Analysis of Optical Propagation in Isotropic Nonlinear Devices
by the Finite Element Method

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Abstract

This work deals with the formulation and implementation of the Finite Element Method (FEM) to the scalar analysis of optical propagation in isotropic nonlinear devices. The resulting computer programmes are used to study structures of practical interest and can be applied to optimize device design.

Starting from Maxwell’s equations, approximations are used to derive specific formulations to treat different classes of problems which include a two-transverse-dimension non-paraxial approach for the steady state case, leading to the Helmholtz equation; and the time domain analysis of slab structures (one dimensional transverse structure).

The numerical treatment is mainly based on the combination of first order finite elements (for the transverse coordinates) and the Crank–Nicolson’s approximation (FEM/CN). A variant of this method, the split operator method (SOM), is also used and a criterion for optimizing the modelling of the nonlinearity is developed.

Practical applications studied for the steady state case include switching, couplers and multi-state devices. Results are tested against previously reported research or analytical results. Numerical stability and convergence are studied for the FEM/CN. Examples are also used to verify the range validity of the SOM and FEM/CN, by investigating stability and convergence of the numerical solution and speed of the algorithms.

The formulation for the time domain analysis, which has been developed for the study of forward propagation of short pulses, includes the modelling of second order dispersion and the Debye equation for modelling the delayed response of the nonlinearity. That approach has been validated with the analysis of practical examples. An extension of this formulation has also been developed to analyze pump-controlled devices.
To María Pía,
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# Contents

1 Introduction ................................................................. 13

1.1 Overview .................................................................................. 13

1.2 Goals ........................................................................................ 15

1.3 Outline of the Thesis .............................................................. 15

2 Physical background and formulations .................................. 17

2.1 Physical representation .......................................................... 17

2.1.1 Maxwell’s equations ............................................................... 18

2.1.2 Helmholtz equation ............................................................... 18

2.1.3 Scalar Approximation (Isotropy) ........................................ 19

2.1.4 Monochromatic approximation ............................................. 20

2.1.5 Quasi-monochromatic approximation .................................... 21

2.1.6 Paraxial approximation and Generalized Nonlinear Schrödinger Equation for the stationary case ............................. 21

2.1.7 Non-paraxial approximation (forward propagation) and mathematical formulation for the stationary case ..................... 22

2.1.8 Time Domain and Noninstantaneous response (Paraxial approximation) ............................................................ 23

2.1.9 Time Domain and Noninstantaneous response (Non-Paraxial approximation) ......................................................... 28

2.1.10 Pumping and First Order Dispersion ..................................... 29
2.2 Methods of Solution ................................................................. 30
  2.2.1 Overview ............................................................. 30
    2.2.1.1 Theta and Crank-Nicolson methods ................. 30
    2.2.1.2 Analysis of CN approximation for the Nonlinear Term . 32
    2.2.1.3 Finite Element Method ........................................ 34
  2.2.2 Paraxial approximation .................................................... 34
    2.2.2.1 Propagation ....................................................... 34
    2.2.2.2 Modal Equation .................................................. 42
    2.2.2.3 Stability ............................................................ 43
  2.2.3 Non-Paraxial approximation for 2D+z ................................. 44
    2.2.3.1 Propagation ....................................................... 44
    2.2.3.2 Modal Equation .................................................. 45
    2.2.3.3 Stability ............................................................ 46
  2.2.4 Time Domain (Paraxial approximation) ............................... 48
    2.2.4.1 Propagation ....................................................... 48
    2.2.4.2 Modal Equation .................................................. 51
    2.2.4.3 Stability ............................................................ 52
  2.2.5 Time Domain (Perturbed Debye equation and Non-paraxiality) . 52
    2.2.5.1 Propagation ....................................................... 52
    2.2.5.2 Modal Equation .................................................. 53
    2.2.5.3 Stability ............................................................ 54
  2.2.6 Pumping and First Order Dispersion .................................. 54
    2.2.6.1 Propagation ....................................................... 54
    2.2.6.2 Modal Equation .................................................. 55
2.2.6.3 Stability ......................................................... 56
2.2.7 Split-Operator/Galerkin Method ....................... 56
2.2.7.1 Paraxial Formulation ........................................ 56
2.2.7.2 Non-paraxial Formulation ............................... 57

