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Hamiltonian structure of propagation equations for ultrashort optical pulses

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Abstract

A Hamiltonian framework is developed for a sequence of ultrashort optical pulses propagating in a nonlinear dispersive medium. To this end a second-order nonlinear wave equation is first simplified using an unidirectional approximation. All non-resonant nonlinear terms are then rigorously eliminated using a suitable change of variables in the spirit of the canonical perturbation theory. The derived propagation equation operates with a properly defined complexification of the real electric field. It accounts for arbitrary dispersion, four-wave mixing processes, weak absorption, and arbitrary pulse duration. Thereafter the so called normal variables, i.e., classical fields corresponding to the quantum creation and annihilation operators, are introduced. Neglecting absorption we finally derive the Hamiltonian formulation. The latter yields the most essential integrals of motion for the pulse propagation. These integrals reflect the time-averaged fluxes of energy, momentum, and classical photon number transferred by the pulse. The conservation laws are further used to control the numerical solutions when calculating supercontinuum generation by an ultrashort optical pulse.

1 Introduction

An evolution of the wave packet is accurately described in terms of a complex envelope [1]. The latter results from the time-scales separation, e.g., when the pulse contains many field cycles. A slowly-varying envelope approximation (SVEA) reduces then the second-order wave equation for the pulse electric filed to a more simple first-order nonlinear Schrödinger equation (NSE) for the pulse envelope [2, 3, 4]. In the frequency domain, the SVEA assumes that the pulse spectrum is narrow, centered around a carrier frequency. On the other hand, situations for which the SVEA lacks precision are also quite common. For instance, we mention self-focusing [5, 6], optical shocks [7], steep pulse edge [8], and supercontinuum (SC) generation [9]. An important example is that of a few-cycle or a sub-cycle optical pulse where the spectrum width is comparable to the carrier frequency [10, 11, 12, 13, 14, 15]. In all such situations the NSE cannot be applied and either a full modeling of Maxwell equations should be undertaken [16, 17, 18, 19, 20, 21, 22, 23] or new effective models for propagation of spectrally broad pulses should be introduced. These models can be developed in different directions.

First, we mention a higher-order NSE which is a direct generalization of the standard NSE. Here, an arbitrary dispersion profile is approximated by a higher-order Taylor

expansion or, more generally, by a polynomial fit in the frequency domain. The dispersion is then accounted for by a differential dispersion operator in the time domain [2, 4]. The nonlinear term in the higher-order NSE is further extended to capture an arbitrary pulse duration [24, 8, 25]. Furthermore, incorporation of Raman scattering [26, 27], diffraction effect [24, 28, 29], and third harmonic generation [30] have been discussed. The higher-order NSE applies to pulse propagation, optical shocks, and SC generation [31, 32, 33, 34, 35, 36, 37, 9, 38]. However, one should note that the dispersion profile for a very broad spectrum a priory cannot be captured by a polynomial expansion [39]. To avoid this problem both a rational approximation to the dispersion function and a nonlocal generalization of the NSE should be used [40].

The second approach to the ultrashort optical pulses is to abandon the envelope concept and to operate directly with the pulse fields. The simplified model equations are derived assuming an unidirectional character of pulse propagation instead of SVEA. A recent review is given in Ref. [41]. In addition, we mention a short pulse equation in which the dispersion function is expanded with respect to the inverse frequency [42, 43] and a more general approach with the Laurent series [44, 45, 46, 47]. Another important class of equations is given by the (mixed) modified Korteweg-de Vries and sine-Gordon models [48, 49, 50, 51, 52, 53].

As a rule, such unidirectional propagation equations in the space-time domain ignore absorption and use a simplified medium response function. In return, the deduced models often allow for an exact treatment [54, 55, 56, 57] or at least for an explicit solitary solution [41, 58, 59, 60, 61, 62, 63, 64]. Also many specific solutions to the higher-order NSE can be found [65, 66, 67, 68, 33, 69, 70, 71, 72, 73, 74, 75, 76, 77].

The third approach is to consider pulse propagation in the spectral domain [78, 79, 80, 22]. Here, again using the unidirectional approximation, one obtains a set of the first-order ordinary differential equations for the field harmonics $E_\omega(z)$. The deduced models are more simple than the full second-order propagation equation and still allow for arbitrary dispersion and spectrum width.

This paper puts emphasis on the improvement of the third class of models. For the basic model introduced in Ref. [78] we demonstrate that the nonlinear terms can to a large extent be removed by a suitable change of variables. This procedure is common in Hamiltonian mechanics [81] and is also useful for nonlinear waves [82]. In our case, the real electric field $E(z,t)$ has to be replaced with a complex one $\mathcal{E}(z,t)$ containing only positive harmonics. The remaining resonant nonlinear terms have a simple "envelope" structure without use of the SVEA. A z-propagated Hamiltonian framework is then introduced for the derived equation in terms of normal variables $\mathcal{A}(z,t)$ and $\mathcal{A}^*(z,t)$. The latter are classical complex fields, they correspond to the quantum creation and annihilation operators. In particular, $|\mathcal{A}_\omega|^2$ is the classical number of photons transferred by the pulse. By construction, the Hamiltonian is an integral of motion. The continuous symmetries of the Hamiltonian yield two more integrals. Physically the integrals are given by the time-averaged fluxes of the relevant physical quantities. They give an effective tool to follow the solution, e.g.,

for the SC generation scenarios.

