Near-field and far-field propagation of beams and pulses in dispersive media

Marek Trippenbach, T. C. Scott, and Y. B. Band

Departments of Chemistry and Physics, Ben Gurion University of the Negev, 84105 Beer-Sheva, Israel

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We formulate an efficient exact method of propagating optical wave packets (and cw beams) in isotropic and nonisotropic dispersive media. The method does not make the slowly varying envelope approximation in time or space and treats dispersion and diffraction exactly to all orders, even in the near field. It can also be used to determine the partial differential wave equation for pulses (and beams) to any order as a power series in the partial derivatives with respect to time and space. The method can treat extremely focused pulses and beams, e.g., from near-field scanning optical microscopy sources whose transverse spatial extent in smaller than a wavelength.

Recently[1,2] a formulation to propagate light pulses in homogeneous dispersive nonisotropic media was developed and experimentally verified.[3] This formulation showed that the wave equation contains terms that rotate the three-dimensional (3D) wave packet of an optical pulse propagating as an extraordinary wave (EW) about an axis perpendicular to the propagation vector. The formulation involved an expansion in terms of the dimensionless parameters $(\omega_0 t_0)^{-1}$ and $\lambda_0/(2\pi\sigma_0)$, where t_0 is the pulse duration, ω_0 is the central frequency, λ_0 is the central wavelength, and σ_0 is the transverse width of the pulse. In this Letter we generalize the treatment of Refs. 1 and 2 by formulating a method for propagating optical pulses and cw beams that is valid to all orders in $(\omega_0 t_0)^{-1}$ and $\lambda_0/(2\pi\sigma_0)$. Therefore, the method can be applied to propagate (without approximation) extremely short pulses and extremely focused pulses and cw beams. Consequently, it can be used to calculate effects of near-field diffraction exactly, not only in vacuum but also in dispersive media and even in nonisotropic dispersive media. For example, in near-field scanning optical microscopy,[4–7] an optical beam with a cross section that is a very small fraction of the incident wavelength can be generated at the end of an optical fiber pulled into a narrow tip and coated with metal. The slowly varying envelope approximation (SVEA) cannot be used to propagate such a nonclassical beam when it leaves the fiber. However, the present method can exactly propagate such beams (or pulses[8]) in vacuum, isotropic, and nonisotropic media. Near-field optical propagation of pulses or beams whose transverse dimensions are comparable with or smaller than the wavelength requires incorporation of evanescent-wave contributions.[9,10] Hence, incorporating radiation tunneling is crucial. In the present formulation, it emerges naturally. Moreover, one cannot adequately propagate pulses shorter than several optical cycles by keeping only small-order time-derivative terms in the wave equation, but one can efficiently and exactly propagate them by using the present method.

We begin by defining the slowly varying envelope (SVE) of the electric field by extracting the wave with central wave vector $\mathbf{K}_0$ and central frequency ω_0 of the pulse, $\mathbf{E}(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t)\exp(i\mathbf{K}_0\mathbf{x} - \omega_0 t)$. The SVE is given by

$$\mathbf{A}(\mathbf{x}, t) = \frac{1}{(2\pi)^4}\int_{-\infty}^{+\infty} \mathrm{d}^3K\,\mathrm{d}\omega\,\mathbf{A}(\mathbf{K}, \omega) \times \exp\{i[(\mathbf{K} - \mathbf{K}_0)\cdot\mathbf{x} - (\omega - \omega_0)t]\}. \quad (1)$$

One can derive the propagation equation for the SVE by differentiating $\mathbf{A}(\mathbf{x}, t)$ with respect to the position coordinate in the direction of $\mathbf{s}_0 = \mathbf{K}_0/|K_0|$, which we choose to be along the space-fixed z axis:

$$\frac{\partial \mathbf{A}(\mathbf{x}, t)}{\partial z} = \frac{1}{(2\pi)^4}\int_{-\infty}^{+\infty} \mathrm{d}^3K\,\mathrm{d}\omega\,\mathbf{A}(\mathbf{K}, \omega)[i(\mathbf{K} - \mathbf{K}_0)\cdot\mathbf{s}_0] \times \exp\{i[(\mathbf{K} - \mathbf{K}_0)\cdot\mathbf{x} - (\omega - \omega_0)t]\}. \quad (2)$$

