Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Padé approximant for refractive index and nonlocal envelope equations

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submitted: 6th January 2009

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No. 1391
Berlin 2009

2000 *Mathematics Subject Classification.* 78A60.

Key words and phrases. Short optical pulses, Envelope equation, Padé approximant.

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Abstract

Padé approximant is superior to Taylor expansion when functions contain poles. This is especially important for response functions in complex frequency domain, where singularities are present and intimately related to resonances and absorption. Therefore we introduce a diagonal Padé approximant for the complex refractive index and apply it to the description of short optical pulses. This yields a new nonlocal envelope equation for pulse propagation. The model offers a global representation of arbitrary medium dispersion and absorption, e.g., the fulfillment of the Kramers-Kronig relation can be established. In practice, the model yields an adequate description of spectrally broad pulses for which the polynomial dispersion operator diverges and can induce huge errors.

An average evolution of the optical field can be described in terms of an envelope [3]. This strategy is especially successful when the spectrum of the oscillations is narrow, centered around a carrier frequency ω_c. A slowly-varying envelope approximation (SVEA) leads then to an envelope equation, e.g., the nonlinear Schrödinger equation (NSE) [1]. A recent progress in the generation of ultrashort optical pulses for which the SVEA does not apply [8] awakened interest in new models. Moreover, even for a longer pulse the SVEA can be broken down by self-focusing [17, 18], a steep pulse edge [9], and supercontinuum generation [6, 5]. Therefore much effort has been directed toward deriving a generalized envelope equation [4, 16, 12, 9, 11, 10]. Broadly speaking, such models assume an unidirectional character of the pulse propagation instead of the SVEA. Medium dispersion is usually taken into account by a standard polynomial dispersion operator like in the higher-order NSE.

Contrary to popular belief, the traditional dispersion operator cannot completely quantify dispersion for ultrashort pulses. This happens when the pulse spectral width becomes comparable with the optical transparency window [14]. Here, taking more terms in the dispersion operator one induces huge errors far from the carrier frequency. In this contribution we overcome the divergence by introducing a rational Padé approximant for the medium refractive index. A local differential dispersion operator in the envelope equation is replaced with a non-local pseudodifferential one. With only the refractive index around ω_c, we completely recover dispersion and obtain an adequate model for spectrally broad pulses.

Medium dispersion, i.e., a relation between the wave vector k and the circular frequency ω of an optical wave, is characterized by specifying the propagation constants

$$\beta_m + i\alpha_m = \left.\frac{d^m k(\omega)}{d\omega^m}\right|_{\omega=\omega_c}, \quad m = 0, 1, 2\ldots \tag{1}$$

The latter are associated with the Taylor expansion

$$k(\omega) = \sum_{m=0}^{\infty} \frac{\beta_m + i\alpha_m}{m!} (\omega - \omega_c)^m \tag{2}$$

and with the differential operator

$$\mathfrak{D}_k = \sum_{m=0}^{\infty} \frac{i^m}{m!} (\beta_m + i\alpha_m) \frac{\partial^m}{\partial t^m} \tag{3}$$

acting on a complex wave amplitude. For instance, consider a linearly polarized electromagnetic pulse with the reference frequency ω_c. In the case of a purely one-dimensional propagation along the z-axis the pulse electric field can be presented as

$$E(z,t) = \frac{1}{2}\Psi(z,t)e^{-i\omega_c t} + \text{c.c.}, \tag{4}$$

where $\Psi(z,t)$ is the complex amplitude with respect to temporal oscillations in a given space point. In what follows we also use the spectral representation of fields

$$E = \frac{1}{2}\sum_{\omega} E_\omega e^{-i\omega t} + \text{c.c.}, \qquad \Psi = \sum_{\Omega} \Psi_\Omega e^{-i\Omega t}$$

in which Eq. (4) yields that $\Psi_\Omega = E_{\omega_c+\Omega}$. The spectral representation of the operator $\mathfrak{D}_k$ is given by

$$(\mathfrak{D}_k \Psi)_\Omega = \left(\sum_{m=0}^{\infty} \frac{\beta_m + i\alpha_m}{m!} \Omega^m \right) \Psi_\Omega.$$