2 Derivation

2.1 Basic equations

A formulation of the problem and notations are described in this section. We consider a sequence of linearly polarized electromagnetic pulses propagating along the z-axis in a bulk dispersive nonlinear medium. The fields $\mathbf{E} = (E(z,t), 0, 0)$ and $\mathbf{B} = (0, B(z,t), 0)$ are governed by Maxwell equations

$$\partial_z E = -\partial_t B, \qquad -\frac{1}{\mu_0}\partial_z B = \partial_t(\epsilon_0 E + P). \tag{1}$$

The induced medium polarization $\mathbf{P} = (P(z,t), 0, 0)$ depends on $E(z,t)$ and is determined by a sequence of nonlocal susceptibility operators $\hat{\chi}^{(i)}$ such that

$$P(E) = \epsilon_0 \left(\hat{\chi}^{(1)}E + \hat{\chi}^{(2)}EE + \hat{\chi}^{(3)}EEE + \cdots\right), \tag{2}$$

where $\hat{\chi}^{(1)}$ is a linear operator, $\hat{\chi}^{(2)}$ is a bilinear one and so on. The power expansion (2) assumes that pulses are propagating in *a weakly nonlinear limit*. In addition, an inverse symmetry is assumed such that $P(-E) = -P(E)$ and $\hat{\chi}^{(2)} = 0$. Equations (1)–(2) are reduced to a scalar nonlinear wave equation

$$\partial_z^2 E - \frac{1}{c^2}\partial_t^2 \left(E + \hat{\chi}^{(1)}E + \hat{\chi}^{(3)}EEE\right) = 0 \tag{3}$$

in which only linear and cubic terms are taken into account. To quantify $\hat{\chi}^{(i)}$ we write $E(z,t)$ in the frequency domain

$$E(z,t) = \sum_{\omega} E_\omega(z) e^{-i\omega t} \qquad \text{with} \qquad \omega \in \frac{2\pi}{T}\mathbb{Z},$$

where T is the period of the pulse sequence and

$$E_\omega(z) = \frac{1}{T}\int_{-T/2}^{+T/2} E(z,t)e^{i\omega t}dt = E^*_{-\omega}(z).$$

Integrating Eq. (3) over one period we obtain

$$\partial_z^2 \int_{-T/2}^{+T/2} E(z,t)dt = 0, \qquad \int_{-T/2}^{+T/2} E(z,t)dt = \text{const},$$

so that the "pulse area" is conserved. We assume that this area is zero, $E_{\omega=0} = 0$. In the continuous spectrum limit ($T \to \infty$) this implies

$$E_\omega \to 0 \qquad \text{for} \qquad \omega \to 0, \tag{4}$$

so that the constant component of electric field vanishes.

The operators $\hat{\chi}^{(1)}$ and $\hat{\chi}^{(3)}$ are given by convolutions

$$\left(\hat{\chi}^{(1)}E\right)_\omega = \chi^{(1)}(\omega)E_\omega,$$
$$\left(\hat{\chi}^{(3)}EEE\right)_\omega = \sum_{\omega_1+\omega_2+\omega_3=\omega} \chi^{(3)}_{\omega_1\omega_2\omega_3\omega}E_{\omega_1}E_{\omega_2}E_{\omega_3},$$

where in the last equation the summation is performed only over the suitable triads $\{\omega_1, \omega_2, \omega_3\}$. The linear susceptibility $\chi^{(1)}(\omega)$ yields the dielectric constant and the propagation parameter

$$\epsilon(\omega) = 1 + \chi^{(1)}(\omega) = \epsilon^*(-\omega),$$
$$k(\omega) = \frac{\omega}{c}\sqrt{\epsilon(\omega)} = \beta(\omega) + i\alpha(\omega) = -k^*(-\omega),$$

where $\beta(\omega)$ and $\alpha(\omega)$ are odd and even functions respectively. In the following we consider *a small absorption limit* such that $|\beta(\omega)| \gg \alpha(\omega) \geq 0$ in a transparency window to which belongs an essential part of the pulse spectrum.

If the nonlinear dispersion can be ignored one is left with the cubic Kerr medium in which

$$\chi^{(3)}_{\omega_1\omega_2\omega_3\omega} = \chi \qquad \text{and} \qquad \left(\hat{\chi}^{(3)}EEE\right)_{\text{Kerr}} = \chi E^3. \tag{5}$$

However, for a spectrally broad pulse such an approximation may be invalid and a more general model should be used. For instance, considering a classical nonlinear oscillator model for electrons, one obtains (Miller's rule, see Ref. [4])

$$\chi^{(3)}_{\omega_1\omega_2\omega_3\omega} = \text{const} \cdot \chi^{(1)}(\omega_1)\chi^{(1)}(\omega_2)\chi^{(1)}(\omega_3)\chi^{(1)}(\omega).$$

In the following we deal with the general nonlinear susceptibility $\chi^{(3)}_{\omega_1\omega_2\omega_3\omega}$ only assuming that it is symmetric with respect to all permutations of frequencies as suggested by Miller's rule. The nonlinear absorption is ignored, i.e., $\chi^{(3)}_{\omega_1\omega_2\omega_3\omega}$ is real and an even function of frequencies. The Kerr model (5) is used as an illustration in the numerical section.

To proceed we write the nonlinear wave equation (3) in the frequency domain

$$\partial_z^2 E_\omega + [\beta(\omega) + i\alpha(\omega)]^2 E_\omega + \frac{\omega^2}{c^2}\left(\hat{\chi}^{(3)}EEE\right)_\omega = 0. \tag{6}$$

Equation (6) is the starting point of our considerations. In the next sections it is simplified using an unidirectional approximation, introducing a proper complex electric field, and eliminating non-resonant terms. Then the Hamiltonian framework and integrals of motion are introduced and interpreted for the resulting model.

2.2 Unidirectional approximation

As explained in the previous section both the nonlinear and the absorption terms in Eq. (6) are taken small. An unidirectional approximation results from this assumption. In a first step, completely neglecting the both small terms in Eq. (6),

we see that $E_\omega(z) \sim e^{\pm i\beta(\omega)z}$ for the forward and the backward waves respectively. Assuming that the forward wave dominates we can write

$$[i\partial_z + \beta(\omega)]E_\omega(z) \approx 0, \tag{7}$$

where a small contribution of the backward wave, nonlinearity, and absorption appears on the right-hand-side in a second step. To calculate this contribution we return to Eq. (6) and apply an exact identity

$$\partial_z^2 + \beta^2(\omega) = 2\beta(\omega)[i\partial_z + \beta(\omega)] - [i\partial_z + \beta(\omega)]^2 \tag{8}$$

According to Eq. (7) the second term in Eq. (8) is now neglected. Then Eq. (6) is transformed to the unidirectional form

$$i\partial_z E_\omega + \beta(\omega)E_\omega = -i\alpha(\omega)E_\omega - \frac{\omega^2}{2c^2\beta(\omega)} \sum_{\omega_1+\omega_2+\omega_3=\omega} \chi^{(3)}_{\omega_1\omega_2\omega_3\omega} E_{\omega_1} E_{\omega_2} E_{\omega_3}, \tag{9}$$

which yields the desired generalization of Eq. (7). One can repeat the procedure using Eq. (9) to better approximate $[i\partial_z + \beta(\omega)]^2$ in Eq. (8) and once again inserting the result into Eq. (6). By doing this we establish which terms (e.g., αE^3 and $\alpha^2 E$) are neglected when deriving Eq. (9).