Equations (1) and (2) present a decomposition of the electric field in terms of the normal modes in the medium; these modes are plane waves that satisfy the medium's dispersion relation (DR) [there are two branches of the DR in general, and a sum over them is necessary in Eqs. (1) and (2)]. Because of the DR, the variables $\mathbf{K}$ and ω are not independent and the four-dimensional integrals in Eqs. (1) and (2) can be reduced to three dimensions. For numerical applications we eliminate integration over K_z, using the DR to express K_z in terms of K_x, K_y, and ω. The DR is derived by substitution of the plane-wave solution into the Faraday and Ampere equations and use of the constitutive equations for the displacement and magnetic induction to obtain the equation $(\mathbf{K}\cdot\mathbf{K})\mathbf{E}(\mathbf{K}, \omega) - \mathbf{K}[\mathbf{K}\cdot\mathbf{E}(\mathbf{K}, \omega)] - \omega^2/c^2\mu\hat{\epsilon}(\mathbf{K}, \omega)\mathbf{E}(\mathbf{K}, \omega) = 0$. Defining the refractive index $n(\mathbf{K}, \omega)$ by the relation $\mathbf{K} = n(\mathbf{K}, \omega)(\omega/c)\mathbf{s}$, where $\mathbf{s}$ is a unit vector in the direction of $\mathbf{K}$, and substituting this definition into the DR, for every $\mathbf{s}$ we obtain a secular equation for the refractive index and a set of equations for the direction of the electric (and magnetic) vector. The detrimental equation is conveniently evaluated in the principal-axis coordinate system $\{X, Y, Z\}$. Here we explicitly consider the uniaxial crystal case (the changes necessary for isotropic or biaxial media are easy to make). For uniaxial crystals, we define the Z-axis in the direction

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of the uniaxial axis and the X axis in the optical plane defined by the uniaxial axis and the wave vector $\mathbf{K}_0$. The secular equation for $n(\mathbf{K}, \omega)$ has two solutions; an ordinary wave (OW) solution, $n = n_o(\omega)$, that is independent of $\mathbf{s}$ and an EW solution with refractive index given by $n(\omega, \theta) = [\cos^2(\theta)/n_o^2(\omega) + \sin^2(\theta)/n_e^2(\omega)]^{-1/2}$, where the angle θ is defined so that $\tan(\theta) = [(K_X^2 + K_Y^2)/K_Z^2]^{1/2}$, $n_e^2(\omega) = \mu(\omega)\epsilon_Z(\omega)$, $n_o^2(\omega) = \mu(\omega)\epsilon_X(\omega) = \mu(\omega)\epsilon_Y(\omega)$. This can be rewritten as

$$(K_X^2 + K_Y^2)/n_e^2(\omega) + K_Z^2/n_o^2(\omega) = \omega^2/c^2. \qquad (3)$$

To use this equation conveniently for propagation, it is useful to rewrite it in the space-fixed coordinate frame with the z axis along $\mathbf{K}_0$ and the x axis in the optical plane. The transformation between the space-fixed (x, y, z) and the principal (X, Y, Z) coordinate frames involves a rotation about the y axis by an angle θ_0. On applying the rotation to Eq. (3), we obtain a quadratic equation for K_z whose solution for EW's in uniaxial media is

$$K_z = \frac{1}{2}\, n^2 \sin(2\theta_0)\left[\frac{1}{n_e^2(\omega)} - \frac{1}{n_o^2(\omega)}\right]K_x + \left[\frac{\omega^2 n^2}{c^2} - \frac{n^2}{n_e^2(\omega)}\, K_y^2 - \frac{n^4}{n_o^2(\omega) n_e^2(\omega)}\, K_x^2\right]^{1/2}, \qquad (4)$$

where $n \equiv n(\omega, \theta_0)$. Note that K_z can be imaginary for any value of ω for sufficiently large K_x and K_y; the argument of the square root in Eq. (4) then becomes negative, yet $\mathbf{K}$ still satisfies the DR, Eq. (3), and as such is included in the Fourier integrals in Eqs. (1) and (2). Hence, evanescent modes are naturally included in our method. For OW's in a uniaxial medium (and for an isotropic medium) one can simply set $n = n_e = n_o$, and K_z is either real or imaginary, but for EW's K_z is either real or complex. This procedure can also be generalized to biaxial media, for which all waves are EW's because of the reduced symmetry; here, two rotations must be applied between space-fixed and principal-coordinate frames, since $n = n(\omega, \theta_0, \phi_0)$.

