SCHRÖDINGER EQUATION FOR PROPAGATION IN PHOTONIC CRYSTAL FIBERS

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Abstract
The propagation of light in a guided medium is generally described by the Maxwell’s equations. For long lengths of fiber, the Nonlinear Schrödinger (NLS) wave equation is typically derived under a few approximations on the waveguide properties of the guiding medium. In theoretical physics, the nonlinear Schrödinger equation is a nonlinear variation of the Schrödinger equation. The propagation of the wave is a fundamental phenomenon occurring in several physical systems. It is a classical field equation whose principal applications are to the propagation of light in nonlinear planar waveguides and optical fibers to the Bose-Einstein condensates confined to highly anisotropic cigar-shaped traps in the mean-field regime. We will focus on the Schrödinger equation for signal propagation in photonic crystal fibers.

Keywords: Schrödinger, nonlinear optics, propagation, photonic crystal, Maxwell's

1. Introduction
The Schrödinger equation is a partial differential equation that describes how the quantum state of a quantum system changes with time. It was formulated in 1926 by the physicist Schrödinger. The nonlinear Schrödinger wave equation has a closed-form solution for no linear dispersion, no Raman effect, and no higher-order fiber nonlinearities, [1]. When the dispersion is present, the Nonlinear Schrödinger equation is generally solved using recursive numerical methods such as the split-step Fourier method or finite-difference methods [1]. The fiber is divided into small segments and the output of each segment is found numerically. Very small segment lengths are required to get accurate results; therefore, the computational cost becomes prohibitively high for long lengths of fibers and short pulse-widths, which are important for future systems. If the segment lengths are increased to reduce these effects, the accuracy. There is no true derivation of this equation, but its form can be motivated by physical and mathematical arguments at a wide
variety of levels of sophistication. The Schrödinger equation has two ‘forms’, one in which time explicitly appears, and so describes how the wave function of a particle will evolve in time. In general, the wave function behaves like a wave, and so the equation is often referred to as the time-dependent Schrödinger wave equation. The generalized nonlinear Schrödinger wave equation may be used to explain the effects of linear dispersion and fiber nonlinearities on the evolution of the complex envelope of the optical field in an optical fiber. The nonlinear Schrödinger wave equation is typically solved using numerical (recursive) methods. Photonic crystals (PhCs), these materials have highly periodic structures that can be designed to control and manipulate the propagation of light. The essential benefit offered by photonic crystals is the high degree of control of the light propagation. Investigations of the physical phenomena occurring in photonic crystals are interesting both from a basic scientific point of view and because of the possibilities for commercial applications for instance in an entire optical network or for new light sources. Like a crystal lattice results from the periodic arrangement of atoms or molecules, a photonic crystal arises from a periodic modulation of the refractive index of the material [2, 3].

2. The objective of the paper

These fibers are based on a new and very promising technology and could provide solutions to many optical problems in telecommunications, light source manufacturing and has already revolutionized the field of frequency metrology. The light itself can also provide periodic structuring through an optical lattice and in this system matter wave propagation will be investigated. The theoretical modeling of light propagation in the PCFs is needed, to get a good understanding of the processes taking place in supercontinuum generation, and to give input to the design and development of new fiber structures and applications.

3. Photonic crystal fibers (PCFs)

Photonic-crystal fibers (PCFs) [14, 15], also referred to as microstructure, or holey, fibers, are optical waveguides of a new type. In PCFs, radiation can be transmitted through a hollow (Fig. 1, a, b) core, surrounded by a microstructured cladding, consisting of an array of cylindrical air holes running along the fiber axis. Such a microstructure is usually fabricated by drawing a perform composed of capillary tubes and solid silica rods.