3 Analysis in Steady State ........................................ 60

3.1 Practical Structures under Paraxial Approximation .... 60
3.1.1 Validation .......................................................... 60
3.1.1.1 Evolution of Overfilling Gaussian Input through a rib structure 61
3.1.1.2 Evolution of Embedded Gaussian Input through a rib structure 64
3.1.1.3 Evolution of a single waveguide mode through a rib coupler 66
3.1.2 Nonlinear Switch ............................................... 73
3.1.3 Nonlinear Coupler ............................................. 77
3.1.4 Three-state Nonlinear Coupler ......................... 81
3.1.5 Wavelength Multiplexor/De-multiplexor .............. 85
3.1.6 Comparison of methods for the simulations .......... 92

4 Analysis in Time Domain ....................................... 95

4.1 Validations ......................................................... 95
4.1.1 Full Inclusion of Debye Equation ....................... 95
4.1.1.1 Linear validation ................................................. 96
4.1.2 Approximated Debye Term ............................... 104
4.1.2.1 Linear validation ............................................... 104
4.1.2.2 Nonlinear validation ....................................... 104
4.2 Applications ....................................................... 111
4.2.1 A Nonlinear Demultiplexer .................................................. 112

5 Conclusions .............................................................................. 117

5.1 General Conclusions .............................................................. 117

5.2 Extensions and Improvements of the Methods ....................... 119

A FEM formulae—Green Integrals ............................................. 122

B First order FEM: Internal Products ......................................... 124

C Comparison of two approximations for the CNG Method ........ 126

D Published Work ...................................................................... 128
List of Figures

2.1 Variation of the amplification factor for the $\theta$-method versus the spectrum $h$ for different values of $\theta$. ......................................................... 44

3.1 Rib structure ................................................................. 61
3.2 Contour plot at 0, 1 and 2 [$\mu m$] .................................................. 62
3.3 Basic structure and final mesh of the structure (3617 elements and 1848 nodes) 63
3.4 Power evolution plot .......................................................... 63
3.5 Basic and final (3654 elements and 1866 nodes) meshes on the structure ... 64
3.6 Contour plot at 1, 2 and 3 [$\mu m$] ............................................... 65
3.7 Contour plot at 4, 5 and 6 [$\mu m$] ............................................... 65
3.8 Contour plot at 7 [$\mu m$] ......................................................... 66
3.9 Power evolution plot .......................................................... 66
3.10 Rib coupler structure ....................................................... 67
3.11 Basic mesh and structure .................................................... 68
3.12 Actual mesh and structure: 3446 elements and 1756 nodes ................. 68
3.13 Power plot: Evolution and Transference ................................. 69
3.14 Contour plot at $z = 1.55[\mu m]$ ............................................... 69
3.15 Contour plot at $z = 77.5[\mu m]$ ................................................ 70
3.16 Contour plot at $z = 155[\mu m]$ ............................................... 70
3.17 Contour plot at $z = 232.5[\mu m]$ .................................................. 70
3.18 Contour plot at $z = 310[\mu m]$ ....................................................... 71
3.19 Contour plot at $z = 387.5[\mu m]$ .................................................... 71
3.20 Contour plot at $z = 465[\mu m]$ ....................................................... 71
3.21 Contour plot at $z = 542.5[\mu m]$ .................................................... 72
3.22 Contour plot at $z = 620[\mu m]$ ....................................................... 72
3.23 Contour plot at $z = 697.5[\mu m]$ .................................................... 72
3.24 Contour plot at $z = 775[\mu m]$ ....................................................... 73
3.25 Strip-based Switch Structure. $\epsilon_{l,cl} = \epsilon_{l,sub} = 2.2500$, $\epsilon_{l,st} = 2.4649$ and $\alpha_{sub} = 6.377266 \cdot 10^{-12}[m^2/V^2]$ .......................................................... 74
3.26 Evolution of the optical beam along the waveguide. Projections on the x=0 plane are shown for values of z from 0 to 12 $\mu m$ .................. 74
3.27 Contour plot of the $E_y$ field component on the $x = 0$ plane showing the evolution of the beam from the excitation to a distance of 65 $\mu m$ .... 75
3.28 Transverse distribution of the $E_y$ field of the input beam and of the switched beam at a distance of 40 free-space wavelengths (20.6 $\mu m$) from the excitation plane. .......................................................... 76
3.29 Switching distance as a function of the power of the input beam. .... 76
3.30 Basic mesh for the lower Cross Section ........................................ 78
3.31 Evolution of the beam in a nonlinear coupler on the symmetry line, Input Power = 1 mW .......................................................... 79
3.32 Comparison of power in one guide of a buried guide coupler, calculated over two complete cycles with the CN method (2.168) and SOM. Total input power in the coupler = 1 mW ........................................ 80
3.33 Total power in the coupler and power in the excitation arm calculated with the CN method based on (2.168) for total input of 10 mW ........ 80
3.34 Total power in the coupler and power in the excitation arm calculated with the CN method based on (2.167) for total input of 10 mW. Small fluctuations are visible. ........................................ 81
3.35 Power in the buried guide coupler calculated with the CN method (2.168) and SOM. The SOM fails to conserve power for total input power of 10 mW.