A scalar first-order propagation model (9) was suggested in Ref. [78]. An arbitrary polarization was discussed in Refs. [79, 80]. In the next sections Eq. (9) is first simplified by eliminating the non-resonant nonlinear terms. This procedure follows a general strategy for a weakly nonlinear system [82]. Thereafter a Hamiltonian framework is introduced for the simplified equation.

2.3 Resonances

A natural approach to Eq. (9) is to simplify it by a suitable change of variables. In the spirit of Eq. (2) we use a power expansion, define

$$\tilde{E}_\omega = E_\omega + \frac{\omega^2}{2c^2\beta(\omega)} \sum_{\omega_1+\omega_2+\omega_3=\omega} \frac{\chi^{(3)}_{\omega_1\omega_2\omega_3\omega} E_{\omega_1} E_{\omega_2} E_{\omega_3}}{\beta(\omega) - \beta(\omega_1) - \beta(\omega_2) - \beta(\omega_3)} + \cdots, \tag{10}$$

write Eq. (9) in terms of $\tilde{E}_\omega(z)$, and obtain an equation

$$i\partial_z \tilde{E}_\omega + \beta(\omega)\tilde{E}_\omega = -i\alpha(\omega)\tilde{E}_\omega + \text{h.o.t.} \tag{11}$$

in which the high-order-terms can be neglected because they correspond to the terms neglected when obtaining Eq. (9). All nonlinearities are then eliminated and we have formally reduced Eq. (9) to a linear model (11). However, such an elimination is possible only for non-resonant triads $\{\omega_1, \omega_2, \omega_3\}$. The resonant frequencies are defined by the conditions

$$\omega_1 + \omega_2 + \omega_3 = \omega, \tag{12}$$

$$\beta(\omega_1) + \beta(\omega_2) + \beta(\omega_3) = \beta(\omega). \tag{13}$$

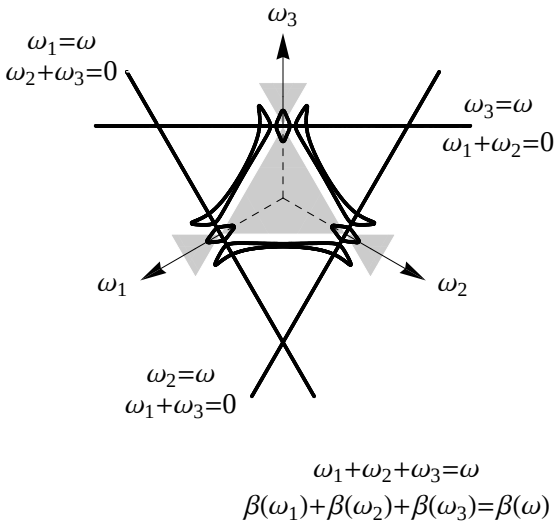

Figure 1: The thick curves show solutions of the resonance conditions (12)–(13) for a bulk fluoride glass (ω corresponds to 0.8 μm, $\epsilon(\omega)$ is taken from [39]). The dashed region corresponds to four-wave mixing processes that change the total number of photons. The dashed part of the resonance curves is usually small. It is neglected in this paper.

In the vicinity of a resonant triad the transformation (10) is singular and cannot be applied. Actually, the nonlinear terms in Eq. (9) can only be eliminated in some subregions of the three-dimensional space of triads.

For a non-dispersive medium with $\beta(\omega)/\omega = \text{const}$ the second resonance condition (13) is trivial, the transformation (10) is always singular, and a further reduction of the unidirectional model (9) is not possible. In a dispersive medium Eqs. (12)–(13) define several resonance curves in the three-dimensional space of triads. Note that for any dispersion law $\beta(\omega)$, the conditions (12)–(13) are satisfied for

$$\{\omega_1, \omega_2, \omega_3\} = \mathfrak{p}\{\omega', -\omega', \omega\}, \qquad \omega' \in \mathbb{R}, \tag{14}$$

where $\mathfrak{p}$ stays for an arbitrary permutation. These universal solutions correspond to the three straight lines shown in Fig. 1. In simple cases (e.g., for the Drude model) no other resonance curves are possible. Further (medium-specific) solutions of Eqs. (12)–(13) may appear for a more complex dispersion law, an example for a bulk fluoride glass is shown in Fig. 1.

In what follows we assume that for $\omega > 0$ the solutions of Eqs. (12)–(13) contain one negative and two positive frequencies. This condition is motivated by the universal solution (14). With respect to the further possible solutions we therefore neglect the dashed parts of the resonance curves shown in Fig. 1. The approximation can easily be understood by analogy with quantum mechanics. The dashed regions correspond to the to four-wave mixing (FWM) processes in which either a photon is decaying into three new ones or vice versa. The only four-wave process that we take into account is the mutual scattering of two photons such that their total number

remains unchanged. This leads to a considerable simplification of Eq. (9), as shown in the next section.

2.4 Complex field

To simplify Eq. (9) we first write it in such a way that contributions of the positive and negative frequencies are explicitly distinguished. To this end we introduce a complex electric field $\mathcal{E}(z,t)$ which, in contrast to the standard real $E(z,t)$, contains only positive harmonics

$$\mathcal{E}(z,t) = 2\sum_{\omega>0} E_\omega(z)e^{-i\omega t}. \tag{15}$$

Here

$$E_{\omega>0} = \frac{1}{2}\mathcal{E}_\omega \qquad \text{and} \qquad E_{\omega<0} = E^*_{-\omega} = \frac{1}{2}\mathcal{E}^*_{-\omega},$$

the latter equations can be combined into a single one

$$E_\omega = \frac{\mathcal{E}_\omega + \mathcal{E}^*_{-\omega}}{2}, \tag{16}$$

because $\mathcal{E}_{\omega<0} = 0$ by construction.