In a linear dispersive medium the complex amplitude is governed by a formally exact differential equation

$$i\partial_z \Psi + \mathfrak{D}_k \Psi = 0, \tag{5}$$

where with respect to Eq. (3) the first two terms in $\mathfrak{D}_k$ are related to the reference wave vector β_0 and the reference group velocity $1/\beta_1$. A standard redefinition

$$\Psi(z,t) = \psi(z,\tau)\exp(i\beta_0 z), \qquad \tau = t - \beta_1 z \tag{6}$$

simplifies Eq. (5) to the form

$$i\partial_z \psi + \sum_{m=0}^{\infty} \frac{i^m}{m!} \gamma_m \frac{\partial^m \psi}{\partial \tau^m} = 0, \tag{7}$$

where $\gamma_0 = i\alpha_0$, $\gamma_1 = i\alpha_1$, and $\gamma_{m\geqslant 2} = \beta_m + i\alpha_m$. The sum in Eq. (7) is referred to as the dispersion operator. The SVEA presupposes that $\omega_c^{-1}\partial_\tau \ll 1$ and that one may break off the infinite sum. Inclusion of the nonlinear terms and a suitable truncation of the dispersion operator transforms Eq. (7) into a general higher-order NSE [1].

It is important to realize that both Eq. (7) and the NSE may become incorrect for ultrashort optical pulses even if one keeps all propagation constants in the dispersion operator [14]. This happens because of the prior resonance nature of the medium response function $\epsilon(\omega)$, where $\omega^2\epsilon(\omega) = k^2c^2$. Both $\epsilon(\omega)$ and $k(\omega)$ have singularity points in the complex plane. Therefore the convergence radius of the Taylor expansion (2) is finite and determined by the singularity nearest to ω_c. If the pulse spectral width exceeds the convergence radius, Eq. (5) cannot be applied. In practice, this happens if the pulse spectral width is comparable with the optical transparency window. Here, taking more terms in Eq. (2) we improve accuracy for $\omega \approx \omega_c$ and cause huge errors for $\omega \simeq 2\omega_c$.

A basic inadequacy of the dispersion operator for the spectrally broad pulses is ignored by all envelope equations in which the operator (3) is used [4, 16, 12, 9, 11, 10]. Thereby the expansion (2) is presupposed to converge for all frequencies of interest thus implying a restriction on the spectrum width and pulse duration. The restriction is relaxed in this contribution. For this purpose we replace the polynomial Taylor series (2) with the rational Padé approximant (see, e.g., [2]) for the complex refractive index

$$n(\omega) = \frac{p_0 + p_1(\omega-\omega_c) + p_2(\omega-\omega_c)^2 + \cdots}{1 + q_1(\omega-\omega_c) + q_2(\omega-\omega_c)^2 + \cdots} \tag{8}$$

in which p_m and q_m are free parameters constricted by Eq. (1) with $k(\omega) = n(\omega)\omega/c$. Furthermore, the differential dispersion operator in the higher-order NSE is abandoned in favor of the pseudodifferential one, $\mathfrak{D}_n$. The latter is associated with Eq. (8) and defined via

$$(\mathfrak{D}_n\Psi)_\Omega = n(\omega_c + \Omega)\Psi_\Omega. \tag{9}$$

A principle advantage of Eq. (8) over Eq. (2) is that the former accounts for complex singularities and with respect to real ω approximates $n(\omega)$ in a larger frequency domain. Moreover, truncating the numerator and denominator of Eq. (8) to polynomials of the same power (i.e., using the diagonal Padé approximant) we additionally ensure that $n(\omega)$ remains bounded. In practice, to a good accuracy the diagonal Padé approximant yields $n(\infty) = 1$ and $n(\omega) - 1 = O(\omega^{-2})$ for $\omega \to \infty$ in accord with the physical intuition (Fig. 1). Also the numerical stiffness of the NSE, which is determined by the highest-order term in the truncation of $\mathfrak{D}_k$, is considerably reduced by transfer to Eq. (8) with the bounded $n(\omega)$.

