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Two facets of simulation in extreme nonlinear optics

Simulations in nonlinear optics will in general reflect two facets of a modeling problem. The first is related to the propagation part of Maxwell's equations, while the second relates to constitutive relations which describe the response of a medium to electromagnetic fields. The first challenge is to describe propagation-related evolution of the optical pulse, and the second is to come up with suitable models of light-matter interactions. A comprehensive approach must therefore address two computer modeling topics, namely Propagation Models, and Medium Models. We start with the former.

1.1 Propagation Models

Form the model point of view, Maxwell's equations can be viewed as describing propagation (as expressed in the curl equations), medium properties (in constitutive relation), and initial constraints (expressed in the divergence equations). It is only natural to split an optical pulse simulator framework accordingly. The "propagation part" of Maxwell's equations, namely

$$\begin{aligned} \nabla \times \boldsymbol{H} &= +\partial_t \boldsymbol{D} + \boldsymbol{J} \\ \nabla \times \boldsymbol{E} &= -\partial_t \boldsymbol{B} \end{aligned} \tag{1.1}$$

has to be implemented into simulator core. In what follows we describe how this can be done specifically in the context of nonlinear optics and without sacrificing any important physics.

Developments in nonlinear optics and particularly in optical filamentation over the last sesquidecade inspired a lot of efforts in computational methods aimed at ultrashort pulses. New regimes, characterized by ultrafast dynamics, super-broad spectra, and approach to wave collapse, meant that the traditional models based on envelope equations, and Nonlinear Schrödinger Equation in particular, had to be replaced by more sophisticated approaches. While open problems remain in emerging areas such as extreme nonlinear optics in structured media with complex geometries, it is fair to say that at least for bulk media the central problem has been solved. State of the art in simulation of femtosecond pulses reached a degree of maturity, and practitioners in the field have a good grasp on proven techniques.

1.2 Nonlinear Medium Models

The medium related part of Maxwell system describes magnetic and electric properties in terms of so-called constitutive relations. Throughout this course we restrict our attention to non-magnetic

materials, so that we only need one relation that connects electric field intensity with electric induction, and a second relation between intensity and the current density induced in the material:

$$\begin{aligned} \boldsymbol{D} &= \epsilon * \boldsymbol{E} + \boldsymbol{P}_{\mathrm{NL}}(\{\boldsymbol{E}\}) \\ \boldsymbol{J} &= \boldsymbol{J}(\{\boldsymbol{E}\}) \end{aligned} \tag{1.2}$$

Here, both nonlinear polarization $\boldsymbol{P}_{\mathrm{NL}}(\{\boldsymbol{E}\})$ and current density $\boldsymbol{J}(\{\boldsymbol{E}\})$ are "functions" of the electric field. It is the purpose of the light-matter interaction model to implement these relations. The current and polarization terms become sources in the propagation equations which drive generation of new frequency components and spatial and temporal reshaping of the optical pulse waveform.

Current situation in this area is rather different than that in dealing with the pulse propagation sub-problem. One can safely say that models to describe nonlinear interaction at time scale of few femtoseconds are very far from satisfactory. There are several reasons this area seems lagging behind the development of Propagation Models. The first and most important is that only recently experiments begin to show that what became a standard model of optical filamentation needs improvement. The standard model is essentially a collection of phenomenological components that describe various aspects of the interaction between light and matter in filaments. It is still believed to capture the picture qualitatively correct. However, as experiments become increasingly more quantitative, gaps become more evident. The second important issue is that first-principle models of light-matter interactions are "too slow" to be integrated into comprehensive ultrafast pulse simulations. It is therefore the grand challenge in this area to develop self-consistent models which go back to first principles, but are at the same time computationally manageable to a degree that will allow their application as integral parts of light-and-matter simulators.

1.3 Brief overview: Standard medium model for femtosecond filaments

This first part of the course concentrates on pulse *propagation* modeling, and our discussion is mostly independent of what exactly are the nature and a concrete implementation of light-matter interaction we want to include. Nevertheless, it will be useful to provide a brief overview of the "standard" way the model is set up for numerical experiments with optical filaments. This is the purpose of this section.

1.3.1 Linear material properties: chromatic dispersion and losses

In general, accurate capture of *linear* properties of the medium in which an ultra-short pulse propagates is crucially important for the modeling of all *nonlinear* interactions. Because the Unidirectional Pulse Propagation Equation (UPPE) approach is spectral in nature, the only potentially difficult issue is the availability of suitable experimental data to model frequency dependent, complex-valued susceptibility. Within the bandwidth in which such data can be obtained, the propagator will capture all linear propagation exactly.

We consider a nonmagnetic, dispersive medium with relative permittivity ϵ that is a function of the transverse coordinates x, y and of the angular frequency ω

$$\epsilon = \epsilon(\omega, x, y) \ , \ \mu = \mu_0 \ . \tag{1.3}$$

This medium specification implies z-invariant geometry (where z is the propagation direction), and includes any dispersive homogeneous medium, such as air or water, as well as structured fiber-like media such as photonic, microstructured and tapered optical fibers.

In bulk media there is an important notion which appears in numerous places in derivation and implementation of propagation equations. It is the dispersion relation for a plane wave solution to Maxwell's equations, namely

$$K_z(\omega, k_x, k_y) = \sqrt{\omega^2 \epsilon(\omega)/c^2 - k_x^2 - k_y^2} \tag{1.4}$$

where k's represent wave-numbers in corresponding transverse directions. We will often refer to K_z as propagation "constant" despite the obvious fact that it is a function of frequency and of two transverse wave-vector components.

In some special cases, permittivity that appears in the above equation can be understood as an effective quantity related to a given mode. For example, to describe propagation of light confined to an effectively two-dimensional, nano-scale thickens glass membrane, ϵ becomes an effective permittivity dependent on the mode confined in the membrane waveguide. Propagation in the plane of the membrane, is then described by usual "plane-wave" expansion with an effective dispersion relation

$$K_z(\omega, k_x)^{\text{eff}} = \sqrt{\omega^2 \epsilon(\omega)^{\text{eff}}/c^2 - k_x^2} \tag{1.5}$$

and concrete $\epsilon(\omega)^{\text{eff}}$ depends on the guided mode, e.g TE or TM.

The important aspect of the approach we are going to discuss is that $\epsilon(\omega)$ (or $\chi(\omega)$) is fully incorporated in the model as a complex-valued function of frequency for all modes of propagation represented in numerics, and the implementation ensures that all these modes exhibit *exact* propagation properties.

1.3.2 Nonlinear medium response

Nonlinear effects are usually described in terms of polarization P through the material constitutive relation:

$$\boldsymbol{D} = \epsilon_0 \epsilon * \boldsymbol{E} + \boldsymbol{P}_{\text{NL}}. \tag{1.6}$$

The star in this formula represents a convolution integral with ϵ being the linear response function corresponding to the frequency dependent $\epsilon(\omega, x, y)$ as described earlier. The non-linear polarization is an "arbitrary" function of the electric field $\boldsymbol{P}_{\text{NL}} = \boldsymbol{P}_{\text{NL}}(\boldsymbol{E})$. We will also include a current density that is driven by the optical field

$$\boldsymbol{j} = \boldsymbol{j}(\boldsymbol{E}) \tag{1.7}$$

to describe interactions with plasma generated by the high-intensity optical pulse. It should be noted that part of medium reaction to the presence of the light field included in the current density may be linear. For example, if free electrons are present, for example generated by another pump pulse, the corresponding current density induced will be linear in $\boldsymbol{E}$.

The main physical effects that influence propagation of ultrashort, high-power light pulses in nonlinear dispersive media include optical Kerr and stimulated Raman effects, free-electron generation, defocusing by the generated free electrons and losses caused by avalanche and multi-photon ionization (MPI). With minor modifications, models including these effects can be used for description of ultra-short optical pulses propagation in gases, condensed bulk media, and in conventional, microstructured, and tapered fibers as well as in ultra-thin silica "wires" and glass membranes.

Form the design point of view and for implementation of an UPPE simulator, the important aspect of medium models is that they are "prescriptions" to evaluate material reactions formulated in the real space (as opposed to spectral space). That is, given the field history $\boldsymbol{E}(t)$ for a

given spatial point, these algorithms calculate either polarization or current density as function of time, and return their results to the solver core. The latter can invoke various modules that evaluate the response independently across all spatial grid points and there is no need for the core to "know" details of such calculations. A uniform communication interface between the core and the response modules is the way to realize this separation in practice.

1.3.3 Optical Kerr effect

The optical Kerr effect is due to electronic response and causes local modification of optical susceptibility

$$\boldsymbol{P}_{\mathrm{NL}} = \epsilon_0 \Delta\chi E \tag{1.8}$$

which is proportional to light intensity I:

$$\Delta\chi = 2n_b n_2 I \tag{1.9}$$

This is the most important effect responsible for the formation of femtosecond light filaments. It causes increase of refractive index where intensity of light is higher, which in turn results in further (self-) focusing of light. In the absence of other effects this would lead to a runaway effect called self-focusing collapse.

Note that the intensity I above is a time-averaged quantity, and the frequency content of P_{NL} is therefore essentially that of the driving pulse. However, because bound electrons react to external fields on atomic time-scales, electronic Kerr effect can be considered as instantaneous. To our knowledge, actual response times have not been detected, e.g. in two-beam coupling experiments, and are believed to be well below femtosecond. That is why a model can implement this effect as reacting to the instantaneous value of an electric field. Importantly, this results in a "new" source of third harmonic frequency.

1.3.4 Third harmonic generation

Consider an instantaneous (electronic) Kerr effect in an isotropic medium. The polarization response that is third-order in E must be constructed solely from $\boldsymbol{E}$ taken at the given moment in time, so there is a single vector to "work with." Consequently, the only possible form of an instantaneous third-order nonlinearity is

$$\boldsymbol{P}_{inst} = \bar{n}_2(\boldsymbol{E}.\boldsymbol{E})\boldsymbol{E} \quad . \tag{1.10}$$

Let us emphasize again, that this simple relation is the only possible for an *instantaneous* response. As soon as there is memory, two frequency dependent components of third-order susceptibility tensor are needed for full description. The frequency content of $\boldsymbol{P}_{\mathrm{inst}}$ consist of both the fundamental frequency of E and its third harmonic. This is the main source of third harmonic radiation observed in femtosecond filaments.

It is worthwhile to note that one can find in the literature also a quite different approach to modeling the third-harmonic generation. In the works and simulations based on *envelope* pulse propagation equations, several authors used two separate envelope functions, one for the fundamental frequency and one for the third harmonic generation. We emphasize that the two-envelope method is incorrect and should be avoided, because situations are frequently encountered in which spectra become extremely broad. Then the distinction between fundamental and third harmonic is impossible, and any two-envelope parametrization is therefore non-unique and the model is fundamentally inconsistent.

1.3.5 Delayed response: stimulated Raman effect

Air is by a large part made of two-atomic molecules with different polarizibilities parallel and perpendicular to their symmetry axes. This leads to a nonlinear effect which is referred to as stimulated Raman effect, although recently the nomenclature acknowledges the fact that reorientation of molecules plays a central role in it.

The interaction energy of a molecule in an external field is such that it prefers to align with the field‘s direction. When a femtosecond pulse “hits” such a molecule, it excites rotational motion; this is a stimulated Raman effect. Molecular rotation in turn changes the effective linear polarizibility of the molecule as projected on the direction of the field. The latter then experiences a modified index of refraction.

Because the interaction Hamiltonian is quadratic in field, the effect is of third-order. It is therefore often considered a “companion” of the electronic Kerr effect. Taken a very different microscopic origins, this may seem arbitrary, but one has to keep in mind that manifestations of the two effects (i.e. self-focusing) are very difficult to distinguish in relatively longer pulses.

A proper, first-principles model would need to integrate quantum mechanical equations of motion for a density matrix describing the rotation state of an ensemble of molecules. Note that such a system is to be solved at each spatial grid location, and at each propagation step, and it requires solutions of a moderat-size system of ordinary differential equations. Instead of this (relatively) difficult calculation, the Raman effect is approximately parametrized with

$$\Delta\chi(t) = 2n_b n_2^{\mathrm{R}} \int_0^\infty \mathcal{R}(\tau) I(t-\tau)\mathrm{d}\tau \ , \tag{1.11}$$

where $\mathcal{R}(\tau) \sim \sin(\Omega\tau)e^{-\Gamma\tau}$ is often sufficient for ultrashort pulses. It is a memory function which represents the response of the system to an excitation by a very short impulse. This simple formula has the advantage of easy implementation that avoids explicit calculation of the convolution integral (1.11). Sometimes an even simpler, exponential memory function $\mathcal{R}(\tau) \sim e^{-\Gamma\tau}$ has been used in simulations. If the actual memory function is sufficiently complex, as is the case in silica for example, a numerical convolution approach may be better suited to calculate the response $\Delta\chi(t)$.

1.3.6 Multiphoton and avalanche ionization

Because of high light intensities occurring in femtosecond pulses, free electrons are generated by Multiphoton Ionization (MPI), tunneling, and avalanche mechanisms. Then it is necessary to account for the response of the optical field to the presence of a dilute plasma. Since the relevant times scales are so short, electron diffusion and ion motion are neglected, and the free-electron density ρ is usually obtained as a solution to an equation of the following form

$$\partial_t \rho = aI\rho + b(I) - c\rho^2 \ . \tag{1.12}$$

Here, I is the light intensity, a parametrizes the avalanche free-electron generation, and $b(I)$ represents the Multi Photon Ionization (MPI) rate that is a highly nonlinear function of the intensity. The last term describes plasma recombination, and is often neglected in sub-hundred femtosecond pulses.

Various representations exist for the ionization rate $b(I)$. Frequently a power-law fit to experimental data or a theoretic formula result is obtained in the form

$$b(i) = \sigma \left(\frac{I}{I_0}\right)^K \tag{1.13}$$

where σ and K (not necessarily an integer!) are ionization cross section and (effective) multi-photon order. Because filaments actually occur at intensities for which multi-photon ionization crosses-over to tunneling regime, the effective order K is usually significantly lower than the number of photons needed to bridge the band-gap of the material.

In extreme intensity regimes, when ionization rate is mostly due to tunneling, b is given as a function of the electric field intensity. Then, because electrons are mostly generated at moments when its amplitude reaches a maximum, a staircase-like temporal profile arises in the free electron density and current. This gives rise to a secondary source of third (and higher) harmonic generation which has recently been detected.