The conjugated field $\mathcal{E}^*(z,t)$ contains only negative harmonics, note that $(\mathcal{E}^*)_\omega$ and $(\mathcal{E}_\omega)^*$ must be distinguished. Namely, taking the complex conjugate of Eq. (15) we obtain

$$(\mathcal{E}^*)_{-\omega} = (\mathcal{E}_\omega)^* = \mathcal{E}^*_\omega. \tag{17}$$

Using Eqs. (16) and (17) we get

$$E_\omega = \frac{\mathcal{E}_\omega + (\mathcal{E}^*)_\omega}{2}, \qquad E(z,t) = \frac{\mathcal{E}(z,t) + \mathcal{E}^*(z,t)}{2},$$

so that $E(z,t)$ is the real part of $\mathcal{E}(z,t)$. Using the latter relations together with the definition of $\hat{\chi}^{(3)}$, we decompose $\hat{\chi}^{(3)}EEE$ and write Eq. (9) as

$$i\partial_z\mathcal{E}_\omega + [\beta(\omega) + i\alpha(\omega)]\mathcal{E}_\omega + \frac{\omega^2}{8c^2\beta(\omega)}\times \\ \left(\hat{\chi}^{(3)}\mathcal{E}\mathcal{E}\mathcal{E} + 3\hat{\chi}^{(3)}\mathcal{E}\mathcal{E}^*\mathcal{E} + 3\hat{\chi}^{(3)}\mathcal{E}^*\mathcal{E}\mathcal{E}^* + \hat{\chi}^{(3)}\mathcal{E}^*\mathcal{E}^*\mathcal{E}^*\right)_\omega = 0. \tag{18}$$

Here, e.g.,

$$\left(\hat{\chi}^{(3)}\mathcal{E}\mathcal{E}^*\mathcal{E}\right)_\omega = \sum_{\omega_1-\omega_2+\omega_3=\omega} \chi^{(3)}_{\omega_1\omega_2\omega_3\omega}\mathcal{E}_{\omega_1}\mathcal{E}^*_{\omega_2}\mathcal{E}_{\omega_3},$$

in accord with the presupposed symmetries of $\chi^{(3)}_{\omega_1\omega_2\omega_3\omega}$ and Eq. (17). The summation is automatically carried out over positive frequencies. Each cubic term in Eq. (18) corresponds to a different four-wave process, all such terms but $\hat{\chi}^{(3)}\mathcal{E}\mathcal{E}^*\mathcal{E}$ can be

eliminated by a suitable redefinition of variables $\mathcal{E}_\omega \to \tilde{\mathcal{E}}_\omega$ in the spirit of Eq. (10) as explained in the previous section. The only remaining term has resonance conditions

$$\omega, \omega_i > 0, \qquad \omega_1 + \omega_3 = \omega + \omega_2,$$
$$\beta(\omega_1) + \beta(\omega_3) = \beta(\omega) + \beta(\omega_2),$$

and corresponds to the scattering of photons. The actual values of $\mathcal{E}_\omega$ and $\tilde{\mathcal{E}}_\omega$ are very close to each other, in other words we can simply neglect the unimportant terms in Eq. (18) and finally write

$$i\partial_z \mathcal{E}_\omega + [\beta(\omega) + i\alpha(\omega)]\mathcal{E}_\omega + \frac{3\omega^2}{8c^2\beta(\omega)} \sum_{\omega_1 - \omega_2 + \omega_3 = \omega} \chi^{(3)}_{\omega_1\omega_2\omega_3\omega} \mathcal{E}_{\omega_1} \mathcal{E}^*_{\omega_2} \mathcal{E}_{\omega_3} = 0. \qquad (19)$$

The new model (19), with which we deal in the rest of this paper, compromises properties of both the spectral propagation models and the envelope models. For instance, an arbitrary $\beta(\omega)$ is captured and a familiar invariance with respect to the phase shifts ($\mathcal{E}_\omega \to \mathcal{E}_\omega e^{i\theta}$ with $\theta = \text{const}$) is retained. Equation (19) can be considered as a simplification of the model (9) introduced in Ref. [78]. In some cases (e.g., for the Drude dispersion model) no further assumptions are required for the derivation of (19) from (9), both models have the same field of applications. The proof originates from the Hamiltonian perturbation theory [81, 82] and is based on a stepwise canceling of the non-resonant nonlinear terms as explained in the previous section. For an arbitrary dispersion law, Eq. (19) is valid if the contribution of $1 \to 3$ and $3 \to 1$ four-wave processes can be neglected. The latter assumption is often harmless, but the vanishing dispersion case in which all FWM interactions are important and reduction of (9) to (19) is not possible.

Last but not least, Eq. (19) operates with the complex electric field $\mathcal{E}(z,t)$ introduced by Eq. (15). This quantity contains only positive frequencies and is a replacement of the familiar complex envelope. Note, that the transformation to normal variables, that is described in the next section, contains $\sqrt{\omega}$ and is naturally applied to $\mathcal{E}(z,t)$. We now turn to the construction of the Hamiltonian framework for Eq. (19).

3 Hamiltonian framework

A standard way to obtain first-order Hamiltonian equations is to perform a Legendre transformation of a second-order Lagrangian equation [83]. This procedure is discussed in Ref. [84] for the second-order nonlinear wave equation and the t-propagated picture. It leads to a complicated multivalued expression for the canonical momentum. The unidirectional Eq. (19) is more simple to deal with because it is of first order. Some care is required because the space coordinate z serves as an effective time. Consider, for instance, a standard continuity equation $\partial_t \rho + \partial_z j = 0$ for a physical quantity with the density $\rho(z,t)$ and the flux density $j(z,t)$ in one space dimension. Normally, the conserved integral is given by the "charge" $\int \rho(z,t)dz$.

For the z-propagated picture we have the mean "current" $\int j(z,t)dt = \text{const}$. Returning to the optical pulses we see that energy and momentum transfered by the pulse for $-\infty < t < \infty$ should not depend on the observation point z. The conserved quantities correspond then to the time-averaged *fluxes* of the relevant physical variables.