3.36 Cross-section of the coupler

3.37 Coupler: 1088 nodes, 2070 elements

3.38 Evolution of the Electric Field on the symmetry line

3.39 Design curves: Absolute Output Power vs. Total Input Power

3.40 Power transfer for different Input Powers

3.41 Normalized signal powers in the two waveguides versus propagation distance

3.42 Normalized signal powers in the two waveguides versus signal wavelength

3.43 Input and output Electric Field Distributions at $\lambda = 1520 \, \text{nm}$

3.44 Input and output Electric Field Distributions at $\lambda = 1548 \, \text{nm}$

3.45 Design curves for the wavelength selective coupler (P1 means power on the co-doped arm, and P2 is the power on the other arm)

3.46 Comparison of total propagated power in the buried guide coupler, calculated over two complete cycles with the CN method (2.168) and SOM. Total input power in the coupler = 1 mW.

4.1 Mesh for the coupler: 703 nodes and 1041 elements

4.2 Total and relative power in the coupler

4.3 Space-time distribution of $E_x$. From top to bottom and left to right: $z = 0.31 \, \mu m$, $z = 153.2 \, \mu m$, $z = 306.4 \, \mu m$, $z = 459.6 \, \mu m$ and $z = 612.49 \, \mu m$.

4.4 Evolution of $E_x(x, y = 20 \, \mu m, z = z_k; k = 1, \ldots)$

4.5 Local time envelopes of the pulse at $z = 0.31 \, \mu m$ and $z = 612.49 \, \mu m$

4.6 Total and relative power in the coupler

4.7 Mesh for the coupler: 1735 nodes and 3386 elements

4.8 Local time envelopes of the pulse at $z = 0.08 \, \mu m$ and $z = 612.8 \, \mu m$
4.9 Space–time distribution of $E_z$. From top to bottom and left to right: $z = 0.08 \mu m$, $z = 153.2 \mu m$, $z = 306.4 \mu m$, $z = 459.6 \mu m$ and $z = 612.8 \mu m$. .......................... 103

4.10 Space–time distribution of $E_z$. From top to bottom and left to right: $z = 0.08 \mu m$, $z = 153.2 \mu m$, $z = 306.4 \mu m$, $z = 459.6 \mu m$ and $z = 612.8 \mu m$. .......................... 105

4.11 Space–time distribution of $E_z$. From top to bottom and left to right: $z = 0.08 \mu m$, $z = 153.2 \mu m$, $z = 306.4 \mu m$ and $z = 459.6 \mu m$. .......................... 107

4.12 Space–time distribution of $E_z$ for $z = 153.2 \mu m$. From top to bottom and left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0 fs$, $\tau = 1.5 fs$, $\tau = 3.0 fs$. .................................................. 108

4.13 Space–time distribution of $E_z$ for $z = 306.4 \mu m$. From top to bottom and left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0 fs$, $\tau = 1.5 fs$, $\tau = 3.0 fs$. .................................................. 109

4.14 Space–time distribution of $E_z$ for $z = 459.6 \mu m$. From top to bottom and left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0 fs$, $\tau = 1.5 fs$, $\tau = 3.0 fs$. .................................................. 110

4.15 Space–time distribution of $E_z$ for $z = 620.46 \mu m$. From top to bottom and left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0 fs$, $\tau = 1.5 fs$, $\tau = 3.0 fs$. .................................................. 111

4.16 Level of confinement for $\tau = 3.0 fs$ (top curve), $\tau = 1.5 fs$ (curve in the middle) and $\tau = 0 fs$ (bottom curve). .................................................. 112