Previously, the partial differential equation (PDE) for the SVE of an optical pulse propagating in a nonisotropic medium was derived to second order in spatial variables and to third order in time,[1,2] and the meaning of each term in the PDE was explained. Using Eq. (2), we obtain exactly the same propagation equation by eliminating the integral over K_z and expanding the expression for K_z appearing in Eq. (4) as a function of K_x, K_y to second order and to third order in ω. The present approach is vastly simpler than the one used in Refs. 1 and 2, since here there exists a direct correspondence between the powers of K_x, K_y, and $(\omega - \omega_0)$ and $i\partial/\partial x$, $i\partial/\partial_y$, and $-i\partial/\partial t$, respectively. The explicit correspondence between the two methods was shown with the Maple computer algebra system[11] to fifth order in time and space, thus demonstrating that the coefficients appearing in the PDE are identical in the two methods. Moreover, Eq. (1) or (2) together with Eq. (4) allows determination or propagation of the SVE to all orders in space and time. The expansion parameters for obtaining the PDE to successively higher orders are $\lambda_0/(4\pi n_0 \sigma_0)$ for space variables and $(\omega_0 t_0)^{-1}$ for time, where $n_0 \equiv n(\mathbf{K}_0, \omega_0)$. The SVEA corresponds to truncation of the expansion of K_z in Eq. (2), and we obtained the paraxial approximation by retaining up to second-order terms in x and y. The mixed space–time second-order terms account for the tilting of the pulse during propagation.[1,2] Higher-order effects become important when either expansion parameter is less than unity or when the propagation distance is much larger than the initial width of the pulse. If K_z is not expanded but the full expression for K_z in Eq. (4) is retained with Eq. (2), the SVEA and the paraxial approximation are avoided and diffraction and dispersion effects are included to all orders.

Keeping terms up to third order, we see that the PDE for $\mathbf{A}$ is

$$\frac{\partial \mathbf{A}}{\partial z} = -\beta_1 \frac{\partial \mathbf{A}}{\partial t} - \frac{i}{2}\beta_2 \frac{\partial^2 \mathbf{A}}{\partial t^2} + \frac{1}{6}\beta_3 \frac{\partial^3 \mathbf{A}}{\partial t^3} + \gamma_x \frac{\partial \mathbf{A}}{\partial x} + i\gamma_{tx}\frac{\partial^2 \mathbf{A}}{\partial t \partial x} + \frac{i}{2}\gamma_{xx}\frac{\partial^2 \mathbf{A}}{\partial x^2} + \frac{i}{2}\gamma_{yy}\frac{\partial^2 \mathbf{A}}{\partial y^2} + \frac{1}{3}\gamma_{txx}\frac{\partial^3 \mathbf{A}}{\partial x^2 \partial t} + \frac{1}{3}\gamma_{tyy}\frac{\partial^3 \mathbf{A}}{\partial y^2 \partial t} + \frac{1}{3}\gamma_{ttx}\frac{\partial^3 \mathbf{A}}{\partial t^2 \partial x} + \cdots. \qquad (5)$$

For an EW in a uniaxial medium, there are only four third-order terms in the PDE: $\beta_3 \partial^3/\partial t^3$, $\gamma_{txx}\partial^3/\partial t \partial x^2$, $\gamma_{tyy}\partial^3/\partial t \partial y^2$, and $\gamma_{ttx}\partial^3/\partial t^2 \partial x$. The first term gives rise to third-order dispersion. The second and third terms are responsible for the curvature of the propagating front of the pulse; they are not included in the paraxial approximation. These terms are present even in an isotropic medium and account for the spherical surface of a propagating front originating from a point source. The explicit expression for γ_{txx} in terms of the refractive index and its derivatives is

$$\gamma_{txx} = \frac{c}{\omega^2 n^2}\left(n + \omega \frac{\partial n}{\partial \omega}\right) - \frac{c}{\omega^2 n^3}\left[\left(n + 2\omega \frac{\partial n}{\partial \omega}\right)\frac{\partial^2 n}{\partial \theta^2} - \omega n \frac{\partial^3 n}{\partial \omega \partial \theta^2}\right] + \frac{2c}{\omega^2 n^4}\frac{\partial n}{\partial \theta}\left[\left(n + 3\omega \frac{\partial n}{\partial \omega}\right)\frac{\partial n}{\partial \theta} - 2\omega n \frac{\partial^2 n}{\partial \omega \partial \theta}\right]. \qquad (6)$$