1.3.7 De-focusing by free electrons

In the spirit of a Drude model, it is assumed that a collective electron velocity $\boldsymbol{v}$ responds to the optical field, and the total current density is governed by the following simple equation

$$\frac{d}{dt}\boldsymbol{j}(t) = \frac{e^2}{m_e}\rho(t)\boldsymbol{E}(t) - \boldsymbol{j}(t)/\tau_c \tag{1.14}$$

where τ_c stands for the mean time between collisions experienced by electrons. Note that v represents an average velocity induced in the ensemble of electrons by the driving field E, it is not an individual electron velocity. This equation is solved together with (1.12) to capture effects of free electrons on the propagation of the optical field, namely defocusing and losses.

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

$$\boldsymbol{P} = \epsilon_0 \Delta\chi_{\mathrm{pla}}(\rho)\boldsymbol{E} = \rho\frac{ie^2}{m_e\omega_{\mathrm{R}}(1/\tau_c - i\omega_{\mathrm{R}})}\boldsymbol{E} \tag{1.15}$$

with ω_{R} being a chosen reference angular frequency. It needs to be emphasized that this approximation completely neglects the plasma induced chromatic dispersion. This may be unacceptable for some numerical experiments, for example pump-probe with fundamental and second harmonic. In such a case, only the current density based description can properly reflect the fact that the second harmonics is experiencing four times weaker de-focusing caused by free electrons. However, in many filamentation modeling scenarios, susceptibility based formulation gives results in practical agreement with those obtained from the more accurate model based on $\boldsymbol{J}$.

It is worthwhile to note that in the framework described so far, electrons interacting with a light pulse are treated as either bound (in their respective atoms and molecules) or completely free and oblivious to the presence of their parent ions. These free electrons are described in terms of a Drude model which is more suitable for true plasma. Here we have to keep in mind that during the first few tens of femtoseconds there is not enough time for plasma to establish itself as a collective ensemble of electrons and ions. Moreover, electrons liberated from atoms and molecules are likely to interact with the parent ions - this effect, which among others leads to High-Harmonic Generation, is completely neglected. These are obviously the issues the "next-generation" modeling will have to account for.

1.3.8 Multiphoton ionization losses

Losses caused by multiphoton ionization are usually incorporated as either an equivalent current or an imaginary susceptibility contribution that extracts the energy needed for the free-electron

generation from the optical field:

$$\boldsymbol{J}_{\text{loss}}.\boldsymbol{E} \approx b(I)E_g \tag{1.16}$$

Here we equate the rate of energy loss suffered by the field with the rate of free electron generation multiplied by an estimated energy cost E_g of one free electron.

Note that although this is a universally utilized approximation in the femtosecond pulse propagation area, it is a very crude model, very likely not adequate when the pulse spectrum broadens in such a way that new frequencies carry a significant portion of its energy. In such a situation the absorption losses as well as MPI generation rates should be frequency selective. This is just one aspect in which the currently standard medium model is less than satisfactory.

2

Maxwell's Equations: The reduction problem

The Maxwell's equations, while efficiently solved by numerical solvers in many areas of computational electromagnetics, are rather ill suited for straightforward computer simulations of nonlinear phenomena in optical pulses of ultra-short duration which deliver TW-scale powers. The following sections explain why is it that direct Maxwell solvers are of limited utility in extreme nonlinear optics. We review various ways this problem has been dealt with in traditional nonlinear optics. We then formulate what we call the "Maxwell reduction problem," which consists in trading the Maxwell system for an effective framework tailored to the pulse propagation context.

2.1 Numerical solvers of Maxwell's equations

Throughout the several past decades, formulation of pulse propagation problems in nonlinear optics has been most often based not directly on the physical fields that appear in Maxwell's equations, but on the so-called envelope equations. These are designed to eliminate the fast oscillatory temporal and spatial variations related to the central frequency and wavenumber of a carrier light wave. Effectively, physical fields are represented by slower evolving complex-valued envelopes. The rationale behind such approximations is twofold. First, envelope equations are natural and accurate approximations to Maxwell's equation in many situations characteristic of nonlinear optics, and provide a useful theoretic basis for building models for phenomena such as harmonic generation. Second, such equations make it feasible to simulate many nonlinear phenomena with sufficient accuracy. While numerical methods for direct simulation of Maxwell's equations have been available, a closer look at the problem will quickly reveal that in a typical nonlinear propagation context direct Maxwell's solvers are of little practical use. One may question this statement and argue that cheap, widely available computing power will surely make the direct attack feasible in the nearest future. Actually, the answer is still negative, and it is the intent of this section to demonstrate that the development of better theoretic models underlying numerical simulators is a much more viable strategy than waiting for the computer power to catch up with our requirements.

So, let us briefly review, the general properties of direct Maxwell solvers in order to understand the implications for description of nonlinear pulse propagation. We will restrict ourselves to the so called Finite Difference Time-Domain (FDTD) solvers because they are the most common representatives of direct Maxwell solution methods. However, the discussed issues are relevant to Maxwell's equations simulators in general.

First, let us consider memory requirements. A direct solver works over a fixed spatial domain, and evolves the grid-based representation of the electric and magnetic fields in discrete time

steps. As a rule of thumb, for accurate simulations one typically needs about 30 grid points per wavelength in space. About the same number of time-steps must be executed per a single wave oscillation. Such a resolution may be practically achievable for radio- or micro-waves and small simulated volumes (as measured in units of cubic wavelengths). But in the optics context, these resolution requirements translate into sub-micrometer spatial, and sub-femtosecond temporal resolution. If an optical pulse beam is only one centimeter wide, and propagates over a laboratory-scale distance of only a few meters, a single snapshot of the field will require of the order of 10^{20} field-variables to store in the memory. Moreover, for each meter of propagation, each of these variables must be updated through tens of millions of integration steps! No matter how fast typical computer memory and performance continue to increase, it becomes clear that a brute-force approach in an optics context is not going to be feasible in any foreseeable future.

The second property which practically disqualifies direct solvers for nonlinear propagation is numerical dispersion. Similar to natural light waves, phase and group velocities of "numerical waves" depend on their frequency - they exhibit so-called numerical dispersion. It is of course a general property of each and every numerical method which simulates wave propagation that the actual wave properties differ from the desired ones because of the discrete nature of the simulation. More precisely, the true relation between wave propagation velocity and its frequency, which is usually called the dispersion relation, is replaced by an artificial one which is significantly different. Typically, a discrete numerical method can only mimic correct dispersion properties of waves for small frequencies. As a consequence, only a very small fraction of the bandwidth which is available to the numerics can actually be utilized. This artificial deformation of the natural relation between the wave velocity and its frequency is very restricting in all discretization schemes for Maxwell's equations, This is because numerical dispersion depends on the grid resolution, and is in general extremely strong from the point of view of nonlinear optics. For example, a "numerical vacuum" simulated by a direct solver will typically exhibit chromatic dispersion orders of magnitude larger than gases and comparable to water or other transparent condensed media. Surely, these unwanted effects decrease in magnitude as we increase the grid resolution. But to get them fully under control, the required resolution would be enormous. Because in the simulation of nonlinear optics it is absolutely crucial to capture the chromatic dispersion *very accurately*, this problem becomes extremely serious.

Last but not least, it turns out that in direct solvers it is actually quite difficult to implement models of nonlinear and dispersive media. The origin of the problem is that dispersion and often also nonlinearity are connected to some kind of memory in the medium. This does not mesh well with the fact that a direct solver scheme is naturally designed to store only a single temporal snapshot of the EM field. If the reaction of the medium at any given point depends on the history of the local field, we must keep sufficient information about this history available to the numerical solver. This can easily multiply the memory needs. The problem gets even worse once we consider that the frequency-dependent properties of the model media are also plagued by numerical dispersion. The artificial "deformation" of the actual numerical medium response can be significantly different from the targeted frequency-dependent properties for the same reason we pointed out for the linear wave propagation.

Thus, it is clear that the direct numerical solution of Maxwell's equations is not feasible for many nonlinear optic phenomena. Next, we will have a look back into the recent history and review how this problem has been by-passed through the use of envelope equations. As a prototype of envelope equations utilized in optics, we first turn our attention to the so called Nonlinear Schrödinger Equation.

2.2 The workhorse of nonlinear optics: Nonlinear Schrödinger Equation

As the name suggests, this equation is closely related to the Schrödinger equation of quantum mechanics. Apart from the nonlinearity, the two are almost equivalent. Indeed, paraxial diffraction of a continuous-wave optical beam is the same as the quantum-mechanical spreading of the wave-packet of a free particle. Moreover, the nonlinear term can be often interpreted as a "potential" that appears in the quantum mechanical version of the equation. However, nonlinearity turns the optical version into a much richer equation. In fact, its applications in physics go way beyond optics and apply to nonlinear dispersive waves in general. This is the reason behind the enormous amount of NLS-related research in both mathematics and physics communities.

The mathematical form of the Nonlinear Schrödinger Equation (NLS) is rather simple:

$$\partial_z A = \frac{i}{2k_0}\Delta A - \frac{k''}{2}\partial_{tt} A + \frac{i\omega_0 n_2}{c}|A|^2 A \ .$$

Here, A represents the complex envelope of an optical pulse centered around the carrier angular frequency ω_0. The first term on the right-hand-side, with k_0 standing for the propagation constant corresponding to the carrier frequency, describes diffraction. The next term captures chromatic dispersion, with k" being the group velocity dispersion. The nonlinear term represents the optical Kerr effect in which the nonlinear modification of the refractive index is simply proportional to the light intensity. The latter is here expressed by $|A|^2$, and n_2 is the so-called nonlinear index of the medium.

Equations of the same form, often with different dimensions of the Laplacian, arise in many areas of physics. In optics, NLS is a prototype equation to describe pulse propagation in nonlinear, dispersive transparent media. Taken its simplicity, it may come as a surprise that it captures a wealth of nonlinear phenomena in fibers and bulk media alike. Often, this equation works qualitatively very well even beyond the "boundaries" given by the paraxial and quasi-monochromatic assumptions under which it is supposed to be valid. That is just one reason this and related equations continue to receive significant attention in the mathematical and physical literature.

We will discuss one of the many ways to derive this important equation in Section 4, where we also specify precisely the physical assumptions that are necessary for its validity. However, at this point it is instructive to be just a little more specific about the relation between the complex amplitude A and its real physical field counterpart E. For simplicity, we restrict ourselves to to a one-dimensional, scalar case of linearly polarized light. Usually, the relation between the two quantities is written as

$$E(x,t) = A(x,t)e^{-i\omega_0 t + ik_0 x} + \text{c.c.} \ .$$

Here, ω_0 and k_0 are the carrier frequency and wavenumber, and the purpose of the oscillatory exponential is to account for the fast changing carrier-wave of the field. The complex amplitude A then can be viewed as a modulation of the carrier. This of course only makes sense if the modulation speed is small in comparison to the angular frequency ω_0. Said in an equivalent way, the spectral content of $A(x,t)$ must be narrow in comparison with ω_0. And this is where the need to improve this equation originates: In modern nonlinear optics, we often deal with waveforms $E(x,t)$ which change their amplitudes significantly within a single oscillation of the carrier. In such a situation even the carrier frequency becomes an ill defined notion. This motivated researchers to propose a number of improved equations which were intended specifically for the modeling of ultra-fast optical pulses. And that is the topic of the next section.

2.3 Beyond the Nonlinear Schrödinger Equation: Correction terms

With the advent of relatively afordable femtosecond lasers and the subsequent accelerated expansion of nonlinear optics into the ultra-fast domain, it became evident that NLS is a rather crude model to describe phenomena such as supercontinuum generation. A single-color optical pulse "explosively" broadening its spectrum such that it can cover the whole visible region and beyond is arguably one of the most spectacular effects in nonlinear optics. Intuition alone tells us that describing such extreme events in terms of envelopes is not realistic. Moreover, it turns out that the white light generation, as the supercontinuum is often called, is an extremely robust and universal phenomenon. The ubiquitous nature of such a nonlinear interaction underlines the need to "go beyond the NLS" and introduce better pulse propagation models.

Researchers therefore developed a whole family of equations which include the so-called correction terms. These are modifications to the NLS equations intended to make it more robust, and especially applicable to very short-duration, high-intensity optical pulses. Some of these "corrected" propagation equation will be described in the next chapter in connection to our nonlinear pulse propagation model. Here, we would like to restrict ourselves to a single example to give the reader an idea about what types of corrections are possible to improve the NLS. The following is the Nonlinear Envelope Equation (NEE), developed by Brabec and Krausz:

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

Similarly to NLS, NEE is an envelope equation, but it is formally free of the quasi-monochromatic approximation. Therefore it is much better suited for very short duration pulses. Without going into details, let us note some of the corrections that take this model well "beyond the NLS". The first is the occurrence of the dispersion operator D on the right hand side of the equation. This is a formal infinite series in temporal derivatives, ∂_t:

$$D(\omega-\omega_\mathrm{R}) = \sum_{n=2}^{\infty}\left(\frac{\partial^n k}{\partial\omega^n}\right)_{\omega=\omega_\mathrm{R}}\frac{(\omega-\omega_\mathrm{R})^n}{n!} \tag{2.1}$$

Setting aside the questions of how to properly define and implement such an operator, let us just say that this can in principle take into account chromatic properties of the medium in a wide range of frequencies. Linear medium properties, specifically its frequency-dependent index of refraction and loss, are encoded in the dispersion operator through the infinite series of coefficients in (2.1). The important point to note is that in comparison with NLS, NEE has a sufficient "number of parameter slots" (in contrast to only two in NLS) to incorporate a detailed medium description.

Another correction to note is the inverse operator in front of the diffraction Laplacian. This is the so-called spatial-temporal diffraction correction term and it takes into account the dependence of diffraction on the color of light. This reflects the well known fact that the longer the wavelength, the more the light diffracts and bends around obstacles.

Yet another important correction stands in the front of the nonlinear polarization $\mathcal{P}$: It is called the self-steepening term which is responsible for strong generation of new spectral components in the trailing edge of a propagating pulse. Intuitively, this correction term can be viewed as a modification of the propagation velocity which depends on the "local" light intensity. The higher the intensity, the slower the propagation. This makes the intensity peaks to lag behind their pedestals, and consequently steepens the trailing edge of the pulse. In turn, the steep edge represents a wide spectral content. This correction is to a large degree responsible for capturing generation of the blue-shifted light as observed in many experiments.