A point to emphasize is that all singularities (and roots) of $n(\omega)$ must belong to the lower half-plane of the complex ω plane. This general property ensures causality and the Kramers-Kronig relation [13]. It is tested by examining both the numerator and the denominator in Eq. (8). If necessary, the approximation order is increased. Finally, from the mathematical point of view it is profitable to change from $\mathfrak{D}_k$ to $\mathfrak{D}_n$ because the refractive index $n(\omega) \neq 0$ for real frequencies and therefore $\mathfrak{D}_n$ can be inverted as opposed by $k(\omega)$ and $\mathfrak{D}_k$. This is an important issue because the previously reported envelope equations for short pulses contain $1/k(\omega)$ or $(\beta_0 + i\beta_1\partial_t)^{-1}$, a singular term resulting from the formal inversion of the truncated $\mathfrak{D}_k \approx \beta_0 + i\beta_1\partial_t$.

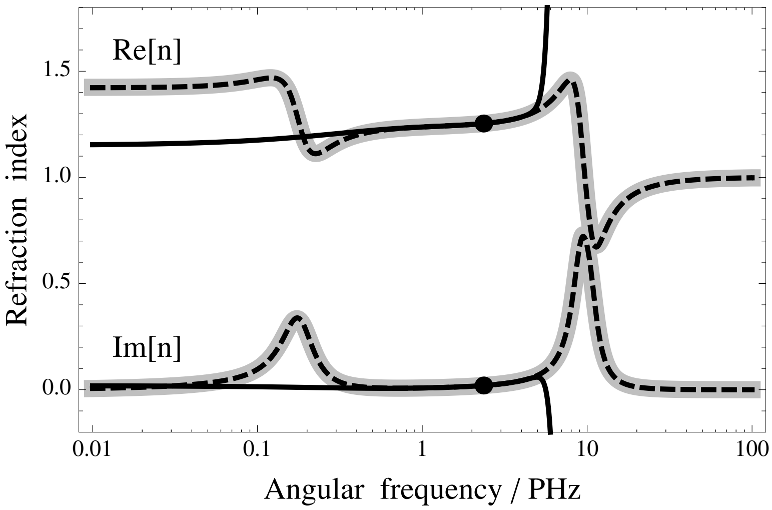

Figure 1: Real and imaginary parts of the refractive index for fluoride glass (light thick lines, double resonance Lorentz model for $n(\omega)=\sqrt{\epsilon(\omega)}$, Ref. [14]) and [5/5] Padé approximant (dashed lines). For comparison, Taylor expansion of the 11th order is also shown (solid lines). Both expansions are calculated at 800 nm (thick points) and are locally identical. The Padé approximant offers better global properties, e.g., relative errors in the transparency window are $< 1.5\%$.

Let us now turn to derivation of the envelope equation. We start with the following model equation for the pulse electric field $E(z,t)$ in a bulk Kerr media [1]

$$c^2\partial_z^2 E - \partial_t^2 D^{\mathrm{lin}} = 4\pi\chi^{(3)}\partial_t^2(E^3), \tag{10}$$

where $D^{\mathrm{lin}}(z,t)$ is the linear part of the electric displacement. In the spectral representation $D_\omega^{\mathrm{lin}} = \epsilon(\omega)E_\omega$. Equation (10) is considered in a weakly nonlinear limit, i.e., the nonlinear polarization on the right-hand-side is a small perturbation to the linear terms. An arbitrary dispersion is a major focus of interest for this work, therefore the radial effects are neglected and the simplest cubic nonlinearity is assumed. Account of a more sophisticated nonlinear medium response will be straightforward. In what follows, we will use the complex amplitude representation (4). Having in mind an arbitrary pulse duration we, however, abandon the SVEA and only assume an unidirectional character of the pulse propagation (see below). The goal is to present a closed equation for $\Psi(z,t)$ compatible with Eq. (8).