3.1 Normal variables

We introduce a new complex field $\mathcal{A}(z,t)$. Like the complex electric field $\mathcal{E}(z,t)$, it contains only positive frequencies

$$\mathcal{A}(z,t) = \sum_{\omega>0} \mathcal{A}_\omega(z) e^{-i\omega t}.$$

The harmonics $\mathcal{A}_\omega(z)$ are defined by the relation

$$\mathcal{E}_\omega(z) = i\omega\sqrt{\frac{2}{\beta(\omega)}}\mathcal{A}_\omega(z), \qquad \omega > 0. \tag{20}$$

Writing Eq. (19) in terms of $\mathcal{A}(z,t)$ we obtain

$$i\partial_z \mathcal{A}_\omega + [\beta(\omega) + i\alpha(\omega)]\mathcal{A}_\omega + \sum_{\omega_1-\omega_2+\omega_3=\omega} T_{\omega_1\omega_2\omega_3\omega}\mathcal{A}_{\omega_1}\mathcal{A}^*_{\omega_2}\mathcal{A}_{\omega_3} = 0, \tag{21}$$

with

$$T_{\omega_1\omega_2\omega_3\omega_4} = \frac{3}{4c^2}\frac{\omega_1\omega_2\omega_3\omega_4\chi^{(3)}_{\omega_1\omega_2\omega_3\omega_4}}{[\beta(\omega_1)\beta(\omega_2)\beta(\omega_3)\beta(\omega_4)]^{1/2}}.$$

Now, defining the Hamiltonian as

$$H = \sum_\omega \beta(\omega)|\mathcal{A}_\omega|^2 + \sum_{\omega_1+\omega_3=\omega_2+\omega_4} \frac{1}{2}T_{\omega_1\omega_2\omega_3\omega_4}\mathcal{A}_{\omega_1}\mathcal{A}^*_{\omega_2}\mathcal{A}_{\omega_3}\mathcal{A}^*_{\omega_4}, \tag{22}$$

and neglecting the α-term (absorption) in Eq. (21), we can write Eq. (21) as

$$i\partial_z \mathcal{A}_\omega + \frac{\delta H}{\delta \mathcal{A}^*_\omega} = 0. \tag{23}$$

Equation (23) is a complex representation of the canonical Hamiltonian equations (see, e.g., Ref. [82]). The fields $\mathcal{A}(z,t)$ and $\mathcal{A}^*(z,t)$ are complex canonical variables. In the next section we demonstrate that they also correspond to the creation and annihilation operators.

3.2 Integrals of motion

In this section we neglect absorption and obtain integrals of motion for the pulse propagation. By construction, the Hamiltonian function (22) conserves for Eq. (23).

Further integrals are obtained from the continuos symmetries of the Hamiltonian (a canonical analog of Noether's theory, see Ref. [83]). Note, that (22) is invariant under the phase shift $\mathcal{A}_\omega \to \mathcal{A}_\omega e^{i\theta}$, this transformation is generated by a differential equation $i\partial_\theta \mathcal{A}_\omega + \mathcal{A}_\omega = 0$, the latter can be written in the Hamiltonian form

$$\mathcal{A}_\omega \to \mathcal{A}_\omega e^{i\theta} \quad \Leftrightarrow \quad i\partial_\theta \mathcal{A}_\omega + \frac{\delta}{\delta \mathcal{A}^*_\omega} \sum_{\omega'} |\mathcal{A}_{\omega'}|^2 = 0.$$

Therefore the quantity

$$N = \sum_\omega |\mathcal{A}_\omega|^2 \tag{24}$$

is an integral of motion for the model (23). Furthermore, (22) is invariant under another continuous transformation $\mathcal{A}_\omega \to \mathcal{A}_\omega e^{i\omega s}$, which we first write in the differential form $i\partial_s \mathcal{A}_\omega + \omega \mathcal{A}_\omega = 0$, and then in the Hamiltonian form

$$\mathcal{A}_\omega \to \mathcal{A}_\omega e^{i\omega s} \quad \Leftrightarrow \quad i\partial_s \mathcal{A}_\omega + \frac{\delta}{\delta \mathcal{A}^*_\omega} \sum_{\omega'} \omega' |\mathcal{A}_{\omega'}|^2 = 0.$$

The quantity

$$P = \sum_\omega \omega |\mathcal{A}_\omega|^2 \tag{25}$$

is another integral of motion for the model (23). It is of interest to relate expressions (22), (24), and (25) to the pulse parameters.

Using an analogy with the quantum mechanics one can interpret $|\mathcal{A}_\omega|^2$ as a classical number of photons for a given frequency. The integrals N, P, and H correspond then to a mean number of photons, energy, and momentum transfered by the pulse (per unit area in the xy-plane). For instance, consider the mean energy flux $\mathfrak{J}_E$ which is given by time-averaging of the Pointing vector

$$\mathfrak{J}_E = \frac{1}{T} \int_{-T/2}^{+T/2} \frac{EB}{\mu_0} dt = \frac{1}{\mu_0} \sum_\omega E_\omega B^*_\omega.$$

Using Eq. (1) and the unidirectional approximation (7) we express the magnetic field

$$B_\omega(z) = \frac{\partial_z E_\omega(z)}{i\omega} = \frac{\beta(\omega)}{\omega} E_\omega(z)$$

and obtain

$$\mathfrak{J}_E = \sum_{\omega>0} \frac{2\beta(\omega)}{\mu_0 \omega} |E_\omega|^2 = \sum_\omega \frac{\beta(\omega)}{2\mu_0 \omega} |\mathcal{E}_\omega|^2 = \sum_\omega \frac{\omega |\mathcal{A}_\omega|^2}{\mu_0},$$

so that $\mathfrak{J}_E = P/\mu_0$. A more complicated but similar calculation relates H and the averaged momentum flux $\mathfrak{J}_M = H/\mu_0$.

The most direct application of the integrals of motion is to control the numerical solutions, e.g., when calculating SC generation by an ultrashort optical pulse. Before addressing these issues we summarize our results by writing them in a space domain.