In comparison to NLS, the Nonlinear Envelope Equation is a very realistic model. Our superficial look at it already makes it evident that its robust numerical implementation requires close

attention to the correction terms. More importantly, it is fair to say that the original derivation of the equation was based on intuitive, but, strictly speaking, unjustified arguments. This is the case for a whole number of corrected equations presented in both optical and mathematical literature. The discussion in later sections will identify cases in which weak arguments resulted in rather poor equations: in one example, physicists were misled by intuition and possibly by their desire for equations easily implemented in numerics which in turn lead to an outright incorrect model. Mathematicians, on the other hand, may be willing to sacrifice realistic models to ones described by "nice" (for example integrable) equations which, however, may turn out to be utterly unsuitable to the very application they were meant for. The celebrated Short Pulse Equation serves as an example here. Because of built-in assumptions, which may seem benign at a first superficial look, this equation can not capture generic behaviour of short pulses in supercontinuum generation in optical fibers. Lessons like these lead us to ask an important question; what kind of qualities do we need to require of our pulse propagation model if it has to aspire to be a truly realistic model applicable in extreme nonlinear optics? We address this in the following.

2.4 The reduction problem

Thus, we have identified the problem of "Maxwell reduction," which means to replace the full set of equations for electromagnetic field with a reduced set capable of handling the extreme conditions encountered in modern nonlinear optics. Specifically, this requires:

- Capability to capture, without any approximations, linear propagation regimes in transparent media, i.e. in media with relatively small, but frequency-dependent absorption, but with potentially complex chromatic dispersion "landscapes."
- Capability to handle spatio-temporal waveforms with extremely wide spectra extending over several octaves of frequency. For this it is necessary to work on the level of physical fields, and avoid introduction of envelopes and related artificial parameters (such as the carrier frequency that appears in envelope propagation equations).
- It is important to implement such models of light-matter interactions that can be valid over broad bandwidth and exhibit "long" response memory (i.e. dependence on the history of the driving field).
- It is crucial that the pulse evolution equations can be implemented in a numerically efficient way that allows simulations of nonlinear pulse propagation over laboratory-scale distances.

Unidirectional Pulse Propagation Equations represent the first approach to put this problem on firm mathematical ground. They are effective Maxwell solvers designed for the pulse propagation context, i.e. especially for situations in which the light propagates in a well defined direction. This can be achieved without sacrificing physics, while eliminating the practical limitations of the direct Maxwell solvers described in the beginning of this section. The next section is devoted to derivation of various forms of Unidirectional Pulse Propagation Equations.

3

Unidirectional Pulse Propagation Equations

In this chapter, we outline the key steps in deriving a physically self-consistent and robust ultrashort pulse propagator that resolves the underlying optical carrier-wave while also enabling propagation over many meter propagation lengths. Our goal is to retain the full rigor of Maxwell's equations while reducing the problem complexity by constraining the model to unidirectional propagation. As our immediate interest is in very short-duration and high-intensity pulse propagation in which the induced nonlinear polarization can have significant impact on the dynamics, we will need to accurately capture the very broad spectral landscape that the pulse experiences during its interaction with a host dielectric material. In many cases, the spectral super-broadening is such that the generated bandwidth exceeds the underlying carrier frequency, i.e $\Delta\omega/\omega_0 >> 1$. In this regime, we expect the Nonlinear Schrödinger Equation (NLSE) to fail. Many attempts have been made to derive nonlinear envelope models that go beyond NLSE. We discuss some of these, and we show explicitly how each can be seamlessly derived from the Unidirectional Pulse Propagation Equation (UPPE).

3.1 Time-propagated and space-propagated equations

Most of the pulse propagation problems in nonlinear optics are solved in one of two formulations: Either the numerical evolution proceeds along the time coordinate, or it follows, or "propagates" the wavepacket along one of the spatial coordinates, usually chosen as z, in the direction of the laser beam. In the first case, termed "time-propagated evolution," one has an initial condition (i.e. some description of the electric and magnetic fields) specified in all space for a given initial time. The evolution is calculated along the time axis, and naturally reflects the structure of the Maxwell's equations. In the second case, termed "z-propagated evolution," the initial condition is given as a function of the local pulse time and of the transverse coordinates (w.r.t. propagation direction). The numerical evolution proceeds along the propagation axis. From the mathematical point of view, this case is an initial value problem very much the same way the t-propagated case is. However, from the physical point of view this is a rather subtle issue because the true "initial" condition requires knowledge of the *total* field in the past *and* in the future. This includes the light which may be nonlinearly "reflected" from the focal region of an experiment. Only if we can assume that this is sufficiently weak, we can solve the corresponding initial value problem. We will refer to the corresponding propagation models as time- and z-propagated equations.

The z-propagated approach is much more common in nonlinear optics simulations based on envelope equations, and is often related to Nonlinear Schrödinger Equation. On the other hand, the time-propagated approach is common for solvers based on direct integration of Maxwell's

equations. The time-propagated versions of UPPE are more suitable for tight-focusing scenarios when the non-paraxial effects start to play a role. On the other hand, the z-propagated equations are easier to use in situations that allow us to neglect the longitudinal field components as contributing sources of nonlinear material responses. That is the main reason the z-propagated approach is more common, specifically in nonlinear optics.

First we focus our attention on the time-propagated UPPEs, because this approach is conceptually simpler. We start with derivation which is based on a formal projection technique designed to separate what we call forward and backward propagating optical field components. We discuss its numerical implementation in Section 4, while its relation to previous envelope models will be discussed together with the z-propagated methods later in the next section.

Most of the room in what follows is devoted to the z-propagated approach. Since the general derivation method, while straightforward in principle, is rather involved, we first show a simple one-dimensional example of scalar propagation equation. This will reveal the mathematical nature of certain assumptions one has to adopt; these are important in that they select from the set of all Maxwell's equations solutions those that fall into the "category of pulsed beams." We then follow with the general case, which is subsequently specialized to equations in the homogeneous bulk media and to wave-guide, or fiber-like structured "media."

3.2 Derivation of T-propagated Unidirectional Propagation Equation

The version of UPPE that is numerically evolved along the time axis is termed a t-propagated equation. It is, strictly speaking, a *pair* of equations, each describing a component of the optical field with a "prevailing" direction of propagation. The derivation is based on the notion of a projection which selects only the forward (or backward) propagating part of the field. It must be emphasized that the forward-backward split is formally exact. However, approximations are necessary for reducing the system into *unidirectional equation*, which we do by assuming that the nature and strength of the nonlinear response is such that it can be accurately calculated from the forward field component only. This in turn implies that the gradients of the nonlinearly modified medium properties are changing on length scales large in comparison to wavelength.

In the next Section, we describe the projector and its properties in detail. We then use it to derive the time-propagated UPPE.

3.2.1 Projection operators for forward and backward propagating fields

Consider general electromagnetic field $\boldsymbol{E}(\boldsymbol{r},t)$ $\boldsymbol{H}(\boldsymbol{r},t)$ and the corresponding induction, $\boldsymbol{D}(\boldsymbol{r},t)$, for a homogeneous nonmagnetic medium characterized by its frequency dependent susceptibility $\chi(\omega)$.

Let us denote $\boldsymbol{E}(\boldsymbol{k})$, $\boldsymbol{H}(\boldsymbol{k})$ and $\boldsymbol{D}(\boldsymbol{k})$ the spatial Fourier transforms of the corresponding fields, e.g.

$$\boldsymbol{D}(\boldsymbol{k}) = \mathcal{F}\{\boldsymbol{D}(\boldsymbol{r})\}(\boldsymbol{k}) \quad \boldsymbol{D}(\boldsymbol{r}) = \mathcal{F}^{-1}\{\boldsymbol{D}(\boldsymbol{k})\}(\boldsymbol{r}) \tag{3.1}$$

In the Fourier representation, i.e. the spatial spectrum space, we can define the following operators

$$\mathcal{P}^{\pm}\begin{pmatrix}\boldsymbol{D}(\boldsymbol{k})\\ \boldsymbol{H}(\boldsymbol{k})\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\boldsymbol{D}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{H}(\boldsymbol{k})\\ \boldsymbol{H}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{D}(\boldsymbol{k})\end{pmatrix}. \tag{3.2}$$

The reader will notice that this pair of operations is diagonal in the wave-vector $\boldsymbol{k}$, and is closely related to the properties of plane-wave solutions of linearized Maxwell's equations. Next we show

that $\mathcal{P}^{\pm}$ have the properties of projectors onto forward and backward propagating fields; they must be idempotent in a certain sense, and have to constitute a decomposition of unity.

Obviously, the two operators $\mathcal{P}^{\pm}$ provide a unity decomposition

$$\mathcal{P}^{-} + \mathcal{P}^{+} = 1 \tag{3.3}$$

which follows directly from their definition.

Further, one can show that as long as they act over the divergence-free subspace, they behave as projectors, namely $\mathcal{P}^2 = \mathcal{P}$. To see this, let $\boldsymbol{U}, \boldsymbol{V}$ be two arbitrary divergence-free vector fields, which satisfy $\nabla.\boldsymbol{U} = \nabla.\boldsymbol{V} = 0$. Then

$$\begin{aligned}
\mathcal{P}^{\pm}\mathcal{P}^{\pm}\begin{pmatrix}\boldsymbol{U}(\boldsymbol{k})\\ \boldsymbol{V}(\boldsymbol{k})\end{pmatrix} &= \tfrac{1}{2}\,\mathcal{P}^{\pm}\begin{pmatrix}\boldsymbol{U}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})\\ \boldsymbol{V}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})\end{pmatrix} = \\
&\tfrac{1}{4}\begin{pmatrix}\boldsymbol{U}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})\\ \boldsymbol{V}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})\end{pmatrix} + \\
&\tfrac{1}{4}\begin{pmatrix}\mp\operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times[\boldsymbol{V}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})]\\ \pm\operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times[\boldsymbol{U}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})]\end{pmatrix} = \\
&\tfrac{1}{4}\begin{pmatrix}\boldsymbol{U}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})\\ \boldsymbol{V}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})\end{pmatrix} + \\
&\tfrac{1}{4}\begin{pmatrix}\mp\operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})\\ \pm\operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})\end{pmatrix} - \\
&\tfrac{1}{4}\begin{pmatrix}\frac{1}{k^2}\boldsymbol{k}\times\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})\\ \frac{1}{k^2}\boldsymbol{k}\times\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})\end{pmatrix} = \\
&\tfrac{1}{2}\begin{pmatrix}\boldsymbol{U}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})\\ \boldsymbol{V}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})\end{pmatrix} - \\
&\tfrac{1}{4}\begin{pmatrix}\frac{1}{k^2}\boldsymbol{k}\boldsymbol{k}.\boldsymbol{U}(\boldsymbol{k})\\ \frac{1}{k^2}\boldsymbol{k}\boldsymbol{k}.\boldsymbol{V}(\boldsymbol{k})\end{pmatrix} = \\
&\tfrac{1}{2}\begin{pmatrix}\boldsymbol{U}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z)\frac{1}{\omega(k)}\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})\\ \boldsymbol{V}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z)\frac{\omega(k)}{k^2}\boldsymbol{k}\times\boldsymbol{U}(\boldsymbol{k})\end{pmatrix} = \\
&\mathcal{P}^{\pm}\begin{pmatrix}\boldsymbol{U}(\boldsymbol{k})\\ \boldsymbol{V}(\boldsymbol{k})\end{pmatrix}
\end{aligned} \tag{3.4}$$

Since the radiation fields $\boldsymbol{D}, \boldsymbol{H}$ are divergence free, the above calculation shows that $\mathcal{P}^{\pm}$ act as projectors on these fields, with $\mathcal{P}^{\pm}\mathcal{P}^{\pm} = \mathcal{P}^{\pm}$.

Finally, it is easy to check that $\mathcal{P}^{+}$ leaves invariant any plane wave solution to Maxwell's equations that propagates with k_z wave-vector component larger than zero (in the positive z-direction): At the same time, it "annihilates" all plane waves propagating in the negative z-direction. To show this, we use the fact that in a plane wave there is a definite relation between the electric and magnetic fields:

$$\begin{pmatrix} \boldsymbol{D}(\boldsymbol{k}) \\ \boldsymbol{H}(\boldsymbol{k}) \end{pmatrix} = \begin{pmatrix} -\frac{1}{\omega(k)}\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ \frac{\omega(k)}{k^2}\boldsymbol{k} \times \boldsymbol{D}(\boldsymbol{k}) \end{pmatrix} . \tag{3.5}$$

Acting with $\mathcal{P}^{\pm}$ on both sides of this equation one obtains

$$\begin{aligned} \mathcal{P}^{\pm} \begin{pmatrix} \boldsymbol{D}(\boldsymbol{k}) \\ \boldsymbol{H}(\boldsymbol{k}) \end{pmatrix} &= \frac{1}{2} \begin{pmatrix} \boldsymbol{D}(\boldsymbol{k}) \mp \operatorname{sgn}(k_z) \frac{1}{\omega(k)}\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ \boldsymbol{H}(\boldsymbol{k}) \pm \operatorname{sgn}(k_z) \frac{\omega(k)}{k^2}\boldsymbol{k} \times \boldsymbol{D}(\boldsymbol{k}) \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} (-1 \mp \operatorname{sgn}(k_z)) \frac{1}{\omega(k)}\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ (+1 \pm \operatorname{sgn}(k_z)) \frac{\omega(k)}{k^2}\boldsymbol{k} \times \boldsymbol{D}(\boldsymbol{k}) \end{pmatrix} \\ &= \frac{+1 \pm \operatorname{sgn}(k_z)}{2} \begin{pmatrix} \boldsymbol{D}(\boldsymbol{k}) \\ \boldsymbol{H}(\boldsymbol{k}) \end{pmatrix} \end{aligned} \tag{3.6}$$

Here, the right-hand-side is either zero or equal to the original field, depending on which direction the plane wave propagates. Naturally, it follows the same way that $\mathcal{P}^{-}$ leaves invariant the backward propagating plane waves while cancelling all forward waves. Therefore, we can summarize that $\mathcal{P}^{\pm}$ each project out from an arbitrary radiation field the component that propagates in the positive (negative) z-direction.