4.17 Mesh for the demultiplexer: 2349 nodes and 4784 elements. .......................... 113

4.18 Time–envelope of the electric field at the input, $1 \mu m \equiv 51.968 fs$. ........ 114

4.19 Space–time distribution of $E_z$, for $z = 75\lambda_0$. .................................. 115

4.20 Mesh for the demultiplexer: 2460 elements and 1278 nodes. ..................... 115

4.21 Space–time distribution of $E_z$. From left to right: $z = \lambda_0$ and $z = 50\lambda_0$. 116
Chapter 1

Introduction

1.1 Overview

Many optical devices and systems are based on isotropic media, either linear or nonlinear. Although design and development for these can be done on a purely experimental basis, mathematical analysis can be an effective complement for the design. Moreover, the theoretical approach can prove to be resource saving. Experimental work is not substituted by numerical analysis but its role is reassigned to the final stages where validation of the practical results can not be avoided. Many of the problems found in this field do not have analytical solution, so they need to be solved applying numerical analysis by means of efficient computer techniques.

The full physical description of an optical material considers anisotropy and nonlinearity but such description is highly complicated due to the number of state variables involved. Many practical applications use materials such as glasses and semiconductors, where anisotropy is negligible and the main effects are both isotropic and nonlinear. Nonisotropic materials are beyond the scope of this work, so the mathematical formulation of the physical problem is limited to problems where the polarization of the fields can be expressed in terms of the main component, leading to a scalar formulation.

Many of the problems already analyzed in nonlinear optics have taken into account only
modal analysis [2]–[4] which means that solutions to those problems are known only for the steady state. Unfortunately, sometimes that steady state is reached after a very long distance of propagation or after a very long time, and sometimes some aperiodicity leads to no mode at all. Modal analysis is not able to produce useful answers for predicting behaviour of discrete optical devices or devices which are subject to very short excitations, so a propagation analysis emerges as the natural solution to that sort of problem.

Propagation analysis accounts for the description of the evolution of the field distribution along the waveguide structure or through time for which an accurate characterization may well lead to very valuable tools for design. Given the usefulness of propagation analysis, it is important to decide on an efficient method for its description, keeping in mind that the local limited computational resources currently suggest that no more than three variables can be used for the modelling. As this problem has been studied by some authors, there are already several methods proposed for analysing propagation for three dimensional problems, like Finite Differences [5]–[7], Finite Elements [8], Fourier Decomposition [7], [9], Lanczos reduction method [10], [11], Split Operator Method [12], Nonparaxial Correction [13], Wide Angle approximation [7], [14], and others. Combinations of these methods have been used for solving the propagation problem, but some of the methods show some disadvantages, for example FDTD-dti (Finite Differences-Time Domain direct time integration) is intensive in memory resources and slow, Lanczos reduction is intensive in memory and execution time, and requires huge computer resources. Other methods restrict the solution to only forward propagation, slow envelope variations, or other constraints. Even though the formulation of Finite Elements is slightly more complex than other approaches, when used as a weak formulation (Galerkin) the problem is usually reduced to a sparse matrix problem, which allows a very efficient and accurate solution. Another advantage of the method is the possibility of using an arbitrary mesh [15], [16] which permits to increase efficiency of the method by improving accuracy where it is required, along with a fast response [17]. A shortcut in terms of execution time has been reported to be the combination of Finite Element Method and Split Operator Method [8]. FEM, CN/G and split operator techniques will be used in this work, in order to allow a thorough description of the physical behaviour of the guiding structures to be studied.
1.2 Goals

This work will concentrate on the development of some software tools and in the study of optical guiding structures, using these tools and others already available. Given the practical limitations of the computer resources, the study is limited to symmetric structures. Thus, from the three spatial coordinates and time, one of the variables can be discarded: in one case, the so called 2D+z, the steady state will be analyzed, in the other case, planar structures will be analyzed on the time-domain (1D+z+t).

During the development of the computer programs, optimum performance and stability are considered in order to maximize robustness and efficiency. Comparisons of the methods are provided where possible. Practical applications analyzed here include couplers, switches and multi-state devices.

