PRA/v60/p5069
[19] P. Kinsler and G. H. C. New, Phys. Rev. A 67, 023813 (2003), physics/0212016v1, URL http://link.aps.org/abstract/PRA/v67/e023813
[20] K. J. Blow and D. Wood, IEEE Journal of Quantum Electronics 25, 2665 (1989), URL http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=1545955
[21] A. Ferrando, M. Zacares, P. F. de Cordoba, D. Binosi, and A. Montero, Phys. Rev. E 71, 016601 (2005).
[22] G. Genty, P. Kinsler, B. Kibler, and J. M. Dudley, Opt. Express 15, 5382 (2007), URL http://www.opticsexpress.org/abstract.cfm?id=132608
[23] S. A. Brown and B. J. Dalton, J. Mod. Opt. 49, 1009 (2002).
[24] P. Kinsler (2002), physics/0212014, URL http://arxiv.org/abs/physics/0212014
[25] D. Gabor, J. Inst. Electr. Eng. (London) 93, 429 (1946).
[26] P. Kinsler and G. H. C. New, Phys. Rev. A 72, 033804 (2005), also see arXiv:physics/0606111 physics/0606111v1, URL http://link.aps.org/abstract/PRA/v72/e033804
[27] P. Kinsler (2006), physics/0606112, URL http://arxiv.org/abs/physics/0606112
[28] L. W. Casperson, Phys. Rev. A 44, 3291 (1991), URL http://link.aps.org/abstract/PRA/v44/p3291
[29] J. Z. Sanborn, C. Hellings, and T. D. Donnelly, J. Opt. Soc. Am. B 20, 152 (2003).
[30] O. Sinkin, R. Holzlo¨chner, J. Zweck, and C. R. Menyuk, IEEE J. Lightwave Technol. 21, 61 (2003).
[31] B. Fornberg, A Practical Guide to Pseudospectral Methods (Cambridge University Press, Cambridge, 1996).
[32] K. S. Yee, IEEE Trans. Antennas Propagat. 14, 302 (1966), URL http://ieeexplore.ieee.org/xpl/freeabs_all.jsp?arnumber=1139353
[33] Zero force condition.
[34] J. E. Sipe, L. Poladin, and C. M. de Sterke, J. Opt. Soc. Am. A 11, 1307 (1994), URL http://josaa.osa.org/abstract.cfm?id=691
[35] C. M. de Sterke, D. G. Salinas, and J. E. Sipe, Phys. Rev. E 54, 1969 (1996), URL http://link.aps.org/abstract/PREP/v54/p1969
[36] W. H. Press, S. A. Teukolsky, W. T. Vettering, and B. P. Flannery, Numerical recipes in C: the art of scientific computing. (Cambridge University Press, Cambridge, 1992).
[37] T. Tanuiti and K. Nishihara, Nonlinear Waves (Pitman, 1983).
[38] J. P. Dowling, M. Scalora, M. J. Bloemer, and C. M. Bowden, J. App. Phys. 75, 1896 (1994).
[39] M. Scalora, J. Dowling, C. Bowden, and M. Bloemer, Phys. Rev. Lett. 73, 1368 (1994), URL http://link.aps.org/abstract/PRL/v73/p1368
[40] M. Scalora and M. E. Crenshaw, Opt. Commun. 108, 191 (1994).
[41] T. Shafer and C. E. Wayne, Physica D 196, 90 (2004).
[42] P. Kinsler, J. Opt. Soc. Am. B. 24, 2363 (2007), the arXiv:0707.0986 version contains an additional appendix., 0707.0986v2, URL http://arxiv.org/abs/0707.0986v2