3.2.2 T-propagated UPPE as a projection of Maxwell's equations

The time-propagated UPPE describes the electric induction rather than the electric field intensity. The rationale behind this is that $\boldsymbol{D}$ is divergence free in the absence of free charges, but this is not the case for $\boldsymbol{E}$. From

$$0 = \nabla.\boldsymbol{D} = \epsilon * \nabla.\boldsymbol{E} + \nabla.\boldsymbol{P} ,$$

we can see that the divergence of the electric vector field is essentially the opposite of that of the polarization. The latter in general possesses a non-zero divergence due to the nonlinear interactions. For example, consider the optical Kerr effect, for which the modification of the index of refraction is proportional to the light intensity. Because of the spatial profile of the latter, the divergence of the polarization is

$$\nabla.\boldsymbol{P} \sim \nabla.(n_2 I \boldsymbol{E}) = n_2 \nabla I.\boldsymbol{E} + n_2 I \nabla.\boldsymbol{E}$$

From this and the previous equations we can see that the gradient of the intensity gives rise to the non-zero divergence of the $\boldsymbol{E}$ field. That is why $\boldsymbol{D}$ is a more natural partner for $\boldsymbol{H}$ as both vector fields are divergence free.

The use of the electric induction $\boldsymbol{D}$ as the primary representation of the electromagnetic field is similar in spirit to the approach utilized in many numerical solvers of Maxwell equations which evolve $\boldsymbol{D}$ and calculate $\boldsymbol{E}$ from a given (nonlinear) constitutive relation at each step

$$\boldsymbol{D} = \epsilon_o \epsilon * \boldsymbol{E} + \boldsymbol{P}_{\mathrm{NL}} \tag{3.7}$$

Here, the $\boldsymbol{D}$ field is supposed to be known in the whole space from previous calculations or from an initial condition. P_{NL} characterizes the medium nonlinearity and is usually specified in terms of a function of the electric field. Consequently, the above equation must be solved for the electric field intensity that becomes a function of the electric induction.

We will use the constitutive relation in the Fourier representation

$$\boldsymbol{D}(\boldsymbol{k}) = \epsilon_o \epsilon(\omega(\boldsymbol{k})) * \boldsymbol{E}(\boldsymbol{k}) + \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) \ , \tag{3.8}$$

where $\omega(\boldsymbol{k})$ is defined implicitly as an angular frequency of a plane wave with a wave-vector $\boldsymbol{k}$, $\omega(\boldsymbol{k})^2 \epsilon(\omega(\boldsymbol{k})) = k^2$.

To isolate the linear part of the Maxwell's equations from the nonlinear, let us introduce a notation for the linear and nonlinear electric field as a function of induction:

$$\boldsymbol{E}_{\mathrm{L}}(\boldsymbol{k}) = \frac{1}{\epsilon_0 \epsilon(\omega(\boldsymbol{k}))} \boldsymbol{D}(\boldsymbol{k}) \tag{3.9}$$

$$\boldsymbol{E}_{\mathrm{NL}}(\boldsymbol{k}) = \boldsymbol{E}(\boldsymbol{k}) - \boldsymbol{E}_{\mathrm{L}}(\boldsymbol{k}) = \frac{1}{\epsilon_0 \epsilon(\omega(\boldsymbol{k}))} \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) \ . \tag{3.10}$$

It must be emphasized that these equations are not expressions of any physics, but merely definitions of the two auxiliary electric vector fields. The reader should note that because the right hand side of the first definition contains the full vector $\boldsymbol{D}$, the quantity $\boldsymbol{E}_{\mathrm{L}}(\boldsymbol{k})$ can not be understood as the "electric field in the linear regime." Rather, the subscript is only meant to indicate that it is the *linear formula* which is used to calculate the electric field from the induction.

Next we use this formal splitting of the electric field intensity in the Maxwell's equations written in the Fourier (plane-wave expansion) domain:

$$\partial_t \begin{pmatrix} \boldsymbol{D}(\boldsymbol{k}) \\ \boldsymbol{H}(\boldsymbol{k}) \end{pmatrix} = \begin{pmatrix} i\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}(\boldsymbol{k}) \end{pmatrix} \equiv \begin{pmatrix} i\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{L}}(\boldsymbol{k}) \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{NL}}(\boldsymbol{k}) \end{pmatrix} \ . \tag{3.11}$$

Now let's act on this equation with $\mathcal{P}^+$ to project out what we will call the forward propagating component of the pulse.

$$\begin{aligned} \partial_t \begin{pmatrix} \boldsymbol{D}_{\mathrm{f}}(\boldsymbol{k}) \\ \boldsymbol{H}_{\mathrm{f}}(\boldsymbol{k}) \end{pmatrix} \equiv \partial_t \mathcal{P}^+ \begin{pmatrix} \boldsymbol{D}(\boldsymbol{k}) \\ \boldsymbol{H}(\boldsymbol{k}) \end{pmatrix} &= \mathcal{P}^+ \begin{pmatrix} i\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}_(\boldsymbol{k}) \end{pmatrix} \\ &\equiv \mathcal{P}^+ \begin{pmatrix} i\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{L}}(\boldsymbol{k}) \end{pmatrix} + \mathcal{P}^+ \begin{pmatrix} 0 \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{NL}}(\boldsymbol{k}) \end{pmatrix} \end{aligned} \tag{3.12}$$

The first term on the right-hand side is simple to evaluate,

$$\mathcal{P}^+ \begin{pmatrix} i\boldsymbol{k} \times \boldsymbol{H}(\boldsymbol{k}) \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{L}}(\boldsymbol{k}) \end{pmatrix} = -i\omega(\boldsymbol{k}) \begin{pmatrix} \boldsymbol{D}_{\mathrm{f}}(\boldsymbol{k}) \\ \boldsymbol{H}_{\mathrm{f}}(\boldsymbol{k}) \end{pmatrix} \tag{3.13}$$

because our projector is diagonal in the plane-wave basis which in turn is the eigen-basis of Maxwell's equations in a homogeneous medium. If this equality seems counterintuitive at first, one has to keep in mind that $\boldsymbol{E}_{\mathrm{L}}(\boldsymbol{k})$ does contain contributions from *nonlinear* interactions. A straightforward evaluation of both sides of this equation proves that it holds.

The second term on the right-hand-side of 3.12 is transformed by applying the definition of the projector and performing a straightforward calculation:

$$\begin{aligned} \mathcal{P}^+ \begin{pmatrix} 0 \\ \frac{-i}{\mu_0} \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{NL}}(\boldsymbol{k}) \end{pmatrix} &= \begin{pmatrix} \frac{i}{2\mu_0 \omega(\boldsymbol{k})} \boldsymbol{k} \times \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{NL}}(\boldsymbol{k}) \\ \frac{-i}{2\mu_0} \boldsymbol{k} \times \boldsymbol{E}_{\mathrm{NL}}(\boldsymbol{k}) \end{pmatrix} \\ &= \begin{pmatrix} \frac{i\omega(\boldsymbol{k})}{2k^2} \boldsymbol{k} \times \boldsymbol{k} \times \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) \\ \frac{-ic^2}{2\epsilon(\omega(\boldsymbol{k}))} \boldsymbol{k} \times \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) \end{pmatrix} \end{aligned}$$

$$= \begin{pmatrix} \frac{i}{2}\omega(\boldsymbol{k})\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) - \frac{i}{2}\omega(\boldsymbol{k})\frac{\boldsymbol{k}\boldsymbol{k}}{k^2}.\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) \\ \frac{-ic^2}{2\epsilon(\omega(\boldsymbol{k}))}\boldsymbol{k} \times \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) \end{pmatrix} \tag{3.14}$$

After inserting expressions (3.13,3.14) into Eqn. (3.12), the first (electric induction) equation becomes the time-propagated UPPE:

$$\partial_t \boldsymbol{D}_{\mathrm{f}}(\boldsymbol{k}) = -i\omega(k)\boldsymbol{D}_{\mathrm{f}}(\boldsymbol{k}) + \frac{i}{2}\,\omega(k)\left[\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) - \frac{1}{k^2}\boldsymbol{k}\;\boldsymbol{k}.\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k})\right]\,. \tag{3.15}$$

Note that the magnetic field equation doesn't provide anything new after the projection. One can check that it can be obtained from the induction equation the same way as the magnetic field is obtained from induction in the plane wave.

In the same way one can obtain the UPPE equation for the backward propagating field component

$$\partial_t \boldsymbol{D}_{\mathrm{b}}(\boldsymbol{k}) = +i\omega(k)\boldsymbol{D}_{\mathrm{b}}(\boldsymbol{k}) - \frac{i}{2}\,\omega(k)\left[\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) - \frac{1}{k^2}\boldsymbol{k}\;\boldsymbol{k}.\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k})\right]\,. \tag{3.16}$$

The two UPPE equations are coupled through their polarization terms, because $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k})$ implicitly depends on the *total* electric field. We emphasize that at this stage this equation pair is still exact; we have not made any approximations so far. However, neither of the equations is *unidirectional* yet. To get there, we have to adopt an approximation which will de-couple the forward and backward equations. Specifically, we will restrict ourselves to those regimes in which it is sufficient to use only the forward propagating electric field to evaluate an approximation for the total nonlinear polarization. In other words, we require

$$\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{k}) \equiv \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{D}_f + \boldsymbol{D}_b, \boldsymbol{k}) \approx \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{D}_f, \boldsymbol{k}) \tag{3.17}$$

which means that the nonlinear polarization is calculated from the forward propagating component of $\boldsymbol{D}$ only, and the second UPPE for $\boldsymbol{D}_b$ can be dropped. This means that the contribution to the nonlinear response from the backward propagating field must be negligible. This is somewhat implicit definition of the one-directional propagation regime, and it is difficult to say a-priori if in a concrete situation this approximation holds. On the other hand, in practice this is actually the assumption which underlines much of the work in the laboratory; it is "known" or rather assumed based on experience that the nonlinear focal regions do not produce strong backward radiation.

While form the practical point of view we know that the above uni-directional approximation is safe to use in practical simulations, the precise characterization of "admissible solutions" is a difficult open mathematical problem. Maybe even more importantly, it is also safe to assume that sooner or later the extreme nonlinear optics research will create scenarios in which the backward-directed radiation *will not* be negligible. On the theoretic level, this question was already posed for the nonlinear Helmholtz equation exhibiting a self-focusing collapse, and it was demonstrated that both directed field components become significant in the collapsing solution. Thus, the detailed understanding of how two UPPE equations couple in the presence of nonlinear interaction is of great interest.

To summarize this part, we have obtained a propagation equation for pulsed beam-like solutions of Maxwell's equations with minimal approximations. The adjective "minimal" means that any uni-directional propagation equations will, in some form use the approximation expressed in Eqn. (3.17). It also means that other optical pulse propagation models can be obtained as approximations to the t-propagated UPPE. We will discuss several such examples in the following Chapter.

3.3 Derivation of Z-propagated Unidirectional Propagation Equation

The UPPE version which is numerically evolved along a spatial direction, say z, is quite similar to its t-propagated counterpart discussed in the previous sections. Not only the mathematical form of the equation is formally the same, but, as we will see shortly, also the approximation which makes it possible to separate two counter-propagation directions is equivalent. However, derivations are rather different, and so far there is no proof that the two approaches are mathematically equivalent. In this case, the derivation is based on expansion into linear propagation modes of the system, and on a coupled mode equation that describes the evolution of a set of complex-valued spectral amplitudes. Similarly as in the t-propagated version, we end up with a formally exact pair of equations, one for each direction of the laser beam. Reduction into a uni-directional system requires that nonlinear response does not generate strong backward component.

It can be shown explicitly that while the pair of forward and backward evolution equation is formally exact as long as they are solved together, the set of all UPPE solutions is smaller than the set of all solutions to Maxwell's equations. It is interesting to note that similar reductions is not encountered for the $t-$propagation. This is one of the reason we believe that the two approaches are in fact not mathematically equivalent.

The most important "ingredient" in unidirectional evolution equations is the separation, or elimination of the wave-form portion which propagates in the opposite direction. To emphasize this, and also to make full derivation easier to digest, we start with a simplified case of one-dimensional Maxwell's equations with a fixed, linear polarization of the electric field. This is of course equivalent to a scalar one-dimensional wave propagation. This simple case is free of notational complications while it still contains all important steps of the fully vectorial treatment.

In the subsequent section, we start by derivation of the coupled mode equations which constitute a common starting point for all "specialized" z-propagated Unidirectional Pulse Propagation Equations.

3.3.1 A warm-up exercise: One-dimensional Maxwell's equations

The one dimensional Maxwell's equations reduced to linearly polarized electric field can be written as

$$\begin{aligned} -\partial_z H &= \partial_t E + \partial_t P \\ -\partial_z E &= \partial_t H \end{aligned} \tag{3.18}$$

where z is the "optical axis" and E and H are implicitly understood to be orthogonal to each other and to z. This system has harmonic waves as solutions in the linear regime when $P = 0$:

$$\mathcal{E}_\lambda(\omega, z, t) = \mathcal{E}_0 \exp\left[-i\omega t + i\lambda k(\omega) z\right] \quad \mathcal{H}_\lambda(\omega, z, t) = \lambda \mathcal{H}_0 \exp\left[-i\omega t + i\lambda k(\omega) z\right] \quad \omega > 0 \quad \lambda = \pm 1$$

The direction "indicator" λ selects forward and backward (or left and right) propagating waves. We can use these as a basis in which to express our full, nonlinear solution as

$$E = \sum_{\mu=\pm 1} \int d\Omega A_\mu(\Omega, z) \mathcal{E}_\mu(\Omega, z, t) \qquad H = \sum_{\mu=\pm 1} \int d\Omega A_\mu(\Omega, z) \mathcal{H}_\mu(\Omega, z, t)$$

Here, $A_\mu(\Omega, z)$ are spectral amplitudes for which we have to find an evolution equation. Taking (3.18) and multiplying with the above basis functions we get

$$\mathcal{E}_\lambda \partial_z H = -\mathcal{E}_\lambda \partial_t E - \mathcal{E}_\lambda \partial_t P$$

$$\mathcal{H}_\lambda \partial_z E = -\mathcal{H}_\lambda \partial_t H \tag{3.19}$$

In these equations and in following formulas, we assume that the arguments of $\mathcal{E}_\lambda$ and $\mathcal{H}_\lambda$ are ω, z, t.