In isotropic media, or for OW's in uniaxial media, n has no dependence on θ, leaving only the first term on the right-hand side of Eq. (6), and $\gamma_{txx} = \beta_1 \gamma_{xx}^2$. The fourth (γ_{ttx}) term is not present in isotropic media or for OW's in uniaxial media. It, too, distorts the pulse but in a fashion that reverses the roles of t and x, as described elsewhere.[11]

As a numerical example, we propagate an EW pulse in a positive uniaxial rutile (TiO_2) crystal. Equation (2) is numerically propagated with the split-step Fourier transform method.[12] This method can be easily applied whether the full expression for K_z in Eq. (4) is retained and evaluated in frequency and momentum space or the expression is

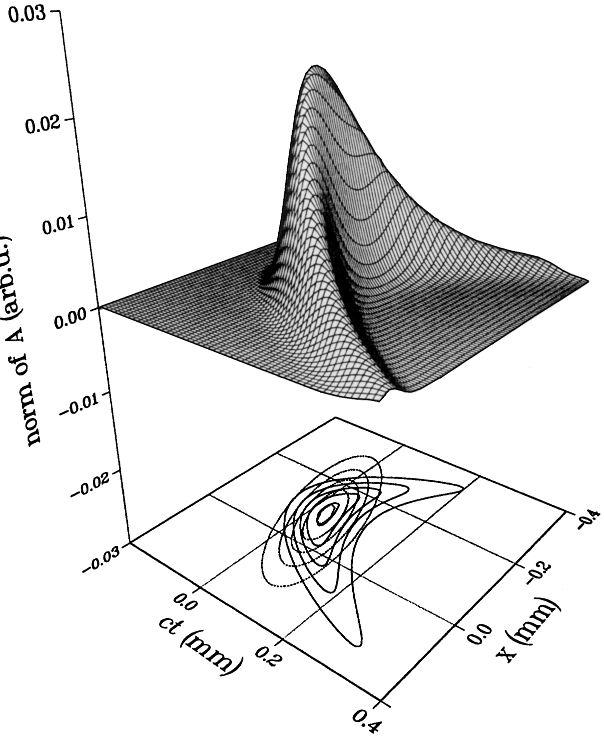

Fig. 1. 3D surface and contour plot of $|\mathbf{A}(x, y, z, t)|$ versus ct and x for a propagation distance of $z = 0.5$ mm in the frame traveling with the z component of the group. The dashed contour plot ellipses show the second-order expansion result.

expanded and the derivatives with respect to time and space are evaluated in frequency and momentum space. We carried out calculations with a pulse of light composed of a frequency superposition of Bethe–Bouwkamp solutions for a circular aperture[9]; the pulse enters a crystal and has both OW and EW polarizations. The boundary-value problem at the surface of the dispersive medium is solved to yield the reflection and transmission amplitudes into the various modes.[10] However, presenting this analysis here would complicate the description of the physical effects that we wish to emphasize, since boundary-matching issues would have to be discussed in detail. Instead, we take an initial EW Gaussian pulse with $\lambda_0 = 410$ nm, spatial width in y $\sigma_y = \infty$ (so that we can display the results in a 3D plot), temporal width $\tau_0 = 33.3$ fs, and $\theta_0 = 50°$ relative to the optic axis. Figure 1 shows a 3D surface and a contour plot of $|\mathbf{A}(x, y, z, t)|$ versus ct and x for a propagation distance of $z = 0.5$ mm in the frame traveling with the z component of the group velocity. For comparison, the second-order expansion result is included in the contour plot as a dashed curve (the third-order result is very similar to the exact result and is not shown). First, let us consider the second-order result. The pulse is not centered at the origin because of the γ_x walk-off term in Eq. (6). Its temporal duration increased by roughly a factor of 2 relative to the input pulse because of group-velocity dispersion (β_2), and its spread in x increased by a factor of $\sim$1000 because of γ_{xx}. The tilt of the elliptical wave packet that is due to γ_{xt} is $\sim$20°. In the exact result, the distortion and curvature are due mainly to the γ_{txx} term (the effect of γ_{ttx} is negligible here). The curvature of the pulse results for the same reason that the wave front from a point source is a sphere. The tilt and walk-off of the exact wave packet are also quite evident.

In summary, the present method can be used to calculate diffraction and propagation of pulses and beams in isotropic and nonisotropic dispersive media efficiently and exactly, even in the near field. To our knowledge, this the only method available to treat the kinds of propagation described here, from the smallest scales, e.g., propagation of light from near-field microscopes in nonisotropic media, to the largest scales, e.g., pulse propagation of light from pulsars in the intergalactic medium (which is nonisotropic because of magnetic fields).

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