3.3 Space formulation

To obtain a space formulation of the pulse propagation model (19) we introduce a real refractive index $n(\omega)$ and a nonlocal pseudodifferential operator $\hat{D}_n$, where

$$n(\omega) = \frac{\beta(\omega)c}{\omega} \qquad \text{and} \qquad \left(\hat{D}_n\mathcal{E}\right)_\omega = n(\omega)\mathcal{E}_\omega. \tag{26}$$

The operator $\hat{D}_n$ is somewhat similar to the dispersion operator which is traditionally used in the higher-order NSE (see Introduction). However, in contrast to the dispersion operator, $\hat{D}_n$ is bounded, nonsingular, and invertible. It is a positive operator so that the square root $\hat{D}_{\sqrt{n}}$ can be defined. Using $\hat{D}_n$ and ignoring absorption we obtain a space form of Eq. (19)

$$\partial_z\mathcal{E} + \frac{1}{c}\partial_t\left[\hat{D}_n\mathcal{E} + \frac{3}{8}\hat{D}_n^{-1}\left(\hat{\chi}^{(3)}\mathcal{E}\mathcal{E}^*\mathcal{E}\right)\right] = 0, \tag{27}$$

which is a nonlinear nonlocal hyperbolic propagation equation. An envelope analogue of Eq. (27) for a Kerr medium was suggested in Ref. [40]. The conserved mean energy flux $\mathfrak{J}_E$ and the mean momentum flux $\mathfrak{J}_M$ are determined by

$$2c\mu_0\mathfrak{J}_E = \sum_\omega n(\omega)|\mathcal{E}_\omega|^2 = \frac{1}{T}\int_{-T/2}^{+T/2}|\hat{D}_{\sqrt{n}}\mathcal{E}|^2dt,$$

and

$$2c^2\mu_0\mathfrak{J}_M = \sum_\omega n^2(\omega)|\mathcal{E}_\omega|^2 + \sum_{\omega_1+\omega_3=\omega_2+\omega_4}\frac{3}{16}\chi^{(3)}_{\omega_1\omega_2\omega_3\omega_4}\mathcal{E}_{\omega_1}\mathcal{E}^*_{\omega_2}\mathcal{E}_{\omega_3}\mathcal{E}^*_{\omega_4} = \frac{1}{T}\int_{-T/2}^{+T/2}\left[|\hat{D}_n\mathcal{E}|^2 + \frac{3}{16}\mathcal{E}^*\left(\hat{\chi}^{(3)}\mathcal{E}\mathcal{E}^*\mathcal{E}\right)\right]dt.$$

The particle number integral reads

$$2cN = \sum_\omega\frac{n(\omega)}{\omega}|\mathcal{E}_\omega|^2 = \frac{1}{T}\int_{-T/2}^{+T/2}\mathcal{E}^*\hat{D}_n(i\partial_t)^{-1}\mathcal{E}dt,$$

and is finite due to the condition (4). If the time-averaged electric field is nonzero, the total number of the involved photons is infinite.

To take absorption into account one should replace Eq. (27) with the full Eq. (19). In particular, $n(\omega)$ becomes complex in the linear part, but still remains purely real in the nonlinear term! This is an important issue, because formally allowing for a complex refractive index in Eq. (27) one obtains an unphysical nonlinear gain. We also note that a traditional polynomial approximation to $\beta(\omega)$ may be unsuitable for Eq. (19). In this case a more flexible rational representation should be used.

4 Numerical solutions

The numerical solution of Eq. (27) with an instantaneous Kerr nonlinearity (5) is described in this section. Here, the direct split-step Fourier approach [3] lacks precision for a few-cycle optical pulse and relatively long (e.g., 1 cm) propagation distance, such that the integrals of motion do not conserve. Therefore we use a de-aliased pseudospectral method, which originates from the computational fluid dynamics [85]. This method calculates all linear operators and derivatives in the frequency domain and performs the nonlinear multiplications in the time domain, with the transformations between the domains achieved by the fast Fourier transform. The integration for the linear and nonlinear part is performed in the frequency domain by a precise Runge-Kutta integration scheme of order eight with adaptive stepsize control depending on the accuracy as described in Ref. [86]. Note, that operator $\hat{D}_n$, which enters Eq. (27), is bounded and numerical stiffness (caused by the unbounded dispersion operator in the higher-order NSE) is avoided in our formulation.

The particle number integral N, the mean energy flux P, and the mean momentum flux H are used as control parameters for the accuracy of the solutions. To assure conservation of N, P, and H for an equidistant mesh of time points we need at least $\Delta t = 0.6\,\mathrm{fs}$. Depending on the initial pulse width, we have to use a resolution of 2^{14} and 2^{15} harmonics for a periodic time window $T = 5\,\mathrm{ps}$ and $T = 10\,\mathrm{ps}$, respectively. Several test calculation were performed for a better resolution, 2^{17}. The increase of the harmonics number does not affect the results.

In the following we study the nonlinear propagation of femtosecond pulses in the anomalous dispersion regime of a microstructured fiber, where complex and comprehensive behavior can be observed. Depending on the input pulse power and width, the interplay of linear and nonlinear effects such as self-phase modulation (SPM), FWM, and soliton dynamics, can lead to the generation of octave-spanning spectra. It is well known, that the physical mechanism of the dramatic spectral broadening process is related to the break-up of higher-order solitons [78]. The soliton fission is caused by the formation of fundamental soliton pulses and the generation of a non-solitonic dispersive wave into the phase-matched wavelength, leading to a spectrum broadened over an octave, even if the injected pulse energy is less than a few nanojoules. Besides soliton propagation, the modulation instability (MI) is another general feature in the anomalous dispersion regime, which affects the propagation of an optical pulse. The MI is a well understood instability phenomenon of the NSE, which results from the interplay between SPM and group velocity dispersion. In [37] the ability of the MI to generate SC and the dominance of the MI for short pulses has been demonstrated. In [38] it has been shown, that soliton fission dominates for low input power and short pulses (100 fs) and the modulation instability has a strong impact for high input powers at arbitrary pulse widths.