![Fig. 1. Cross-section of photonic-crystal fibers: (a) large-mode-area PCF, and (b) hollow-core PCFs](image)

Along with conventional waveguide regimes, provided by total internal reflection, PCFs under certain conditions can support guided modes of electromagnetic radiation due to the high reflectivity of their cladding within the photonic band gaps (PBGs) or regions of low densities of photonic states [6, 7], as well as by the antiresonance mechanism of waveguiding [5, 8]. Such regimes can be supported by fibers with a hollow [9, 7, 10] or solid [11] core and a two-dimensionally periodic (photonic crystal) cladding. A high reflectivity provided by the PBGs in the transmission of such a cladding confines radiation in a hollow core, substantially reducing the loss, which is typical of hollow-core-guided modes in conventional, capillary-type hollow waveguides and which rapidly grow with a decrease in the diameter of the hollow core [12, 13]. Unique properties of PCFs open up new routes for a long-distance transmission of electromagnetic radiation [4, 5], as well as for nonlinear-optical transformation of laser pulses [14]. As shown by Knight
et al. [15], PCFs can support single-mode waveguiding within a remarkably broad frequency range. Photonic-crystal fibers offer new solutions for laser physics, nonlinear optics, and optical technologies, as they combine dispersion tuneability and a high degree of light-field confinement in the fiber core. Dispersion of such fibers is tailored by changing their core–cladding geometry [16, 17], while a strong light-field confinement is achieved due to the high refractive-index step between the core and the microstructure cladding [18]. Controlled dispersion of PCFs is the key to new solutions in optical telecommunications and ultrafast photonics. The high degree of light-field confinement, on the other hand, radically enhances the whole catalogue of nonlinear-optical processes and allows observation of new nonlinear-optical phenomena.

4. Maxwell’s equations

To get the dispersion characteristics ($\omega$ versus $\beta$) of the fiber structure, the Maxwell’s equations have to be solved. Decoupling the Maxwell’s equations with no free charges and currents, assuming linear response of the medium and no losses leads to a wave equation for the $H_\omega(r)$ field

$$\nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times H_\omega(r) \right] = \left( \frac{\omega}{c} \right)^2 H_\omega(r),$$

where $\varepsilon$ is the dielectric function. Here the fields have been expanded into a set of harmonic modes $H_\omega(r, t) = \text{Re} \left( H_\omega(r)e^{-i\omega t} \right)$ with frequency $\omega$. This can be done without further loss of generality since the Maxwell’s equations have already been assumed linear [19,20]. Because of translational symmetry along the $z$-axis, the dielectric function only depends on $(x, y)$, consequently the harmonic modes can be expressed in the following form:

$$H_m(r) = \sum_m \alpha_m h_m(x, y)e^{-i\beta_m(\omega)z},$$

where $m$ denotes the $m$th eigenmode with transverse part $h_m(x, y)$ and propagation constant $\beta_m(\omega)$. After expanding in a plane wave basis, the matrix eigenvalue problem is solved leading to the (fully vectorial) eigenmodes. The method is described in [19, 21]. Johnson and Joannopoulos have developed a freely available code to solve the Maxwell’s equations [22]. With this code and a dielectric function based on Fig. 2

![Image of the end face of a PCF with a core diameter of 1.7μm. The picture is provided by Crystal Fibre A/S.](Fig. 2)

Niels Asger Mortensen and Jes Broeng from Crystal Fibre have calculated the transverse part $h_m(x,y)$ of the eigenmodes and propagation constants $\beta_m(\omega)$ [23] (Fig. 3).
Both the material dispersion of silica and the dispersion due to the micro-structuring of the fibers contribute to the effective refractive index of the fundamental mode

\[ n_{\text{eff}} = n_{\text{material}} + n_{\text{eff,bandstructure}} - n_{\text{constant}}, \]  

(3)

The effective propagation constant \( \beta \) of the fundamental mode can subsequently be found from Eq. (1) by inserting \( n_{\text{eff}} \). The refractive index of silica \( n_{\text{material}} \) has been calculated from the Sellmeier formula

\[ n_{\text{material}}^2(\lambda) = 1 + \sum_{j=1}^{3} \frac{B_j}{1 - (\frac{\lambda_j}{\lambda})^2}, \]