We now add these two equations and collect terms that constitute full derivatives:

$$\partial_z[\mathcal{E}_\lambda H + \mathcal{H}_\lambda E] = -\partial_t[\mathcal{E}_\lambda H + \mathcal{H}_\lambda E] - \mathcal{E}_\lambda \partial_t P \tag{3.20}$$

The next step is to integrate over the whole domain perpendicular to the direction of propagation. In this simplified case it means the t domain alone. We can see that after t integration, we obtain boundary terms at past and future temporal infinity. To get rid of these, we will restrict our solution space to those functions which satisfy

$$\lim_{t\to\pm\infty}[\mathcal{E}_\lambda H(z,t) + \mathcal{H}_\lambda E(z,t)] = 0 \tag{3.21}$$

This condition eliminates the middle term in (3.20), and the rest can be transformed as follows. First, in the left-hand side we use the fact that the basis solutions are orthogonal, and after time integration they eliminate the sum over Ω and the modal index μ:

$$\begin{aligned}
&\int dt \partial_z[\mathcal{E}_\lambda(\omega,z,t)H + \mathcal{H}_\lambda(\omega,z,t)E] = \\
&= \int dt \partial_z \mathcal{E}_\lambda(\omega,z,t) \sum_{\mu=\pm1} \int d\Omega A_\mu(\Omega,z)\mathcal{H}_\mu(\Omega,z,t) + \\
&+ \int dt \partial_z \mathcal{H}_\lambda(\omega,z,t) \sum_{\mu=\pm1} \int d\Omega A_\mu(\Omega,z)\mathcal{E}_\mu(\Omega,z,t) = \\
&= 2\lambda \mathcal{E}_0 \mathcal{H}_0 \partial_z A_\lambda(\omega,z)
\end{aligned} \tag{3.22}$$

On the right-hand side of (3.20), the polarization term yields essentially a Fourier transform

$$-\int dt \mathcal{E}_\lambda(\omega,z,t)\partial_t P = i\omega \exp[-i\lambda k(\omega)z]\hat{P}(\omega,z)$$

Collecting both sides, we arrive at an evolution equation for spectral amplitudes:

$$\partial_z A_\lambda(\omega,z) = \frac{i\omega}{2\lambda\mathcal{E}_0\mathcal{H}_0} \exp[-i\lambda k(\omega)z]\hat{P}(\omega,z) \tag{3.23}$$

To obtain a corresponding equation for the electric field, we recall that

$$\hat{E}_\lambda(\omega,z) = A_\lambda(\omega,z)\exp[i\lambda k(\omega)z]$$

and expressing its z derivatives using the evolution equation for the spectral amplitudes (3.47) we have:

$$\partial_z \hat{E}_\lambda(\omega,z) = i\lambda k(\omega)\hat{E}_\lambda(\omega,z) + i\lambda \frac{\omega}{2\mathcal{E}_0\mathcal{H}_0}\hat{P}(\omega,z)$$

This is a pair of equations for forward and backward ($\lambda = \pm 1$) propagating fields. The two are coupled through the polarization which depends on their sum. Explicitly,

$$P(z,t) = P[E_+(z,t) + E_-(z,t)]\ .$$

where the concrete functional form of this dependence is not important for the present purpose, but as an example one can consider the instantaneous Kerr nonlinearity for which the polarization

is simply proportional to the cube of the electric field (for more examples, see introductory sections of these notes):

$$P(z,t) = P[E_+(z,t) + E_-(z,t)] \sim [E_+(z,t) + E_-(z,t)]^3$$

We should note that as soon as nonlinear polarization exhibits memory effects the above expression *does not* capture the most general form of cubic nonlinearity in isotropic media.

The above derivation illustrates the scheme we will use in the next section to derive the general, fully vectorial Unidirectional Pulse Propagation Equation. The important point to note here is that in the course of derivation we had to restrict the space of our solutions by the condition (3.21). This means that the UPPE solution set is smaller than the set of all Maxwell's equations solutions. However, within the admissible subspace, unidirectional equations are exact, as long as we can solve them simultaneously while always calculating the nonlinear polarization term from the *total* field.

So let us have a look at the assumption (3.21). What it says is that for every fixed location z along the laser beam axis, if we wait for a sufficiently long time, the field at this location will tend to zero. In other words, light energy will dissipate into positive and negative z-infinities. This is certainly very benign condition in the context of pulse propagation, because this is exactly what happens to localized pulsed wavepackets - they eventually disappear from our sight. On the other hand, one can easily think of an example which does not satisfy (3.21): a pulse trapped within a perfect cavity filled with a loss-less medium. Obviously, its field will continue to exhibit in-cavity values which will not tend to zero at long times (they may not have such limits, of course). Of course, a perfect cavity is an extreme idealization, as is the notion of a loss-less medium which must be also dispersion-less and therefore in fact a vacuum. Thus we see that while there is a condition on the UPPE solutions, it is not practically restricting. Situation will turn out to be completely analogous in the fully three-dimensional case discussed in the next section.

3.3.2 Maxwell equations as a boundary value problem for pulsed beam propagation

As a first step in derivation of various versions of UPPE, we derive an exact coupled-modes system of equations. Electromagnetic fields of a light pulse propagating along the z axis can be expanded into modal contributions that reflect the geometry of the waveguide (we can consider a homogeneous medium as a special case of the latter).

$$\begin{aligned}\boldsymbol{E}(x,y,z,t) &= \sum_{m,\omega} A_m(\omega,z)\boldsymbol{\mathcal{E}}_m(\omega,x,y)e^{i\beta_{\mathrm{m}}(\omega)z-i\omega t} \\ \boldsymbol{H}(x,y,z,t) &= \sum_{m,\omega} A_m(\omega,z)\boldsymbol{\mathcal{H}}_m(\omega,x,y)e^{i\beta_{\mathrm{m}}(\omega)z-i\omega t}\end{aligned} \tag{3.24}$$

Here, m labels all transverse modes, and an initial condition $A_m(\omega, z=0)$ is supposed to be given or calculated from the known field values at $z=0$. Note that the above expansion is valid for the transverse components only, and that the modal index m is a short hand for all quantities which are required to specify a unique propagation mode. For example, in a homogeneous bulk medium, the eigen modes are the well known plane waves, and the index m represents polarization, two transverse wavenumbers, and a binary value selecting the forward or backward direction of propagation.

To save space, the following short-hand notation will be used below

$$\begin{aligned}\boldsymbol{\mathcal{E}}_m &\equiv \boldsymbol{\mathcal{E}}_m(\omega,x,y)e^{i\beta_{\mathrm{m}}(\omega)z-i\omega t} \\ \boldsymbol{\mathcal{H}}_m &\equiv \boldsymbol{\mathcal{H}}_m(\omega,x,y)e^{i\beta_{\mathrm{m}}(\omega)z-i\omega t}\end{aligned}\ . \tag{3.25}$$

We consider a non-magnetic medium ($\mu = \mu_0$) with a linear permittivity $\epsilon(\omega, x, y)$ that doesn't depend on the propagation coordinate z which coincides with what we consider forward and backward propagation direction. Note that the permittivity or, equivalently, the index of refraction may depend on the transverse coordinates x, y. That would be the case for example in a micro-structured waveguide, or in a hollow-core fiber or capillary; at this first stage, we want to treat bulk media and fiber-like geometries together. Later we will "branch" and derive separate, specialized equations for waveguides and for bulk media.

The starting point of our derivations is of course the Maxwell's equations:

$$\begin{aligned} \boldsymbol{j} + \partial_t \boldsymbol{P} + \epsilon_0 \partial_t \epsilon * \boldsymbol{E} &= \nabla \times \boldsymbol{H} \\ -\mu_0 \partial_t \boldsymbol{H} &= \nabla \times \boldsymbol{E} \end{aligned} \tag{3.26}$$

where the star represents a convolution so that the term is a short hand for

$$\epsilon_0 \partial_t \epsilon * \boldsymbol{E} = \epsilon_0 \partial_t \int_0^\infty \mathrm{d}\tau \epsilon(\tau) \boldsymbol{E}(t - \tau)$$

Here $\epsilon(\tau)$ is the temporal representation of frequency-dependent permittivity $\epsilon(\omega)$. The same notation will be used for both quantities, and their arguments will serve to distinguish them where needed.

As a first step, we scalar-multiply Maxwell's equations by complex conjugate modal fields

$$\begin{aligned} \boldsymbol{\mathcal{E}}_m^* . (\boldsymbol{j} + \partial_t \boldsymbol{P}) + \epsilon_0 \boldsymbol{\mathcal{E}}_m^* . \partial_t \epsilon * \boldsymbol{E} &= \boldsymbol{\mathcal{E}}_m^* . \nabla \times \boldsymbol{H} \\ -\mu_0 \boldsymbol{\mathcal{H}}_m^* . \partial_t \boldsymbol{H} &= \boldsymbol{\mathcal{H}}_m^* . \nabla \times \boldsymbol{E} \ . \end{aligned} \tag{3.27}$$

Using the formula $\boldsymbol{b}.(\nabla \times \boldsymbol{a}) = \nabla.(\boldsymbol{a} \times \boldsymbol{b}) + \boldsymbol{a}.(\nabla \times \boldsymbol{b})$, we transform both right-hand sides to obtain

$$\begin{aligned} \boldsymbol{\mathcal{E}}_m^* . (\boldsymbol{j} + \partial_t \boldsymbol{P}) + \epsilon_0 \boldsymbol{\mathcal{E}}_m^* . \partial_t \epsilon * \boldsymbol{E} &= \nabla . [\boldsymbol{H} \times \boldsymbol{\mathcal{E}}_m^*] + \boldsymbol{H} . [\nabla \times \boldsymbol{\mathcal{E}}_m^*] \\ -\mu_0 \boldsymbol{\mathcal{H}}_m^* . \partial_t \boldsymbol{H} &= \nabla . [\boldsymbol{E} \times \boldsymbol{\mathcal{H}}_m^*] + \boldsymbol{E} . [\nabla \times \boldsymbol{\mathcal{H}}_m^*] \ . \end{aligned} \tag{3.28}$$

Now we can take advantage of the fact the modal fields themselves satisfy the Maxwell's equations

$$\begin{aligned} \nabla \times \boldsymbol{\mathcal{E}}_m^* &= -\mu_0 \partial_t \boldsymbol{\mathcal{H}}_m^* \\ \nabla \times \boldsymbol{\mathcal{H}}_m^* &= \epsilon_0 \partial_t \epsilon * \boldsymbol{\mathcal{E}}_m^* \ , \end{aligned} \tag{3.29}$$

and therefore the previous equations can be written as

$$\begin{aligned} \boldsymbol{\mathcal{E}}_m^* . (\boldsymbol{j} + \partial_t \boldsymbol{P}) + \epsilon_0 \boldsymbol{\mathcal{E}}_m^* . \partial_t \epsilon * \boldsymbol{E} &= \nabla . [\boldsymbol{H} \times \boldsymbol{\mathcal{E}}_m^*] - \mu_0 \boldsymbol{H} . \partial_t \boldsymbol{\mathcal{H}}_m^* \\ -\mu_0 \boldsymbol{\mathcal{H}}_m^* . \partial_t \boldsymbol{H} &= \nabla . [\boldsymbol{E} \times \boldsymbol{\mathcal{H}}_m^*] + \epsilon_0 \boldsymbol{E} . \partial_t \epsilon * \boldsymbol{\mathcal{E}}_m^* \end{aligned} \tag{3.30}$$

Next, we subtract the two equations and collect terms that constitute full time derivatives

$$\boldsymbol{\mathcal{E}}_m^* . (\boldsymbol{j} + \partial_t \boldsymbol{P}) + \partial_t [\epsilon_0 \boldsymbol{\mathcal{E}}_m^* . \epsilon * \boldsymbol{E}] = \nabla . [\boldsymbol{H} \times \boldsymbol{\mathcal{E}}_m^*] - \partial_t [\mu_0 \boldsymbol{\mathcal{H}}_m^* . \boldsymbol{H}] - \nabla . [\boldsymbol{E} \times \boldsymbol{\mathcal{H}}_m^*] \ . \tag{3.31}$$

Now we integrate over the whole xyt domain. Note that all terms except the first and ∂_z, which is implicit in the $\nabla.$ operator, are derivatives that give rise to "surface terms" after integration over x, y, t. These surface terms are supposed to vanish far from the axis of the laser beam, as well as in past and future temporal infinities. Intuitively, admissible solutions include spatially and temporally localized pulse-like solutions, which we are interested in. As a consequence, the only surviving derivatives will be ∂_z:

$$\int \boldsymbol{\mathcal{E}}_m^* . (\boldsymbol{j} + \partial_t \boldsymbol{P}) \mathrm{d}x\mathrm{d}y\mathrm{d}t = \partial_z \int \boldsymbol{z} . [\boldsymbol{H} \times \boldsymbol{\mathcal{E}}_m^*] \mathrm{d}x\mathrm{d}y\mathrm{d}t - \partial_z \int \boldsymbol{z} . [\boldsymbol{E} \times \boldsymbol{\mathcal{H}}_m^*] \mathrm{d}x\mathrm{d}y\mathrm{d}t \tag{3.32}$$

Here and in what follows, t integrations are understood like this: $\int \mathrm{d}t \equiv \frac{1}{T}\int_{-T/2}^{+T/2}\mathrm{d}t$ where T is a large normalization "volume," and integrals over x, y are understood in a similar way. This will give us a convenient way to obtain the correct normalization and "translate" it into implementation which will be in terms of numerical Fourier transforms.
Because only transverse field components enter the above equation, we can use our modal expansion here (recall that those are only valid for transverse vector components):

$$\begin{gathered}\int \boldsymbol{\mathcal{E}}_m^*.(\boldsymbol{j}+\partial_t\boldsymbol{P})\mathrm{d}x\mathrm{d}y\mathrm{d}t = \\ \partial_z \int \boldsymbol{z}.[\textstyle\sum_{n,\Omega} A_n(\Omega,z)\boldsymbol{\mathcal{H}}_n(\Omega)\times\boldsymbol{\mathcal{E}}_m^*(\omega)]e^{i\beta_{\mathrm{n}}(\Omega)z-i\Omega t}e^{-i\beta_{\mathrm{m}}(\omega)z+i\omega t}\mathrm{d}x\mathrm{d}y\mathrm{d}t \\ -\partial_z \int \boldsymbol{z}.[\textstyle\sum_{n,\Omega} A_n(\Omega,z)\boldsymbol{\mathcal{E}}_n(\Omega)\times\boldsymbol{\mathcal{H}}_m^*(\omega)]e^{i\beta_{\mathrm{n}}(\Omega)z-i\Omega t}e^{-i\beta_{\mathrm{m}}(\omega)z+i\omega t}\mathrm{d}x\mathrm{d}y\mathrm{d}t\ .\end{gathered} \tag{3.33}$$