For our simulations the dispersion profile of the highly nonlinear microstructured fiber is taken from [87]. The real refractive index is then represented by a proper

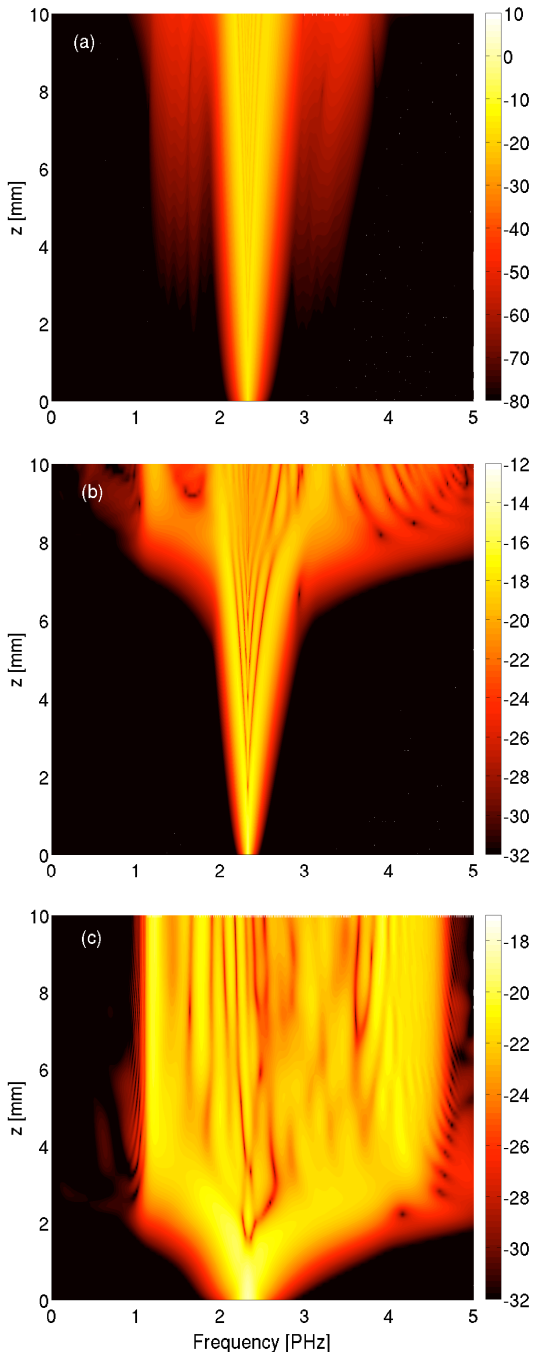

Figure 2: Density plots of the spectral evolution for (a) $t_0 = 100\,\mathrm{fs}$ pulse with typical signature of the modulation instability, (b) $t_0 = 50\,\mathrm{fs}$, and (c) $t_0 = 10\,\mathrm{fs}$ pulses generating SC by soliton fission. The spectra are shown in logarithmic scale (dB).

rational approximation

$$n(\omega) = \frac{p_0 + p_1(\omega/\mathrm{PHz}) + \cdots + p_5(\omega/\mathrm{PHz})^5}{1 + q_1(\omega/\mathrm{PHz}) + \cdots + q_5(\omega/\mathrm{PHz})^5}$$

with parameters: $p_0 = 1.00654$, $p_1 = -2.31431$, $p_2 = 1.95942$, $p_3 = -0.678111$, $p_4 = 0.120882$, $p_5 = -0.00911063$ and $q_1 = -2.29967$, $q_2 = 1.94727$, $q_3 = -0.673382$, $q_4 = 0.120015$, $q_5 = -0.00905104$.

As an initial condition we consider an input pulse electric field having a central angular frequency ω_0

$$\sqrt{\chi}E(z,t)|_{t=0} = \frac{1}{2}\Psi(t)e^{-i\omega_0 t} + \text{c.c.},$$

and a hyperbolic-secant shape for the initial envelope $\Psi(t) = \Psi_0 \operatorname{sech}(t/t_0)$ with the dimensionless amplitude $\Psi_0 = 0.03$ and temporal width $t_0 = 10$–$100\,\mathrm{fs}$. The electric field is normalized by $\chi^{-1/2}$. The pulses are injected at a central frequency $\omega_0 = 2.32548\,\mathrm{PHz}$, corresponding to a pump wavelength $\lambda_0 = 810\,\mathrm{nm}$ in the vicinity of the zero dispersion wavelength in the anomalous dispersion regime.

Figure 2 shows the density plots in the (ω, z)-plane of the spectral evolution for different input pulse widths. The spectra are shown on a logarithmic scale to illustrate the fine structure of the spectrum generated. For a 100 fs-pulse spectral broadening in the range $z = 1$–$10\,\mathrm{mm}$ is mainly dominated by SPM. However the significant features of the MI can be observed. The underlying MI acts in the initial stage on the pulse and leads to the generation of a Stokes and an anti-Stokes component. Fig. 2a shows the appearance of two sidebands after $z = 3.7$ mm. This demonstrates that also for short pulses with durations of 100 fs the modulation instability is present and can have an impact on the propagation dynamics.

The simulations in Fig. 2b,c illustrate the typical scenario of spectral broadening by soliton-related dynamics, for input pulses with $t_0 = 50\,\mathrm{fs}$ and $t_0 = 10\,\mathrm{fs}$. Three different stages are clearly observed. The initial stage of propagation is dominated by symmetrical spectral broadening induced by SPM. An extreme spectral broadening is then caused by pulse contraction due to the first step of soliton propagation (Fig. 3b,d at $z = 7.9\,\mathrm{mm}$ for 50 fs and $z = 2.1\,\mathrm{mm}$ for 10 fs). In the second stage the spectral broadening becomes asymmetric and energy is shifted to to the blue side of the spectrum, due to soliton fission accompanied by the excitation of dispersive waves. This is associated with the development of distinct temporal peaks that sit upon a broader low-amplitude background (Fig. 3e,f at $z = 9.9\,\mathrm{mm}$). The extension of the spectrum to the blue side is related to the dispersion profile of the optical fiber and to the input pulse power. The spectral broadening is limited by the broadening of the temporal waveform of the pulses. In the third stage the spectral width is already saturated, but FWM generates complicated substructures. The appearance of the fine structure is an essential phenomenon and is extremely sensitive with respect to the initial pulse energy.