(4)

where \( \lambda_j \) is an atomic resonance in the fused silica. For the calculations, the parameters given in [24] have been used: \( B_1=0.6961663 \), \( B_2=0.4079426 \), \( B_3=0.8974794 \), \( \lambda_1=0.0684043 \mu m \), \( \lambda_2=0.1162414 \mu m \), \( \lambda_3=9.896161 \mu m \). The contribution to the effective refractive index from the micro-structuring \( n_{\text{eff,bandstructure}} \) has been calculated by assuming a frequency independent refractive index of silica \( n_{\text{constant}}=1.45 \) in the dielectric function \( \varepsilon(x, y) \) in Eq. (6). By solving the equation, the propagation constant of the fundamental mode \( \beta^{(1)} \) is found, giving \( n_{\text{eff,bandstructure}} = c \beta^{(1)}/\omega \). To include the contribution to \( n_{\text{eff}} \) from silica only once, the constant offset \( n_{\text{constant}} \) in Eq. (8) is introduced. In fact, this constant term will have no impact on the simulations in the following chapters, since a frame of reference moving with the group velocity of the propagating pulse is chosen. Based on an SEM-picture of the fiber end face shown in Fig. 5, the propagation constant of the shown 1.7\( \mu m \) core diameter PCF has been calculated using the method sketched above. The group velocity dispersion \( \beta^2 \), calculated from the propagation constant, is shown in Fig. 3. A mode corresponding to the other polarization state exists, but in the calculations presented in the following chapters only propagation in one polarization mode will be considered, even though for example the fiber in Fig. 5 is not polarization maintaining. The frequency dependency of the refractive index of silica can also be taken into account initially through a frequency dependent dielectric function \( \varepsilon(x, y, \omega) \). The equation (6) then has to be solved self-consistently. When comparing the two methods, no major differences appear. An effective area of a mode in a fiber can be defined as [23, 24]

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**Fig. 3.** Effective area of the same fiber. Calculations are carried out by Niels Asger Mortensen/Jes Broeng from Crystal Fibre A/S.
where $|\mathbf{h}(x, y)|^2$ is proportional to the intensity distribution in the fiber. Fig. 6 shows the effective area of the fundamental mode for the 1.7 $\mu$m core diameter PCF. It is the high index contrast between silica and air that makes the relatively low effective areas in PCFs possible [23].

5. Derivation of a nonlinear Schrödinger equation

Decoupling the Maxwell’s equations with no free current sand charges gives the following wave equation for the electric field $E(t, t)$

$$
\nabla \times \nabla \times E(r, t) = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} t^2 E(r, t) - \mu_0 \frac{\partial^2}{\partial t^2} P(r, t),
$$

where $P(r, t)$ is the polarization, having a contribution from the linear polarization with susceptibility $\chi^{(1)}(t-t1)$ and a contribution from the nonlinear polarization with susceptibility $\chi^{(3)}$, in the following approximated by

$$
\chi^{(3)}(t-t1, t-t2, t-t3)=\chi^{(3) g}(t-t1)\delta(t-t2)\delta(t-t3).
$$

Through the delay function $g(t-t1)$, the interaction of the light with the vibration almodes of silica can be included in the description (Raman scattering). $\chi^{(3)}(t-t1, t-t2, t-t3)$ can be approximated by a product of three delta functions if only the electronic response of the material is wanted, since it is almost instantaneous, in which case one speaks of a Kerr nonlinearity. Because of inversion symmetry of the fibers, the second-order polarization disappears. Further, the induced charges at the surfaces between air and silica are neglected, corresponding to assuming $\nabla E(r, t) = 0$, which leads to the following approximation

$$
\nabla \times \nabla \times E(r, t) \approx \nabla(\nabla E(r, t) - \nabla E(r, t) \times \nabla E(r, t)).
$$