1.3 Outline of the Thesis

Chapter 2 deals mainly with theoretical aspects of wave propagation in nonlinear media and with the formulation of the methods used later in conjunction with the finite element method to describe wave propagation. The approximations used are here explained and the Crank–Nicolson method is detailed and expanded. Both time–independent and time–domain formulations are introduced, analyzing the transverse mode solutions and also stability of quasi–linear formulations. In this chapter the following aspects are introduced for the first time:

- Analysis of the Crank–Nicolson approximation for the nonlinear term, giving useful results for many nonlinear problems (section 2.2.1.2)
- Analysis of stability of the non–paraxial approximation for 2D + z (section 2.2.3.3)
- Study of the modal equations and stability for the time domain analysis with the paraxial approximation (sections 2.2.4.2 and 2.2.4.3)
1: Introduction

• Analysis of the modal equations and stability for the perturbed Debye equation and for the nonparaxial case (sections 2.2.5.2 and 2.2.5.3)

• Analysis of modes and stability for devices with signal and pump beams, considering first order dispersion (sections 2.2.6.2 and 2.2.6.3)

• Application of the split-operator/Galerkin method to the non-paraxial formulation (section 2.2.7.2).

Chapter 3 gives validation of the numerical methods and presents practical applications of the time-independent problem. Results are compared with physical predictions and the methods and programs used are checked for stability, reliability and optimum performance in the use of computer resources. The validations concern the computer programs using Crank–Nicolson/Galerkin alongside with the finite element method. These methods are applied for the first time to problems of propagation along structures of constant cross-section (section 3.1.1). Three examples of application are analyzed with the same program developed here to solve the propagation problem (see sections 3.1.2, 3.1.3 and 3.1.4). A new design of a wavelength multiplexor/demultiplexor is introduced (section 3.1.5) and studied using the methods described in Chapter 2, and for the first time a practical comparison of these methods is done (section 3.1.6).

Chapter 4 describes validation of the computer programs for the analysis in the time-domain, and also includes an application. Physical interpretation is made of all the main features of the validations and the example analyzed. The validations make use of the programs where propagation is studied using Crank–Nicolson/Galerkin and finite elements for the first time in the time-domain analysis. The example analyzed here is the first practical application of the programs created here (section 4.2).

Chapter 5 presents the conclusions of this work and overviews the research that is being carried out to optimize and extend the scope of the applications. A new suggestion on the computational method for dealing with the nonlinear matrix is introduced (section 5.2).

Finally, Appendix C presents an original contribution to the comparison of two approximations for the Crank–Nicolson/Galerkin method.
Chapter 2

Physical background and formulations

The main purposes of modelling in any physical situation are to describe the phenomena and to predict behaviour of the device. Maxwell's equations [18], [19] describe very well the optical phenomena, but their exact analytical solutions are generally hard to achieve. In order to get practical solutions some approximations need to be done. These approximations may constrain the validity range of the model, but for the situations under these assumptions, the solutions should then be reliable and quickly obtained, so the approximations would be worthwhile.

2.1 Physical representation

For the materials that are currently being used in the fabrication of optical devices, their macroscopic behaviour will be taken into account; this means that either permittivity and permeability or refractive index will usually be explicitly given. In other more complex cases, those indices will be given implicitly through equations that will describe more non-linear complexity. For the particular case of bichromatic operation, two excitations will be considered: signal and pump, where the pump —i.e. local oscillator— is intended to control
the behaviour of the material for the propagation of the signal [20], [21].

2.1.1 Maxwell’s equations

Mathematical modelling of the electromagnetic physical behaviour is described by Maxwell’s Equations. According to the nature of the problem to be solved, Maxwell’s Equations may require some simplifications; this means that once the solution is reached, its analysis is valid under the already made assumptions.

As a starting point Maxwell’s Equations are presented here:

\[ \nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \]  
\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \]  
\[ \nabla \times \vec{D} = \rho \]  
\[ \nabla \times \vec{B} = 0 \]

And the following relations hold [22]:

\[ \vec{D} = \varepsilon_0 \vec{E} + \vec{P} \]  
\[ \vec{P} = \sum_{n=1}^{\infty} \int \cdots \int_{-\infty}^{\infty} \chi^{(n)}(t - t_1, \ldots, t - t_n) \vec{E}(\vec{r}, t_1) \cdots \vec{E}(\vec{r}, t_n) dt_1 \cdots dt_n \]  
\[ \vec{B} = \mu_0 \vec{H} + \vec{M}, \]

where \( \chi \) represents the electric susceptibility of the medium, and includes both linear and nonlinear contributions. For the optical problems treated here, \( \vec{M} \) will always be zero, and so will be \( \rho \). Also, on most of the cases, \( \vec{J} \) will be zero. If that is not the situation, conductivity will be included as part of permittivity.