Integration over time gives a Kronecker delta between angular frequencies, $\delta_{\Omega\omega}$, which in turn reduces the sum over Ω:

$$\begin{gathered}\int \boldsymbol{\mathcal{E}}_m^*.(\boldsymbol{j}+\partial_t\boldsymbol{P})\mathrm{d}x\mathrm{d}y\mathrm{d}t = \\ \partial_z \int \boldsymbol{z}.[\textstyle\sum_{n} A_n(\omega,z)\boldsymbol{\mathcal{H}}_n(\omega,x,y)\times\boldsymbol{\mathcal{E}}_m^*(\omega,x,y)]e^{i\beta_{\mathrm{n}}(\omega)z}e^{-i\beta_{\mathrm{m}}(\omega)z}\mathrm{d}x\mathrm{d}y \\ -\partial_z \int \boldsymbol{z}.[\textstyle\sum_{n} A_n(\omega,z)\boldsymbol{\mathcal{E}}_n(\omega,x,y)\times\boldsymbol{\mathcal{H}}_m^*(\omega,x,y)]e^{i\beta_{\mathrm{n}}(\omega)z}e^{-i\beta_{\mathrm{m}}(\omega)z}\mathrm{d}x\mathrm{d}y\ .\end{gathered} \tag{3.34}$$

Collecting like terms results in an equation

$$\begin{gathered}\int \boldsymbol{\mathcal{E}}_m^*.(\boldsymbol{j}+\partial_t\boldsymbol{P})\mathrm{d}x\mathrm{d}y\mathrm{d}t = \partial_z \sum_n A_n(\omega,z)e^{i\beta_{\mathrm{n}}(\omega)z}e^{-i\beta_{\mathrm{m}}(\omega)z}\times \\ \int \boldsymbol{z}.[\boldsymbol{\mathcal{H}}_n(\omega,x,y)\times\boldsymbol{\mathcal{E}}_m^*(\omega,x,y)-\boldsymbol{\mathcal{E}}_n(\omega,x,y)\times\boldsymbol{\mathcal{H}}_m^*(\omega,x,y)]\mathrm{d}x\mathrm{d}y\ .\end{gathered} \tag{3.35}$$

At this point we are going to use a general property of electromagnetic modal fields which constitute an orthogonal basis: all radiative waveforms can be expressed as their linear combinations. To calculate such expansions, one can utilize the following orthogonality relation

$$\int \boldsymbol{z}.[\boldsymbol{\mathcal{E}}_m\times\boldsymbol{\mathcal{H}}_n^*-\boldsymbol{\mathcal{H}}_m\times\boldsymbol{\mathcal{E}}_n^*]\ \mathrm{d}x\mathrm{d}y = 2\delta_{m,n}N_m(\omega) \tag{3.36}$$

Here $N_m(\omega)$ is a normalization constant, whose explicit functional form has to be derived for each concrete set of modes.

Orthogonality of modes is used to reduce the sum over n in (3.35)

$$\int \boldsymbol{\mathcal{E}}_m^*.(\boldsymbol{j}+\partial_t\boldsymbol{P})\mathrm{d}x\mathrm{d}y\mathrm{d}t = -\partial_z \sum_n A_n(\omega,z)e^{i\beta_{\mathrm{n}}(\omega)z}e^{-i\beta_{\mathrm{m}}(\omega)z}2\delta_{m,n}N_m(\omega)\ , \tag{3.37}$$

and we finally obtain an evolution equation for our expansion coefficients:

$$\begin{aligned}\partial_z A_m(\omega,z) = -\frac{1}{2N_m(\omega)\ XYT}\int_{-T/2}^{+T/2}\mathrm{d}t\int_{-Y/2}^{+Y/2}\mathrm{d}y\int_{-X/2}^{+X/2}\mathrm{d}x\times \\ e^{-i\beta_m(\omega)z+i\omega t}\boldsymbol{\mathcal{E}}_m^*(\omega,x,y).[\boldsymbol{j}(x,y,t)+\partial_t\boldsymbol{P}(x,y,t)]\end{aligned} \tag{3.38}$$

This is the starting point for the z-propagated unidirectional equations. In the following sections, we will specialize this to the case of bulk media and then continue on with waveguides.

3.3.3 Z-propagated UPPE for homogeneous media: General case

In this section, Eq. (3.38) is specialized for the case of a homogeneous medium. This is done by inserting explicit expressions for a given family of modal fields.

In bulk media, field modes are plane waves, They can be labeled by transverse wavenumbers k_x, k_y, by a polarization index $s = 1, 2$, and by a $\pm$ sign signifying the direction of propagation along the z direction. So the index m, which we used to label modes in the preceding section, is actually a list:

$$m \equiv k_x, k_y, s, \pm \; . \tag{3.39}$$

The following notation will be used for the frequency- and wavenumber-dependent propagation constant of a plane wave characterized by its angular frequency ω:

$$\beta_{k_x,k_y,s,\pm}(\omega) \equiv k_z(\omega, k_x, k_y) = \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2} \; , \tag{3.40}$$

Electric and magnetic amplitudes in plane waves are mutually determined by the Maxwell's equations. We fix them as

$$\boldsymbol{\mathcal{E}}_{k_x,k_y,s,\pm} = \boldsymbol{e}_s \exp\left[ik_x x + ik_y y \pm ik_z(\omega, k_x, k_y)\right] \tag{3.41}$$

$$\boldsymbol{\mathcal{H}}_{k_x,k_y,s,\pm} = \frac{1}{\mu_0\omega}\boldsymbol{k} \times \boldsymbol{\mathcal{E}}_{k_x,k_y,\omega,s,\pm} \; . \tag{3.42}$$

We can choose one of the amplitudes (the electric one in this case) arbitrarily, and the choice will be naturally reflected in the modal normalization constants, but is otherwise inconsequential. The polarization of modal fields is determined by polarization vectors $\boldsymbol{e}_{s=1,2}$ which are of unit length and are normal to the wave-vector

$$\boldsymbol{k} = \{k_x, k_y, k_z \equiv \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2}\} \; . \tag{3.43}$$

Using the above formulas, it is straightforward to calculate the modal normalization constant

$$\begin{aligned} 2N_{k_x,k_y,s,\pm}(\omega) = \int \boldsymbol{z}.[\boldsymbol{\mathcal{E}}_m \times \boldsymbol{\mathcal{H}}_m^* - \boldsymbol{\mathcal{H}}_m \times \boldsymbol{\mathcal{E}}_m^*] \, \mathrm{d}x\mathrm{d}y = \\ 2\boldsymbol{z}.[\boldsymbol{e}_s \times (\boldsymbol{k} \times \boldsymbol{e}_s)]\frac{1}{\mu_0\omega} = \pm 2k_z(\omega, k_x, k_z)\frac{1}{\mu_0\omega} \end{aligned} \tag{3.44}$$

$$N_{k_x,k_y,s,\pm}(\omega) = \pm\frac{k_z(\omega, k_x, k_z)}{\mu_0\omega} \; . \tag{3.45}$$

Now we can insert expressions for modal fields and the corresponding normalization constant into coupled mode equation Eq. (3.38) to obtain

$$\begin{aligned} \partial_z A_{k_x,k_y,s,\pm}(\omega, z) = \mp\frac{\omega\mu_0}{2k_z}e^{\mp ik_z z}\int \frac{\mathrm{d}x\mathrm{d}y\mathrm{d}t}{L_x L_y T}e^{i(\omega t - k_x x - k_y y)} \times \\ \boldsymbol{e}_s.[\boldsymbol{j}(x, y, z, t) + \partial_t \boldsymbol{P}(x, y, z, t)] \end{aligned} \tag{3.46}$$

The above integral is nothing but a spatial and temporal Fourier transform, so one can write it down in the spectral domain as

$$\partial_z A_{k_x,k_y,s,+}(\omega, z) = \frac{\omega}{2\epsilon_0 c^2 k_z}e^{-ik_z z}\boldsymbol{e}_s.[i\omega\boldsymbol{P}_{k_x,k_y}(\omega, z) - \boldsymbol{j}_{k_x,k_y}(\omega, z)] \; . \tag{3.47}$$

This is the propagation equation that will actually be solved numerically because it is cast in terms of the slowest variables our propagation problem has. We can see that the only source of evolution in spectral amplitudes is nonlinearity.

For those who prefer to see evolution equations for electric fields proper, we express the above in terms of the electric field rather than in terms of modal expansion coefficients. From a modal expansion, the transverse part of the electric field is

$$\boldsymbol{E}^{\perp}_{k_x,k_y,+}(\omega,z) = \sum_{s=1,2} \boldsymbol{e}^{\perp}_{s} \boldsymbol{A}_{k_x,k_y,s,+}(\omega,z) e^{ik_z(k_x,k_y,\omega)z} \ , \tag{3.48}$$

and therefore its z derivative reads

$$\begin{aligned} \partial_z \boldsymbol{E}^{\perp}_{k_x,k_y,+}(\omega,z) = ik_z(k_x,k_y,\omega)\boldsymbol{E}^{\perp}_{k_x,k_y,+}(\omega,z) + \\ \sum_{s=1,2} \boldsymbol{e}^{\perp}_{s} \partial_z \boldsymbol{A}_{k_x,k_y,s,+}(\omega,z) e^{ik_z(k_x,k_y,\omega)z} \end{aligned} \tag{3.49}$$

Using Eq. (3.47), we obtain the full-vectorial UPPE for a homogeneous medium:

$$\begin{aligned} \partial_z \boldsymbol{E}^{\perp}_{k_x,k_y,+}(\omega,z) = +ik_z \boldsymbol{E}^{\perp}_{k_x,k_y,+}(\omega,z) + \\ \sum_{s=1,2} \boldsymbol{e}^{\perp}_{s} \boldsymbol{e}_{s} \cdot [\frac{i\omega^2}{2\epsilon_0 c^2 k_z} \boldsymbol{P}_{k_x,k_y}(\omega,z) - \frac{\omega}{2\epsilon_0 c^2 k_z} \boldsymbol{j}_{k_x,k_y}(\omega,z)] \end{aligned} \tag{3.50}$$

This is an exact system of equations that describes evolution of modal amplitudes along the z-axis for the forward propagating field. Of course, an analogous equation holds for the backward propagating component:

$$\begin{aligned} \partial_z \boldsymbol{E}^{\perp}_{k_x,k_y,-}(\omega,z) = -ik_z \boldsymbol{E}^{\perp}_{k_x,k_y,+}(\omega,z) - \\ \sum_{s=1,2} \boldsymbol{e}^{\perp}_{s} \boldsymbol{e}_{s} \cdot [\frac{i\omega^2}{2\epsilon_0 c^2 k_z} \boldsymbol{P}_{k_x,k_y}(\omega,z) - \frac{\omega}{2\epsilon_0 c^2 k_z} \boldsymbol{j}_{k_x,k_y}(\omega,z)] \end{aligned} \tag{3.51}$$

This pair of equation is exact and completely analogous to the pair of z-propagated equations discussed in the previous section. Because the nonlinear polarization in these equations results as a response to the *complete* electric field, they can't be used to calculate the forward field in isolation (i.e. without its backward propagating counterpart). The equation becomes unidirectional only when the following approximation can be adopted:

$$\boldsymbol{P}(\boldsymbol{E}), \boldsymbol{j}(\boldsymbol{E}) \rightarrow \boldsymbol{P}(\boldsymbol{E}_f), \boldsymbol{j}(\boldsymbol{E}_f) \tag{3.52}$$

In other words, to obtain a closed system *which is restricted to a single direction* and which can be solved numerically, we must require that nonlinear polarization can be calculated accurately from only the forward propagating field. This means that UPPE is only applicable when the back-reflected portion of the field is so small that its contribution to the nonlinearity can be neglected.

3.3.4 Z-propagated UPPE: Simplified, practical version

Eq. 3.50, with nonlinear polarization approximated by Eq. 3.52 can easily become a rather large system to solve numerically. This is especially true for experiments with wide-beam multi TW lasers. Fortunately, in most cases transverse dimensions of resulting structures remain relatively large in comparison to wavelength, and further approximations are possible. For example in

femtosecond filamentation in gases, the typical diameter of the filament core is about hundred micron which dimension is large in comparison with the laser wavelength. Consequently, the longitudinal vector component of the electric field is much smaller than the transverse (x, y) components, and can be neglected in calculation of the nonlinear medium response. It thus makes sense to take advantage of this fact to obtain a simpler equation.
Concretely, one can neglect the z components of the field and polarization vectors. In such a situation the sum over polarization vectors reduces approximately to unity

$$\sum_{s=1,2} \boldsymbol{e}_s^{\perp} \boldsymbol{e}_s \approx 1 \,. \tag{3.53}$$

To see this, it is enough to recall that the left-hand side constitutes a projector onto the wave-vector (recall that these vectors are mutually orthogonal). As the wave-vector is pointing in the direction almost parallel to the beam axis, it is also approximately a unity "operator" in the vector subspace spanned by x, y.

Replacing the transverse projection by unity, the full UPPE simplifies into an equation for transverse component(s)

$$\begin{aligned} \partial_z E_{k_x,k_y}(\omega, z) &= ik_z E_{k_x,k_y}(\omega, z) + \frac{i\omega^2}{2\epsilon_0 c^2 k_z} P_{k_x,k_y}(\omega, z) - \frac{\omega}{2\epsilon_0 c^2 k_z} j_{k_x,k_y}(\omega, z) \,, \\ k_z &= \sqrt{\omega^2 \epsilon(\omega)/c^2 - k_x^2 - k_y^2} \,. \end{aligned} \tag{3.54}$$

This is the most useful form for practical calculation, and is therefore called simply UPPE in the following. While we write it as a scalar equation, it should be understood that it is in general coupled to its counterpart governing the other polarization. The two polarization components of the electric field both contribute to the nonlinear polarization and this is how they become mutually coupled.

3.4 Other propagation models as approximations of UPPE

The previous section showed the the Unidirectional Pulse Propagation Equations can be rigorously derived under very general assumptions. They are based on a single approximation, an that is that nonlinear interaction between light and matter occurs in such a regime that the medium response to the field can be calculated with sufficient accuracy from only the forward-going field component. Because this is how *all* one-way pulse propagation equation include nonlinearity, one can expect that other types of equations can be derived from UPPE. We want to demonstrate this in what follows. We will in fact show a universal scheme to derive all other propagation models.