Equation (27) reproduces all essential features of the SC evolution seen in a number of experiments [88, 9] and in simulations with the higher-order NSE. Moreover, it

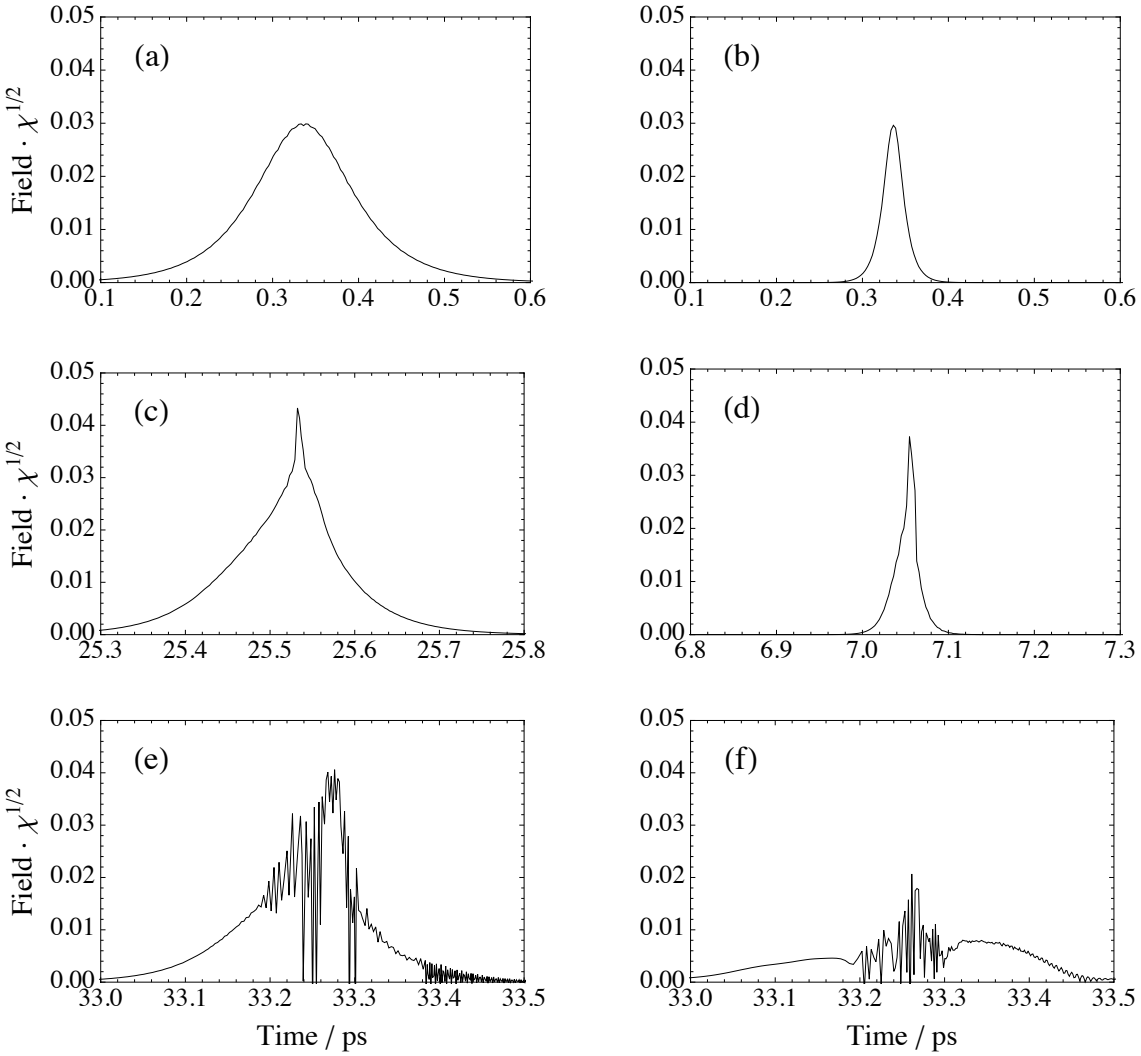

Figure 3: Temporal evolution for selected propagation distances for a 50 fs pulse at (a) $z = 0.1$ mm, (c) $z = 7.6$ mm, (e) $z = 9.9$ mm and for a 10 fs pulse at (b) $z = 0.1$ mm, (d) $z = 2.1$ mm, (f) $z = 9.9$ mm. Pulse envelopes are shown.

goes beyond the envelope approximation and allows for an arbitrary pulse duration. The numerical solutions are effectively controlled by the conservation laws.

5 Conclusions

Let us summarize our results. Propagation of spectrally broad ultrashort optical pulses is considered. In a first step, we show that known propagation equations can be simplified by a rigorous elimination of the non-resonant terms. This technique originates from the dissipationless Hamiltonian mechanics, however, the linear absorption effect can also be taken into account. The resulting non-envelope Eq. (19) applies to a properly chosen complex electric field in the frequency domain. The

model (19) combines advantages of both envelope and non-envelope approaches, it accounts for arbitrary dispersion, four-wave mixing processes, weak absorption, and arbitrary pulse duration. The space formulation (27) is obtained in terms of a nonlocal operator $\hat{D}_n$, the latter provides a natural generalization of the common dispersion operator. It is of interest, that the linear absorption does not affect the nonlinear term in Eq. (19). This is an important issue because careless use of the complex refractive index, e.g., in Eq. (27), leads to an unphysical nonlinear gain in the numerical solutions.

In a second step we neglect the absorption term and obtain a Hamiltonian framework for Eq. (19). To this end the classical normal variables are introduced. These classical creation and annihilation operators are of interest, e.g., for interpretation of the optical experiments with event horizons [89]. As such, the Hamiltonian formulation of a nonlinear wave equation has many important applications — integrability analysis, conservation laws, stability of solitons, and power-spectrum of turbulent states to name just a few [82, 90, 91]. Specifically we obtain the conservation laws for the z-propagated picture. They are given by the time-averaged fluxes of relevant physical quantities and provide a useful tool to control numerical solutions.

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