2.1.2 Helmholtz equation

Taking the curl of (2.2) the following relation is obtained:

\[ \nabla \times \nabla \times \vec{E} = -\nabla^2 \vec{E} + \nabla \left( \nabla \times \vec{E} \right) \]
\[ = -\varepsilon_0 \frac{\partial^2 (\vec{E} + \vec{P})}{\partial t^2} \]
This equation will be regarded as the complete Helmholtz equation for $\vec{E}$. Following a similar procedure with (2.1), $\vec{H}$ is described by:

$$\vec{\nabla} \times \vec{\nabla} \times \vec{H} = -\vec{\nabla}^2 \vec{H} = -\mu_0 \varepsilon_0 \frac{\partial^2 \vec{H}}{\partial t^2} + \frac{\partial (\vec{\nabla} \times \vec{P})}{\partial t}$$

(2.10)

(2.11)

This equation will be regarded as the complete Helmholtz equation for $\vec{H}$.

Sometimes it will be necessary to return to (2.9) and (2.11), where the polarization vector appears explicitly.

Main simplifications of the Helmholtz equation are combinations of the following choices:

- Monochromatic/Time Domain
- Scalar/Full Vector
- Paraxial/Non-Paraxial

The following sections will deal with these approaches.

2.1.3 Scalar Approximation (Isotropy)

Assuming that the media are isotropic materials with instantaneous response, $\vec{P}$ must be proportional to $\vec{E}$. So now, (2.5) can be written as:

$$\vec{D} = \varepsilon \varepsilon_0 \vec{E}$$

(2.12)

where

$$\varepsilon = \varepsilon_1 + \varepsilon_n(\vec{r}, \vec{E})$$

(2.13)

From (2.9) and another two restrictions:

- the slow variation of the permittivity $\varepsilon$: $\frac{\partial \varepsilon}{\partial t} \simeq 0$, and

- $\varepsilon$ is weakly dependent on the coordinates: $\vec{\nabla} \cdot (\vec{\nabla} \cdot \vec{E}) = -\vec{\nabla} \cdot (\vec{E} \cdot \vec{\nabla} (\varepsilon \varepsilon_0)) \simeq 0$, 

it is possible to rewrite Helmholtz Equation for $\vec{E}$, constrained to isotropy as well, in the form:

$$
\nabla^2 \vec{E} - \varepsilon_0 \varepsilon_\mu \frac{\partial^2 \vec{E}}{\partial t^2} = 0
$$

(2.14)

Again, taking (2.11), considering isotropy and the following two restrictions:

- slow variations of $\varepsilon$: $\frac{\partial \varepsilon}{\partial t} \approx 0$ and
- $\varepsilon$ weakly dependent on the coordinates, but usually stronger than as assumed in (2.1.3): $\nabla \varepsilon \approx 0$,

the new Helmholtz equation for $\vec{H}$ is:

$$
\nabla^2 \vec{H} - \varepsilon_0 \mu_0 \frac{\partial^2 \vec{H}}{\partial t^2} = 0
$$

(2.15)

With the approximations made here and assuming that reflections are negligible during propagation, it is possible to demonstrate that only one component of the field is needed to obtain solutions of the problem, so both versions of the Helmholtz equation turn into scalar equations. The assumption of negligible reflections is very strong but is correct when refractive indices do not vary greatly; that is quantitatively [22]:

$$
\left( \frac{n_{co}^2 - n_{cl}^2}{2n_{co}^2} \right) = \Delta
$$

(2.16)

$$
\Delta \lesssim 10\%
$$

(2.17)

### 2.1.4 Monochromatic approximation

In linear problems, it is shown that the superposition principle applies with no further assumptions, but in nonlinear problems the extension of this principle means that high order terms are being neglected, specially self modulation terms. For the present case, monochromatic approximation stands for the case where only one frequency component is taken into account. And this also means that this approximation assumes steady state, because any fluctuation requires extra frequency components to describe the phenomenon.
The monochromatic approximation will be described here by the following expressions:

\[ E(r, t) = \tilde{E}(x, y, z) \exp(j(\omega t - \beta_0 z)) + \tilde{E}_b(x, y, z) \exp(j(\omega t + \beta_0 z)) \]  
\[ H(r, t) = \tilde{H}(x, y, z) \exp(j(\omega t - \beta_0 z)) + \tilde{H}_b(x, y, z) \exp(j(\omega t + \beta_0 z)) \]  

where \( \beta_0 \) is a reference propagation constant to be chosen as closer as possible to the inverse of the phase velocity and \( \omega \) is the angular frequency. \( \tilde{E}_b \) and \( \tilde{H}_b \) represent backwards propagation fields.