The first purpose of this section is to illustrate that what we have identified as the Maxwell reduction problem in Introduction, has been receiving a lot of attention in the literature for many years. Researchers proposed a number of various solutions and new results continue to appear in the literature.

The motivation for such research is obviously different in different research communities. The optics community is mostly interested in practical wave propagation solvers as tools to utilize in experimental and theoretic work. But there is also an applied mathematics community which studies these equations as weakly nonlinear systems, not necessarily restricted to the optical contexts. The goal is a rigorous analysis of resulting equations rather than their practical application. These divergent interests are, in our opinion, one of the reasons why the Maxwell reduction problem still enjoys attention of researchers.

The second purpose of the Section is to bring various derivations and different version of propagation equations "under one roof." We present a unifying view as a means to elucidate exactly what approximations went into original derivations. The reader might expect that assumptions behind an equation should be be clearly established, but it is actually not the case; derivations often suffer from lack of control over the neglected terms or effects. This is why we consider useful to discuss some successful propagation models along with a couple of examples when the results turn out to be "less than solid." This should give our reader "tools" to evaluate the plethora of propagation models scattered over the literature of last ten years.

3.4.1 General method to obtain pulse propagation models from UPPE

Several types of unidirectional propagation equation appear frequently in the literature on nonlinear optics. The most important examples are Non-Linear Schrödinger (NLS) equation [**?**], Nonlinear Envelope Equation [**?**] (NEE), the First-Order Propagation equation [**?**] (FOP), Forward Maxwell's equation [**?**] (FME), and several other equations that are closely related to these.

In this section, we explain a unified method which will be subsequently used to derive several of the light-pulse propagation equations. The main benefit of re-deriving known equations from a common starting point while using the same method, is that it allows us to compare physical assumptions and approximation underlying different equations. It also reveals relations between equations which may not be obvious either because of their apparently different form, or because of different methods used in the original derivations.

It is instructive to break the derivation procedure into several steps. As a first step, we adopt a scalar, one-component approximation and write the Unidirectional Pulse Propagation Equation in the following form:

$$\partial_z E_{k_x,k_y}(\omega,z) = iKE_{k_x,k_y}(\omega,z) + iQP_{k_x,k_y}(\omega,z) \tag{3.55}$$

where

$$K(k_x,k_y,\omega) = \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2} \tag{3.56}$$

is the linear field propagator in the spectral representation, and

$$Q(k_x, k_y, \omega) = \frac{\omega^2}{2\epsilon_0 c^2 \sqrt{\omega^2 \epsilon(\omega)/c^2 - k_x^2 - k_y^2}} \tag{3.57}$$

will be called nonlinear coupling term. In most cases, the concrete form of the nonlinear polarization P is unimportant, and we will assume that it can be specified in terms of an algorithm which accepts the electric field (in general as a function of time), at a given spatial location as its input.

Let us note that this one-component, or scalar representation can be still understood as a description of a single polarization in a coupled system describing two transverse vector components of an optical field. While each equation appears scalar, the two become coupled through the polarization term, for example due to the nonlinear birefringence. These coupling effects can play a role even if a laser beam is much wider than the light wavelength, and can lead to a rich polarization dynamics within femtosecond filaments. What *is* neglected at this step is the longitudinal part of the electric field. That only becomes important when the beam focuses to a size comparable with wavelength. However, in the naturally occurring filaments such extreme focusing is never achieved, because self-focusing collapse is always arrested either by chromatic dispersion or by the free-electron induced de-focusing. Thus, for many practical purposes, the above representation is sufficiently rich and accurate.

In the second derivation step, we replace couplings K and Q by suitable approximations. In most cases, they are closely related to Taylor expansions in frequency and in transverse wavenumbers. It is at this stage that artificial parameters are introduced into a propagation model (a typical example is the reference frequency). It is important to keep in mind that "knowledge" extracted from simulations should not depend on such degrees of freedom. In this respect, we aim to show that the improvements introduced into pulse evolution equations can be often viewed as corrections which (partially) restore the invariance of a model with respect to these free-will choices.

Having chosen our approximations for the linear and nonlinear coupling, we are still in the real-field representation. However, most of the published models are written using envelopes. Thus, in the next step, we obtain *envelope* equations. To do this, one can expresses 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 $k_\mathrm{R} = K(0, 0, \omega_\mathrm{R})$:

$$E(x, y, z, t) = \mathcal{A}(x, y, z, t) e^{i(k_\mathrm{R} z - \omega_\mathrm{R} t)} \tag{3.58}$$

A similar factorization is of course introduced for the nonlinear polarization $P(x, y, z, t)$ as well.

The final step consist in transforming the equation from the spectral- to the real-space representation. Mathematically, this is nothing but a Fourier transform, and the following standard replacement rules for differential operators provide quick and easy way to do this transformation:

$$(\omega - \omega_\mathrm{R}) \to i\partial_t \qquad ik_x \to \partial_x \qquad ik_y \to \partial_y \qquad \partial_z \to ik(\omega_\mathrm{R}) + \partial_z \tag{3.59}$$

Finally, in most cases we also transform to a frame moving with a suitable group velocity such that the pulse remains close to the center of the computational domain.

3.4.2 Derivation of Non-Linear Schrödinger Equation from UPPE

The Nonlinear Schrödinger Equation (NLS) is a prototype propagation equation ubiquitous in the nonlinear optics, and its importance can hardly be overstated. It is therefore only natural

to start our model discussions with this equation. It is also the simplest case to illustrate the derivation method outlined above, and an opportunity to point out some important issues which are also relevant in other pulse propagation models.

Following the general procedure, we replace the K and Q "coefficients" with their appropriate approximations. We denote by $k_{\mathrm{R}} = k(\omega_{\mathrm{R}})$ the reference wavenumber corresponding to an "arbitrarily" chosen reference frequency ω_{R}, and take

$$\begin{aligned} K(k_x, k_y, \omega) &= \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2} \\ &\approx k_{\mathrm{R}} + v_g^{-1}(\omega - \omega_{\mathrm{R}}) + \frac{k''}{2}(\omega - \omega_{\mathrm{R}})^2 - \frac{1}{2k_{\mathrm{R}}}(k_x^2 + k_y^2) \end{aligned} \tag{3.60}$$

This is a second-order Taylor expansion in $\omega - \omega_{\mathrm{R}}$ and in k_x, k_y. It should be noted that the parameter ω_{R} has nothing to do with the *solution* of the equation and in particular it does not need to be equal to the central frequency of the simulated optical pulse. In fact, below we give a very good reason why it *should not*, and why simulation runs obtained for different choices should be compared to asses their robustness. The point is that this is an example when an artificial parameter, originally absent from Maxwell's equations, makes its way into a theoretical model. Such a parameter must be regarded as a "gauge variable" from whose concrete choice all physical results must be independent. This is never the case, strictly speaking. In practice, we choose a value and this choice has a measurable effect on the numerical solution: this is a consequence of the equation not being strictly invariant. A blessing in disguise is that both the accuracy of the numerical solution, as well as the robustness of the propagation equation itself, can and *should be* "measured" in how big or small these unwanted parameter-dependencies are. Clearly, the NLS equation will be manifestly dependent of our choice for the reference frequency in the above approximation of K, and its solutions will inherit the same. In the next subsections, it will become evident that the so called correction terms introduced into the NLS equation can be actually viewed as corrections which eliminate at least partly the dependence of the equation on ω_{R}.

Now, let us return to our derivation. In the nonlinear coupling coefficient, we neglect all variable dependencies and replace it with its value at the reference frequency and zero transverse wavenumbers:

$$Q(k_x, k_y, \omega) = \frac{\omega^2}{2\epsilon_0 c^2\sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2}} \approx \frac{\omega_{\mathrm{R}}}{2\epsilon_0 n(\omega_{\mathrm{R}})c} \tag{3.61}$$

In the context of the Nonlinear Schrödinger Equation, the nonlinear polarization term only accounts for the instantaneous optical Kerr effect. The polarization envelope is usually expressed in terms of the light intensity I and of the field-envelope A:

$$\mathcal{P} = 2\epsilon_0 n(\omega_{\mathrm{R}}) n_2 I \mathcal{A} \tag{3.62}$$

Inserting this into (3.55,3.58) we obtain

$$\partial_z \mathcal{A} = +iv_g^{-1}(\omega - \omega_{\mathrm{R}})\mathcal{A} \; + \frac{ik''}{2}(\omega - \omega_{\mathrm{R}})^2\mathcal{A} - \frac{i}{2k_{\mathrm{R}}}(k_x^2 + k_y^2)\mathcal{A} + \frac{i\omega_{\mathrm{R}}}{c} n_2 I \mathcal{A} \tag{3.63}$$

The NLS is usually written in units suitable for the given geometry, be it a fiber or a bulk medium. In the latter, it is customary to normalize the envelope amplitude such that $|\mathcal{A}|^2 = I$. Using rules (3.59) we finally obtain the NLS equation:

$$(\partial_z + v_g^{-1}\partial_t)\mathcal{A} = \frac{i}{2k_{\mathrm{R}}}\Delta_\perp \mathcal{A} - \frac{ik''}{2}\partial_{tt}\mathcal{A} + \frac{i\omega_{\mathrm{R}}}{c} n_2 |\mathcal{A}|^2 \mathcal{A} \tag{3.64}$$

The above derivation shows explicitly what approximations need to be adopted to obtain NLS: Approximating K to second order in frequency and transverse wavenumber amounts to the paraxial, and quasi-monochromatic approximations for the linear wave propagation. The approximation in the nonlinear coupling Q also requires a narrow spectrum in order to be able to represent Q by a constant.

Despite the underlying assumption of a narrow spectrum, NLS is in practice often pushed into a regime with significant spectral broadening. This immediately invites a question: which portion of the simulated spectrum can be correct?

One characteristic feature of NLS and of other envelope equations is the reference frequency. It is usually chosen equal to the central frequency of the initial pulse, and beginner's implementations often hard-code this particular choice in the program. This is not necessary, and not even a good practice. It is useful to keep in mind that ω_R is a free parameter, and as such it provides an opportunity to test the robustness of obtained simulation results. Comparative runs with small variations in reference frequency will readily reveal which parts of simulated spectra "react" to these changes - these are artifacts and only the stable, robust portions of the solution can be accepted. This is naturally applicable to any pulse propagation model that contains artificial parameters not present in the original Maxwell's equations.

3.4.3 Nonlinear Envelope Equation

Nonlinear Envelope Equation [**?**] is a paraxial equation with some additional approximations related to chromatic dispersion.

Once again, we follow the general procedure and approximate the linear propagator by its paraxial version:

$$K(k_x, k_y, \omega) = \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2} \approx +k(\omega) - \frac{c}{2\omega n_b(\omega_\mathrm{R})}(k_x^2 + k_y^2) \tag{3.65}$$

This is the second-order (paraxial) Taylor expansion in transverse wavenumbers with an additional approximation. Namely, we replaced $n_b(\omega) \to n_b(\omega_\mathrm{R})$ in the denominator of the diffraction term, and thus partly neglected chromatic dispersion.

Further, the first term in the above approximation, which is an exact propagation constant for a plane wave propagating along the z axis, is re-expressed as a sum of its two lowest-order Taylor expansion terms plus the rest:

$$k(\omega) = k(\omega_\mathrm{R}) + v_g^{-1}(\omega - \omega_\mathrm{R}) + D(\omega - \omega_\mathrm{R}) \tag{3.66}$$

where

$$D(\omega - \omega_\mathrm{R}) = \sum_{n=2}^{\infty} \left(\frac{\partial^n k}{\partial \omega^n}\right)_{\omega=\omega_\mathrm{R}} \frac{(\omega - \omega_\mathrm{R})^n}{n!} \tag{3.67}$$

This is formally exact and can be practically implemented in the spectral domain without further approximations, but sometimes a finite number of series expansion terms is used to fit the linear chromatic dispersion of a medium or of a waveguide.

Next, we approximate the nonlinear coupling term. Unlike in NLS, we preserve the frequency dependence exactly, but neglect the transverse wave-number dependence:

$$Q(k_x, k_y, \omega) \equiv \frac{\omega^2}{2\epsilon_0 c^2 \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2}} \approx \frac{(\omega - \omega_\mathrm{R}) + \omega_\mathrm{R}}{2\epsilon_0 c n(\omega_\mathrm{R})} \tag{3.68}$$

Here, as in the free propagation term, we neglect the chromatic dispersion of the background index of refraction.

After inserting the above approximations for K and Q into the original UPPE, we obtain

$$\begin{aligned}\partial_z \mathcal{A} = & iv_g^{-1}(\omega-\omega_{\mathrm{R}})\mathcal{A} + iD(\omega-\omega_{\mathrm{R}})\mathcal{A} \\ & - \frac{ic}{2\omega_{\mathrm{R}} n(\omega_{\mathrm{R}})}(1+\frac{\omega-\omega_{\mathrm{R}}}{\omega_{\mathrm{R}}})^{-1}(k_x^2+k_y^2)\mathcal{A} \\ & + \frac{i\omega_{\mathrm{R}}}{2\epsilon_0 cn(\omega_{\mathrm{R}})}(1+\frac{\omega-\omega_{\mathrm{R}}}{\omega_{\mathrm{R}}})\mathcal{P}\end{aligned} \tag{3.69}$$

Finally, transforming into the real-space representation, we arrive at NEE

$$\partial_z \mathcal{A} + v_g^{-1}\partial_t \mathcal{A} = iD(i\partial_t)\mathcal{A} + \frac{i}{2k_{\mathrm{R}}}(1+\frac{i}{\omega_{\mathrm{R}}}\partial_t)^{-1}\Delta_\perp \mathcal{A} + \frac{ik_{\mathrm{R}}}{2\epsilon_0 n_b^2(\omega_{\mathrm{R}})}(1+\frac{i}{\omega_{\mathrm{R}}}\partial_t)\mathcal{P} \tag{3.70}$$

Thus, approximations underlying the NEE are 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 spatio-temporal correction term and in the nonlinear coupling term. Note that the latter approximations are usually not serious at all.