Transforming to the frequency domain. Using the following convention for the Fourier transforms

$$
E^*(r, \omega) = \int_{-\infty}^{\infty} dte^{i\omega t} E(r, t)
$$

And the above listed approximations the wave equation can be transformed into frequency space

$$
\nabla^2 E(r, \omega) + \varepsilon(x, y, \omega) \frac{\partial^2}{\partial z^2} E(r, \omega) = -\mu_0 \omega^2 P(r, \omega),
$$

where

$$
P(r, t) = \varepsilon_0 \chi^{(3) g}(r, t) \int_{-\infty}^{\infty} dt1 g(t-t1) E^2(r, t1).
$$

And $\varepsilon(x, y, \omega)=1+\chi(1)(x,y,\omega)$. As the dielectric function used does not depend on the z coordinate because of translational symmetry along the z-axis. Separating the electric field by assuming weak coupling between the transverse and longitudinal degrees of freedom through the nonlinearity, the electric field can to a good approximation be separated into a product of a function with longitudinal dependence $\tilde{G}(z, \omega)$ and a function with transversal dependence $\tilde{h}(x, y, \omega)$ [25, 26]. Furthermore, the fields are assumed to be linearly polarized along the vector $x$.  

$$
A_{eff,n}(\omega) = \left[ \frac{\int_{-\infty}^{\infty} dxdy |h_n(x,y)|^2}{\int_{-\infty}^{\infty} dxdy |h_n(x,y)|^2} \right]^2.
$$
\[ \mathbf{E}(r, \omega) = x \frac{\hat{h}(x, y, \omega)}{\sqrt{S(\omega)}} \tilde{G}(z, \omega), \]  
(12)

where the normalization factor \( S(\omega) \) is given by

\[ S(\omega) = \int dxdy |\hat{h}(x, y, \omega)|^2, \]  
(13)

\[ \nabla^2 \hat{h}(x, y, \omega) + \varepsilon(\mathbf{r}, \omega) \frac{\omega^2}{c^2} \hat{h}(x, y, \omega) = \beta(\omega)^2 \hat{h}(x, y, \omega), \]  
(14)

\[ \frac{d^2}{dz^2} \tilde{G}(z, \omega) + \beta(\omega)^2 \tilde{G}(z, \omega) = -\frac{\omega^2}{c^2} \chi^{(3)}(\omega) p(z, \omega), \]  
(15)

\[ \tilde{p}(z, \omega) = \left( \frac{1}{2\pi} \right)^2 \int d\omega_1 \int d\omega_2 \tilde{g}(\omega_1 - \omega_2) \times \tilde{G}(z, \omega - \omega_1 + \omega_2) \tilde{G}^*(z, \omega_1) \tilde{G}(z, \omega_1), \]  
(16)

\[ p(z, t) = G(z, t) \int dt' g(t - t') G(z, t') \right|^2, \]  
(17)

\[ A_m(\omega) = \left( \frac{\int dxdy |\hat{h}(x, y, \omega)|^2}{\int dxdy |\hat{h}(x, y, \omega)|^2} \right)^2, \]  
(18)

\[ G(z, t) = \text{Re}[G(z, t) + G(z, t)] = \frac{1}{2} \left[ G(z, t) + G(z, t) \right], \]  
(19)

\[ \tilde{G}(z, \omega) = \frac{1}{2} [\tilde{G} + (z, \omega) + \tilde{G} - (z, \omega)] = \frac{1}{2} [\tilde{U} + (z, \omega) e^{i\beta z} + \tilde{U} - (z, \omega) e^{-i\beta z}] \]  
(20)

\[ \left( \frac{d^2}{dz^2} + \beta(\omega)^2 \right) \tilde{G}(z, \omega) = \left( \frac{d}{dz} + i\beta(\omega) \right) \tilde{G}(z, \omega), \]  
(21)

\[ 2i\beta(\omega) \left( \frac{d}{dz} - i\beta(\omega) \right) \tilde{G}(z, \omega), \]  
(22)

\[ \frac{d}{dz} \tilde{G} + (\omega) = i\beta(\omega) \tilde{G} + \omega + \frac{\omega^2}{c^2} \chi^{(3)}(\omega) \int_\infty^\infty dt' g(t - t') \times \{ 2G(t) + (t_i)G(t_i)G(t) + G(t) + G(t_i)G(t_i) + G(t) + G(t_i)G(t_i) \} \]  
(23)