This approximation reduces the complexity of the problem to only 3 independent variables (transverse and longitudinal coordinates), because under Fourier transformation, the \( \frac{\partial}{\partial t} \) operator can be replaced by \( j\omega \) as a multiplier, eliminating the time variable.

### 2.1.5 Quasi–monochromatic approximation

When time fluctuations are significant, the technique used for the monochromatic behaviour can be applied, but keeping the time variable. This approximation can be called quasi–monochromatic because it allows the existence of other frequency components closer to the main frequency (usually the excitation frequency).

In order to keep the size of the problem restricted to three independent variables, other kind of approximations are needed if the monochromatic approximation needs to be implemented.

### 2.1.6 Paraxial approximation and Generalized Nonlinear Schrödinger Equation for the stationary case

If propagation is assumed to be along the \( z \)-axis, \( \nabla \) can be expressed as:

\[ \nabla = \nabla_t + \frac{\partial}{\partial z} \]  

Partially differentiating (2.18) or (2.19) with respect to \( z \), we get for a particular choice of the parameter \( \beta_0 \):

\[ \frac{\partial^2 \tilde{E}}{\partial z^2} = \left( \frac{\partial^2 \tilde{E}}{\partial z^2} - 2j\beta_0 \frac{\partial \tilde{E}}{\partial z} - \beta_0^2 \tilde{E} \right) \exp(j(\omega t - \beta_0 z)) \]
but this approximation means that second order fluctuations of $\vec{E}$ are negligible with respect to $2j\beta_0 \frac{\partial \vec{E}}{\partial t}$. So the paraxial approximation leads to:

$$\frac{\partial^2 \vec{E}}{\partial z^2} \approx (-2j\beta_0 \frac{\partial \vec{E}}{\partial z} - \beta_0^2 \vec{E}) \exp(j(\omega t - \beta_0 z) + b.t., \quad (2.22)$$

and

$$\frac{\partial^2 \vec{H}}{\partial z^2} \approx (-2j\beta_0 \frac{\partial \vec{H}}{\partial z} - \beta_0^2 \vec{H}) \exp(j(\omega t - \beta_0 z) + b.t., \quad (2.23)$$

where b.t. means backward term.

Once any of the last two relations is replaced in Helmholtz equation, it is obvious that only one sign is allowed; one means forward propagation, and the other backward propagation. Here forward propagation will be used, so the other terms will be excluded. When both the monochromatic and the paraxial approximations are combined, the equation is reduced to:

$$-\nabla^2 \vec{E} + \left( \beta_0^2 - \epsilon \left( \frac{\omega}{c} \right)^2 \right) \vec{E} = -2j\beta_0 \frac{\partial \vec{E}}{\partial z}, \quad (2.24)$$

symbolically (2.24) can be written as:

$$-2j\beta_0 \frac{\partial \vec{E}}{\partial z} = \left( \mathcal{L} + \mathcal{N} \right) \vec{E}, \quad (2.25)$$

where the operators $\mathcal{L}$ and $\mathcal{N}$ are given by:

$$\mathcal{L} = -\nabla^2_t + \left( \beta_0^2 - \epsilon_t \left( \frac{\omega}{c} \right)^2 \right), \quad (2.26)$$

$$\mathcal{N} = -\epsilon_{nl} \left( \frac{\omega}{c} \right)^2. \quad (2.27)$$

Equation (2.25) is usually called the Generalized Nonlinear Schrödinger Equation (GNSE).

2.1.7 Non-paraxial approximation (forward propagation) and mathematical formulation for the stationary case

Starting from the following equation, which is nonparaxial, but includes a reference propagation constant:

$$\frac{\partial^2 \vec{E}}{\partial z^2} - 2j\beta_0 \frac{\partial \vec{E}}{\partial z} = \left( \mathcal{L} + \mathcal{N} \right) \vec{E}, \quad (2.28)$$
where \( \mathcal{L} \) and \( \mathcal{N} \) are the linear and nonlinear operators previously defined in (2.26) and (2.27), and setting:

\[
\mathcal{F} = \frac{\partial \mathcal{E}}{\partial z},
\]  

(2.29)

it is possible to write the following equivalent matrix equation:

\[
\frac{\partial}{\partial z} \begin{bmatrix} \mathcal{E} \\ \mathcal{F} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \mathcal{L} + \mathcal{N} & 2j\beta_0 \end{bmatrix} \begin{bmatrix} \mathcal{E} \\ \mathcal{F} \end{bmatrix}.
\]  

(2.30)

The variable transformation has reduced the order of the differential equation but has doubled the order of the matrix, if compared to the paraxial approximation. Usefulness of this matrix equation is considered by analyzing its stability (see section 7.2.3).