Before proceeding it is useful to remind some facts concerning the linear medium response [13]. A general linear relation between the input signal $a(t)$ and the output $b(t)$ is given by the convolution

$$b(t) = a(t) + \int_0^\infty \mathfrak{f}(s)a(t-s)ds \tag{11}$$

with the memory function $\mathfrak{f}(s)$ describing the induced medium response. Equation (11) implies a linear proportionality between the spectral components

$$b_\omega = f(\omega) a_\omega, \qquad f(\omega) = 1 + \int_0^\infty \mathfrak{f}(s) e^{i\omega s} ds \tag{12}$$

in which the spectral function $f(\omega)$ allows an analytic continuation into the complex ω plane. It is natural to assume that $f(\omega) \neq 0, \infty$ for real ω and that $f(\omega) \to 1$ as $\omega \to \infty$. It follows that $f(\omega) \neq 0, \infty$ in the upper half-plane, in this respect $f(\omega)$ and $1/f(\omega)$ have the same analytic properties and a backward transformation is possible. Therefore, a set of the spectral functions is a commutative group with respect to multiplication.

If the input signal is centered around the carrier frequency ω_c, we can introduce two complex amplitudes

$$a(t) = \frac{1}{2} A(t) e^{-i\omega_c t} + \text{c.c.}, \quad b(t) = \frac{1}{2} B(t) e^{-i\omega_c t} + \text{c.c.},$$

and rewrite Eq. (11) as

$$B(t) = A(t) + \int_0^\infty \mathfrak{f}(s) A(t-s) e^{i\omega_c s} ds \tag{13}$$

or in a full analogy with Eq. (9)

$$B = \mathfrak{D}_f A, \qquad (\mathfrak{D}_f A)_\Omega = f(\omega_c + \Omega) A_\Omega. \tag{14}$$

For a short-range memory function $\mathfrak{f}(s)$ one can expand $A(t-s)$ into the Taylor series, insert the expansion into Eq. (13), and obtain a differential representation

$$\mathfrak{D}_f = \sum_{m=0}^\infty \frac{i^m}{m!} f^{(m)}(\omega_c) \frac{\partial^m}{\partial t^m}, \tag{15}$$

where the derivatives $f^{(m)}(\omega_c)$ are calculated from the integral representation (12). The mapping $f \to \mathfrak{D}_f$ provides a representation of the spectral functions group. Indeed, it is easy to check that if $f(\omega) = g(\omega) h(\omega)$ then

$$\mathfrak{D}_{gh} A = \mathfrak{D}_g (\mathfrak{D}_h A) = \mathfrak{D}_h (\mathfrak{D}_g A) \tag{16}$$

and one can invert $\mathfrak{D}_f$ by defining $\mathfrak{D}_f^{-1} = \mathfrak{D}_{1/f}$.

For a ultrashort pulse the amplitude $A(t-s)$ changes rapidly and the Taylor expansion in Eq. (13) is not suitable. Equation (15) should be abandoned in favor of the spectral definition (14) with a suitable approximation of $f(\omega_c + \Omega)$. Following these lines we will use $\mathfrak{D}_n$ defined by Eq. (9) and approximate $n(\omega_c + \Omega)$ by Eq. (8). The group property (16) yields that $\mathfrak{D}_\epsilon = \mathfrak{D}_n^2$ and $\mathfrak{D}_n^{-1} = \mathfrak{D}_{1/n}$.

We now return to Eq. (10) and note that the material relation $D_\omega^{\text{lin}} = \epsilon(\omega) E_\omega$ indicates that $\mathfrak{D}_n^2 \Psi$ is a complex amplitude for the electric displacement. Therefore

$$\partial_t^2 D^{\text{lin}} = -\frac{1}{2} \left[(\omega_c + i\partial_t)^2 \mathfrak{D}_n^2 \Psi \right] e^{-i\omega_c t} + \text{c.c.},$$

where the last expression and the representation (4) are further inserted into Eq. (10). For simplicity the cubic harmonic term is neglected, though one may keep it in the spirit of [7]. We write the nonlinear term as

$$\partial_t^2(E^3) \approx -\frac{3}{8}\left[(\omega_c + i\partial_t)^2|\Psi|^2\Psi\right] e^{-i\omega_c t} + \text{c.c.}$$

and transform Eq. (10) to the form

$$(ic\partial_z)^2\Psi = \mathfrak{T}^2\left(\mathfrak{D}_n^2\Psi + 3\pi\chi^{(3)}|\Psi|^2\Psi\right), \tag{17}$$

where $\mathfrak{T} = \omega_c + i\partial_t$ is introduced for brevity sake.