6. The nonlinear Schrödinger equation

The simplest form of the nonlinear Schrödinger equation is given by

\[ \frac{d}{dz} A = -i \frac{\beta_z}{2} \frac{\partial^2}{\partial t^2} A + i|A|^2 A. \]  
(24)
On the way to the equation above, a more general version of the nonlinear Schrödinger equation will be found. The first term describes the second-order dispersion determined by the material and the geometrical structure of the fiber as described in the previous chapter. The second term is the nonlinearity, which depends upon the polarizability of the material through $\chi^{(3)}$ and scales with the third power of the electric field. The nonlinear Schrödinger equation has been applied in fiber optics since the beginning of the eighties, where it was used to describe Mollenauer’s first experimental observations of solitons in optical fibers [27]. Solitons emerge as fundamental solutions to the nonlinear Schrödinger equation because the dispersion term can balance the nonlinear term. In quantum optics, the Gross-Pitaevskii equation is used to describe the evolution of the Bose-Einstein condensate ground state wave function. The propagation constant can be achieved either through calculations or experimental investigations of the fiber and is often expressed in terms of a Taylor expansion

$$\beta(\omega) = \frac{n_{\text{eff}}(\omega)\omega}{c} = \sum_{m} \frac{1}{m!} \beta_m (\omega - \omega_0)^m; \beta_m = \frac{\partial^n \beta}{\partial \omega^n} \bigg|_{\omega_0}. \ (25)$$

Any dispersion profile can be fitted with a Taylor polynomial, the question is only how many terms are needed to make a good fit over the width of the spectrum.

**The propagation:**

The linear part is

$$\frac{d^2}{dz^2} G(z, \omega) + \beta(\omega)^2 \tilde{G}(z, \omega) = -\frac{\omega^2}{c^2} \frac{\chi^{(3)}}{A_{\text{eff}}(\omega)} \tilde{p}(z, \omega), \ \ (26)$$

$$\frac{d^2}{dz^2} \tilde{G}(z, \omega) = -\beta(\omega)^2 \tilde{G}(z, \omega), \ \ (27)$$

and Eq. (1) both originate from the Maxwell’s linear equations. By considering the magnetic field $\mathbf{H}(\omega) \mathbf{r}$ as given by Eq. (2) and taking the second derivative with respect to $z$, the following equation arises

$$\frac{d^2}{dz^2} \mathbf{H}_m(\mathbf{r}) = -\beta(\omega)^2 \mathbf{H}_m(\mathbf{r}). \ \ (28)$$

The magnetic and electric fields are related by

$$E_m(\omega) = -\frac{ic}{\omega \varepsilon(x, y)} \nabla \times \mathbf{H}_m(\mathbf{r}), \ \ (29)$$

where with translational symmetry $\varepsilon(x, y)$ is independent of $z$. Consequently, $E_m(\omega)$ also fulfills Eq. (30) and $\beta(\omega)$ in this and the previous chapter is the same.

7. Conclusion

The transverse micro-structuring makes the dispersion of the fibers highly tunable and together with the high index contrast it leads to the small effective area, cadre of nonlinear effects can take place in the fibers. The interplay between the special dispersion of the fibers and these nonlinear effects makes the phenomenon of supercontinuum generation possible. The linear Maxwell’s equations have been solved for the transverse structure of the fibers. Starting with the Maxwell’s equations it has been sketched how a nonlinear Schrödinger equation for wave propagation in the PCFs can be achieved. The full frequency dependency of the propagation constant as well as the effective transverse area serve as input for the model and these parameters can either be calculated or measured. The model includes the instantaneous nonlinear response of silica. Additionally, the effects of the Raman scattering, self-steepening and shock formation can be included.
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