An important point is that NEE should not be implemented in the form it was originally introduced. Handling higher order time derivatives any other way than spectral would necessarily cause additional numerical dispersion which may spoil linear propagation properties. However, if implemented in a spectral representation, NEE transforms into another propagation model discussed latter in these notes. Readers should be aware that authors in the literature sometimes claim to use NEE even if, in the above sense, they are not.

As in all envelope equations a reference frequency and a reference wave-number appear in the NEE. They are normally chosen equal to the central frequency and wave-number of the input pulse. But as we pointed out in connection to NLS, one has to keep in mind that these quantities are artificial and arbitrary "gauge" parameters which do not appear in the Maxwell's equations. Consequently, numerical solutions should not depend on how the reference is chosen. In other words a propagation equations should be "reference-frequency-invariant." While NLS is manifestly dependent on the reference choice, NEE is nearly invariant although ω_{R} appears in it several times. To appreciate this consider the spatio-temporal focusing correction term (operator) $\omega_{\mathrm{R}}^{-1}(1+\frac{1}{\omega_{\mathrm{R}}}\partial_t)^{-1}$ It seems to depend on the reference ω_{R}, but it is in fact proportional to ω^{-1} as long as it is implemented in the spectral domain which allows to include all orders of the series expansion. Note that this (approximate) invariance is only achieved in the infinite order, and can be properly implemented only in the spectral representation. Truncating operators at a finite order of series expansion breaks the invariance and causes undesirable artifacts. We illustrate this point in the following example.

3.4.4 Partially corrected NLS

The Partially Corrected NLS (PC-NLS) equation can be viewed as a "simplification" of NEE. It is derived from the UPPE in the same way, with one additional step. Namely, the following first order series expansion is applied in the correction term of the free propagator in Eqn.(3.69):

$$(1+\frac{\omega-\omega_{\mathrm{R}}}{\omega_{\mathrm{R}}})^{-1} \approx (1-\frac{\omega-\omega_{\mathrm{R}}}{\omega_{\mathrm{R}}}) \tag{3.71}$$

This step is meant to make it easy to implement a numerical solver in the real space, as it results in the equation that only contains "simple" differential operators in the real-space representation:

$$\partial_z \mathcal{A} + v_g^{-1}\partial_t \mathcal{A} = iD(i\partial_t)\mathcal{A} + \frac{i}{2k_{\mathrm{R}}}(1-\frac{i}{\omega_{\mathrm{R}}}\partial_t)\Delta_\perp \mathcal{A} + \frac{ik_{\mathrm{R}}}{2\epsilon_0 n_b^2(\omega_{\mathrm{R}})}(1+\frac{i}{\omega_{\mathrm{R}}}\partial_t)\mathcal{P} \tag{3.72}$$

While it may seem that the Partially Corrected NLS is essentially NEE with a "little more" approximation, this equation is not to be recommended. Because of the arbitrary truncation of an infinite series, the dispersion properties of the linear part of this equation are unphysical. While the PC-NLS provides better-than-NLS approximation around the reference frequency ω_{R}, its dispersion properties become rather pathological around $\omega \approx 2\omega_{\mathrm{R}}$ where its diffraction term changes sign as a consequence of the truncated correction factor. Artifacts in the angular distribution of the spectrum can be observed at high frequencies beyond $\omega \approx 2\omega_{\mathrm{R}}$. Consequently, this equation is only applicable in the same regime as the NLS, namely when the spectrum of the pulse remains relatively narrow.

3.4.5 First-order propagation equation

The previous three examples represented field envelope propagation equations. Next we discuss a non-envelope, First-Order Propagation equation (FOP), introduced by Geissler et al. [**?**]. Though it resolves the carrier wave, this equation is equivalent to NEE from the point of view of the approximations required for its derivation as we shall see shortly. Following the original authors, we neglect linear chromatic dispersion in order to obtain the same equation as Geissler et al.

In Eqn.(3.54) , we approximate

$$K(k_x, k_y, \omega) \equiv \sqrt{\omega^2/c^2 - k_x^2 - k_y^2} \approx \frac{\omega}{c} - \frac{c}{2\omega}(k_x^2 + k_y^2) \tag{3.73}$$

Note that the corresponding approximation made in NEE reduces to the present case if there is no linear chromatic dispersion (vacuum).

Similarly,

$$Q(k_x, k_y, \omega) \equiv \frac{\omega^2}{2\epsilon_0 c^2 \sqrt{\omega^2/c^2 - k_x^2 - k_y^2}} \approx \frac{\omega}{2\epsilon_0 c} \tag{3.74}$$

is the same approximation as the one in NEE only with vacuum in the role of the linear medium.

Thus, the propagation equation obtained with these expressions is

$$\partial_z E_{k_x,k_y,\omega} = \frac{i\omega}{c} E_{k_x,k_y,\omega} - \frac{ic}{2\omega}(k_x^2 + k_y^2) E_{k_x,k_y,\omega} + \frac{i\omega}{2\epsilon_0 c} P_{k_x,k_y,\omega} \tag{3.75}$$

which is equivalent to Eqn. (2) of Ref. [**?**].

When transforming into the real-space domain, ω^{-1} gives rise to an integral over time, and we arrive at the FOP equation

$$(\partial_z + \frac{1}{c}\partial_t) E(r_\perp, t) = \frac{c}{2}\Delta_\perp \int_{-\infty}^{t} d\tau E(r_\perp, \tau) - \frac{1}{2\epsilon_0 c}\partial_t P(r_\perp, t) \tag{3.76}$$

Comparing the derivation steps for NEE and FOP it becomes clear that despite of rather different ways they were originally derived, these two equations become equivalent in a non-dispersive medium.

3.4.6 Forward Maxwell Equation

Another non-envelope equation free of any reference frequency is the Forward Maxwell Equation, introduced by Husakou and Herrmann [**?**]. Although it was written in a vector form, it was derived from the wave equation with a neglected $\nabla\nabla.\boldsymbol{E}$ term. That is why vector nature of light is not captured completely correctly. The result is a "two-component" equation rather than a true

vectorial one. The polarization scrambling terms only come from the nonlinear polarization term in the equation. One can therefore derive the equation component-by-component in the same way as previous propagation equations.

The linear propagator and the nonlinear coupling approximations are similar to those used for NEE:

$$K(k_x, k_y, \omega) = \sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2} \approx k(\omega) - \frac{c}{2\omega n_b(\omega)}(k_x^2 + k_y^2) \tag{3.77}$$

and

$$Q(k_x, k_y, \omega) \equiv \frac{\omega^2}{2\epsilon_0 c^2\sqrt{\omega^2\epsilon(\omega)/c^2 - k_x^2 - k_y^2}} \approx \frac{\omega}{2\epsilon_0 c n_b(\omega)} \tag{3.78}$$

The only difference from NEE is that here chromatic dispersion of the index of refraction is correctly preserved.

The resulting equation is then obtained by transforming to the real space in transverse coordinates only, keeping the spectral frequency-time representation:

$$\partial_z E(x, y, \omega, z) = ik(\omega)E(x, y, \omega, z) + \frac{i}{2k(\omega)}\Delta_\perp E(x, y, \omega, z) + \frac{i\mu_0\omega c}{2n_b(\omega)}P(x, y, \omega, z) \tag{3.79}$$

This equation is equivalent to FME Eqn.(2) of Ref. [**?**]. A small difference is that we have not transformed the equation to the coordinate frame moving with the vacuum light velocity. The reason is that in a strongly dispersive medium it is necessary to use the frame that moves with a suitable *group* velocity.

Formulas (3.78) and (3.65,3.68) show that there is very little difference between FME and NEE. Because of the operator series expansion, the only acceptable way to solve NEE is in the spectral domain. But there, the correct frequency dependence of the background index of refraction can be easily taken into account - but that is when NEE becomes FME.

3.4.7 Maxwell's equations versus Wave equation in pulse-propagation

This subsection is devoted to the relation between the Unidirectional Pulse Propagation Equations and the wave equation. Naively, one may think that because the wave equation follows directly from the Maxwell's equations, we should be able to derive from it all pulse evolution. Several previously published results discussed in previous subsections were obtained just like that. One motivation for what follows is to demonstrate that such an approach has an inherent problem, and that is the fact that a *one-way equation must not be equivalent to the wave equation!* To start, we recall that the total field is a sum of left- and right-propagating components:

$$E(\boldsymbol{r}, t, z) = E^+(\boldsymbol{r}, t, z) + E^-(\boldsymbol{r}, t, z) \tag{3.80}$$

where each is expressed through Fourier amplitudes in transverse space ($\boldsymbol{r}$) and time:

$$E^+(\boldsymbol{r}, t, z) = \int \hat{E}^+(\boldsymbol{k}, \omega, z)e^{-i\omega t + i\boldsymbol{k}.r}dk^2 d\omega \quad E^-(\boldsymbol{r}, t, z) = \int \hat{E}^-(\boldsymbol{k}, \omega, z)e^{-i\omega t + i\boldsymbol{k}.r}dk^2 d\omega \tag{3.81}$$

The following is the *total nonlinear* polarization. Its functional dependence on the electric field is irrelevant for now; it may include the optical Kerr effect (i.e. self-focusing), the defocusing induced by free electron, the nonlinear losses due to multiphoton and avalanche ionization, and other effects...

$$P(\boldsymbol{r}, t, z) = \int \hat{P}(\boldsymbol{k}, \omega, z)e^{-i\omega t + i\boldsymbol{k}.r}dk^2 d\omega \tag{3.82}$$

(We assume that the linear portion of polarization has been included in the mediums frequency-dependent permittivity $\epsilon(\omega)$, and therefore it does not appear explicitly in our equations.) The nonlinear polarization serves as a source for one-way propagating fields:

$$\partial_z \hat{E}^+(\boldsymbol{k},\omega,z) = +ik_z(\omega,k)\hat{E}^+(\boldsymbol{k},\omega,z) + \frac{i\omega^2}{2\epsilon_0 c^2 k_z(\omega,k)}\hat{P}(\boldsymbol{k},\omega,z) \tag{3.83}$$

$$\partial_z \hat{E}^-(\boldsymbol{k},\omega,z) = -ik_z(\omega,k)\hat{E}^-(\boldsymbol{k},\omega,z) - \frac{i\omega^2}{2\epsilon_0 c^2 k_z(\omega,k)}\hat{P}(\boldsymbol{k},\omega,z) \tag{3.84}$$

where $k_z(\omega,k) = \sqrt{\frac{\omega^2\epsilon(\omega)}{c^2} - k^2}$ is a short-hand for the plan-wave propagation constant.

It is shown next that the unidirectional propagation equations give *together* a total field which satisfies the wave equation, while the single forward (or backward) propagating component does not. First, let us evaluate the ∂_{zz} term in two ∂_z steps:

$$\partial_z E^+(\boldsymbol{r},t,z) = \int \partial_z \hat{E}^+(\boldsymbol{k},\omega,z) e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega \tag{3.85}$$

after using the propagation equation to express the z-derivative in the spectral representation one gets

$$\partial_z E^+(\boldsymbol{r},t,z) = \int \left[+ik_z(\omega,k)\hat{E}^+(\boldsymbol{k},\omega,z) + \frac{i\omega^2}{2\epsilon_0 c^2 k_z(\omega,k)}\hat{P}(\boldsymbol{k},\omega,z) \right] e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega \tag{3.86}$$

Add to this its backward-going counterpart to get the derivative of the total field. Note that the polarization terms cancel each other, and a forward-backward field difference appears:

$$\begin{aligned} \partial_z E(\boldsymbol{r},t,z) &= \partial_z (E^+(\boldsymbol{r},t,z) + E^-(\boldsymbol{r},t,z)) = \\ &= \int \left[+ik_z(\omega,k)(\hat{E}^+(\boldsymbol{k},\omega,z) - \hat{E}^-(\boldsymbol{k},\omega,z)) \right] e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega \end{aligned} \tag{3.87}$$

From here, we take the second z-derivative to obtain:

$$\partial_{zz} E(\boldsymbol{r},t,z) = \int \left[+ik_z(\omega,k)(\partial_z \hat{E}^+(\boldsymbol{k},\omega,z) - \partial_z \hat{E}^-(\boldsymbol{k},\omega,z)) \right] e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega \tag{3.88}$$

which, after using the propagation equations once again, and grouping into terms of total field and polarization, yields:

$$\partial_{zz} E(\boldsymbol{r},t,z) = \int \left[-k_z(\omega,k)^2 \hat{E}(\boldsymbol{k},\omega,z) - \frac{\omega^2}{\epsilon_0 c^2}\hat{P}(\boldsymbol{k},\omega,z) \right] e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega \tag{3.89}$$

Having evaluated the ∂_{zz} term, we continue on with the remaining, transverse part of the Laplacian:

$$(\partial_{xx} + \partial_{yy}) E(\boldsymbol{r},t,z) = \int -(k_x^2 + k_y^2)\hat{E}(\boldsymbol{k},\omega,z) e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega \tag{3.90}$$

The remaining piece of the wave equation is the temporal derivative, which is also written in the spectral domain:

$$\partial_{tt}\epsilon * E(\boldsymbol{r},t,z) = \int -\omega^2 \epsilon(\omega)\hat{E}(\boldsymbol{k},\omega,z) e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega \tag{3.91}$$

Now, put everything together to form left-hand side of a wave equation. In the process, terms corresponding to the linear propagation cancel out, and only the nonlinear polarization survives:

$$(\partial_{zz} + \partial_{xx} + \partial_{yy})E(\boldsymbol{r}, t, z) - 1/c^2 \partial_{tt} \epsilon * E(\boldsymbol{r}, t, z) = \int \frac{-\omega^2}{\epsilon_0 c^2} \hat{P}(\boldsymbol{k}, \omega, z) e^{-i\omega t + i\boldsymbol{k}.r} dk^2 d\omega = \frac{1}{\epsilon_0 c^2} \partial_{tt} P(\boldsymbol{r}, t, z) \tag{3.92}$$

On the right-hand side of the above equation, we find exactly what there should be, namely the second temporal derivative of the polarization. We have shown that the sum of the forward and backward solutions to the UPPE obeys the wave equation. Importantly, it is also evident that each of the one-way fields alone does not. This observation explains the difficulties encountered in derivation of previous pulse propagation equations which started from the wave equation, and worked with a single amplitude representing the one-directional field. A prime example is the Nonlinear Envelope Equation which was obtained for the price of more or less arbitrary neglecting a number of undesirable terms. Now we can see that this was a consequence of an attempt to satisfy, with a single envelope solutions, an equation which in fact must not be satisfied...