Ignoring first the nonlinear term in Eq. (17) we obtain $(ic\partial_z \pm \mathfrak{T}\mathfrak{D}_n)\Psi = 0$ for the two counter-propagating waves. We take the first one as the main wave and account for the small contribution of the nonlinearity by putting $ic\partial_z\Psi \approx -\mathfrak{T}\mathfrak{D}_n\Psi$ and

$$\left[(ic\partial_z)^2 - \mathfrak{T}^2\mathfrak{D}_n^2\right]\Psi \approx (ic\partial_z + \mathfrak{T}\mathfrak{D}_n)(-2\mathfrak{T}\mathfrak{D}_n)\Psi. \tag{18}$$

Equation (17) is then simplified to the form

$$ic\partial_z\Psi + (\omega_c + i\partial_t)\left[\mathfrak{D}_n\Psi + \frac{3\pi\chi^{(3)}}{2}\mathfrak{D}_{1/n}|\Psi|^2\Psi\right] = 0 \tag{19}$$

which is the general envelope equation we are interested in. Equation (19) can be applied as long as the approximation (18) holds, the latter condition replaces SVEA. A similar condition was first introduced in [4] and was referred to as the slowly-evolving wave approximation. It also ensures an unidirectional pulse propagation.

Let us compare Eq. (19) to previously reported envelope models. The identity $k(\omega)c = \omega n(\omega)$ yields for $\omega = \omega_c + \Omega$ that $c\mathfrak{D}_k = (\omega_c + i\partial_t)\mathfrak{D}_n$. We use this fact to return to $\mathfrak{D}_k$ in Eq. (19) and formally allow for both $\mathfrak{D}_k^{-1}$ and representation (3). Equation (19) takes the form

$$i\partial_z\Psi + \mathfrak{D}_k\Psi + \frac{3\pi\chi^{(3)}}{2c^2}\frac{(\omega_c + i\partial_t)^2}{\mathfrak{D}_k}|\Psi|^2\Psi = 0 \tag{20}$$

which is a nonlinear counterpart of Eq. (5). Now assuming $i\partial_t \ll \omega_c$, using the approximations

$$(\omega_c + i\partial_t)^2 \approx \omega_c^2 + 2i\omega_c\partial_t, \quad D_k^{-1} \approx (\beta_0 + i\beta_1\partial_t)^{-1},$$

and changing to $\psi(z,\tau)$ in accord with Eq. (6) we simplify Eq. (20) to a well known nonlocal envelope equation

$$i\partial_z\psi + \sum_{m=0}^{\infty}\frac{i^m}{m!}\gamma_m\frac{\partial^m\psi}{\partial\tau^m} + \frac{3\pi\chi^{(3)}}{2c^2}\frac{\omega_c^2 + 2i\omega_c\partial_\tau}{\beta_0 + i\beta_1\partial_\tau}|\psi|^2\psi = 0$$

first introduced in [4] and then refined in [9, 11, 10]. Expanding the last fraction with respect to $i\partial_\tau$ we arrive at a generalized NSE with the "optical shock" term (see,

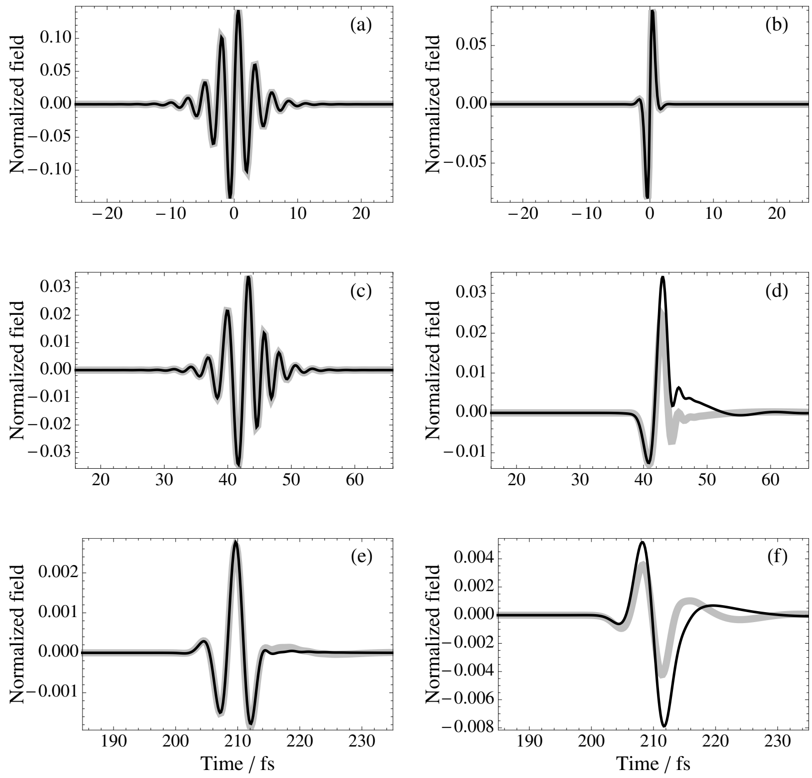

Figure 2: Pulse electric field $E(z,t)$ normalized by $1/\sqrt{\chi^{(3)}}$ versus time for a few-cycle pulse (left) and a sub-cycle pulse (right). Solutions are evaluated from the Padé based propagation Eq. (19) (thin line) and the Taylor based Eq. (20) (thick line). (a,b) $z = 0$; (c,d) $z = 10\,\mu$m; (e,f) $z = 50\mu$m.

e.g., [19, 15, 6]). Moreover, completely ignoring $i\partial_t$ in the nonlinear part of Eq. (20) and approximating $\mathfrak{D}_k^{-1}$ with $1/\beta_0$ we reduce Eq. (20) to the standard higher-order NSE [1]. We conclude, that the basic Eq. (19) contains all these models as special cases. It should be emphasized that for an ultrashort pulse the polynomial dispersion operator can diverge and the term $(\beta_0 + i\beta_1\partial_\tau)^{-1}$ can become singular. That is why a more general model (19) should be used. The latter, as opposed by the NSE, also provides an adequate approximation for the medium absorption near the resonance frequencies (see Fig. 1).

Equation (19) can be solved numerically by a straightforward application of the split-step Fourier method [1]. Two exemplary solutions are shown in Fig. 2. The initial pulse envelope is shaped as $1/\cosh$ and the reference frequency corresponds to 800 nm. The diagonal Páde approximant for the complex refractive index depicted in Fig. 1 is used. The numerical solution is calculated using 2^{12} harmonics for $|t| < 256\pi/\omega_c$ and periodic boundary conditions, the propagation distance is $50\,\mu$m. For comparison, the solutions of the Taylor expansion based Eq. (20) in which an artificial spectral filter is implemented to avoid divergence are also shown. The initial pulse width at half maximum of the intensity envelope is 3.75 fs (Fig. 2a) and

0.75 fs (Fig. 2b). In the former case Eqs. (19) and (20) yield similar results. In the latter case the deviations caused by the broad pulse spectrum are clearly seen and Eq. (20) can not be applied.

In conclusion, to gain the most benefit from the propagation constants, one can construct the diagonal Páde approximant for the complex refractive index $n(\omega)$ and the corresponding pseudodifferential operator $\mathfrak{D}_n$. The latter, as opposed by the standard dispersion operator, can quantify dispersion for practically any frequency (Fig. 1). Moreover, one can guarantee the Kramers-Kronig relation and an accurate description of medium absorption. Our results are most important with respect to spectrally broad pulses governed by the new unidirectional Eq. (19). The model is suitable for the further mathematical analysis of few-cycle and even sub-cycle pulses. Equation (19) is also favorable for computing because its numerical stiffness is reduced as compared to that of NSE. This work was supported by the DFG Research Center MATHEON under project D 14.

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