### 2.1.8 Time Domain and Noninstantaneous response (Paraxial approximation)

Time domain analysis under the paraxial approximation is intended to model propagation in nonlinear materials. In order to do so, material models must take into account not only their nonlinearity but also relaxation times or noninstantaneous response. Failure to model this behaviour will lead to a monochromatic approximation.

As in (2.6) a convolution integral in time appears; this means that usually higher frequency components will be found in the expression for polarization.

The time domain analysis restricted to the scalar case with isotropy will be considered at the beginning. But it is necessary to return to (2.9) and (2.6) before applying those approximations. Assuming the same behaviour for \( \varepsilon \), as before in (2.1.3) (weak dependence on coordinates):

\[
\nabla^2 \vec{E} - \mu_0 \frac{\partial^2}{\partial t^2} \left( \varepsilon_0 \vec{E} + \vec{P} \right) = 0.
\]  

(2.31)

In order to use (2.31), some considerations will be made about polarization and other features of the media. The polarization vector \( \vec{P} \) is separated into its linear and nonlinear
parts and then (2.31) may be rewritten as:

\[ \nabla^2 \vec{E} - \mu_0 \frac{\partial^2}{\partial t^2} \left( \varepsilon_0 \vec{E} + \vec{P}_1 + \vec{P}_n \right) = 0 \]  

(2.32)

Now it is essential to develop a good approximation for the polarization, but it should be considered that \( \chi(\Omega) \) is actually a function that depends on \( \Omega \) which is the combination of sums and differences of all the exciting frequencies. That is a very important fact, because as the study is going to be concentrated near the fundamental frequency (quasi-monochromatic approximation), \( \chi^{(2n)} \) with \( n = 1, 2, \ldots \) will produce interactions at more than twice the input frequency, when exciting with only one frequency. Usually, the first and the third order components of the polarization vector will be enough for a good description of the behavior of the media. Application of the scalar approximation and other criteria briefly mentioned, yields linear and nonlinear parts of \( \vec{P}_n \), that are introduced as [21]:

**Linear response of the media:**

\[ P_1 = \frac{1}{2} \left( \int_{-\infty}^{\infty} \chi^{(1)}(t-t_1)E(\vec{r}, t_1)dt_1 + \text{c.c.} \right) \]  

(2.33)

**Nonlinear instantaneous response of the media:**

\[ P_{nl} = \varepsilon_{nl} \varepsilon_0 E \]  

(2.34)

\[ \varepsilon_{nl} = \frac{3}{4\varepsilon_0} \chi^{(3)} \int |E|^2 \]  

(2.35)

Now assuming \( E = \mathcal{E} e^{j(\omega t - \beta_0 z)} \) (neglecting backwards propagation) and applying the Fourier Transformation to (2.32):

\[ \nabla^2 \mathcal{E}(\omega - \omega_0) e^{-j\beta_0 z} = \mathcal{F} \left\{ \frac{\partial^2 \varepsilon_{nl} \mathcal{E} e^{j\omega t}}{\partial t^2} \right\} e^{-j\beta_0 z} \mathcal{E}(\omega - \omega_0) e^{-j\beta_0 z} - \beta^2(\omega) \mathcal{E}(\omega - \omega_0) e^{-j\beta_0 z}, \]

where

\[ \beta^2(\omega) = \left( 1 + \frac{\chi^{(1)}(\omega)}{\varepsilon_0} \right) k_0^2 \]  

(2.36)

\[ (\nabla_1^2 + \frac{\partial^2}{\partial z^2} - 2j\beta_0 \frac{\partial}{\partial z} - \beta_0^2)\mathcal{E}(\omega - \omega_0) + \beta^2 \mathcal{E}(\omega - \omega_0) - \frac{4\mathcal{E}}{c^2} \mathcal{F} \left\{ \frac{\partial^2 \varepsilon_{nl} \mathcal{E} e^{j\omega t}}{\partial t^2} \right\} = 0, \]  

(2.37)

clearly \( \beta \) is the linear constant of propagation, which has a dependence on the frequency.

Now introducing in (2.37) the paraxial approximation:

\[ \chi^{(3)}_{xxxx} \text{ is the third order nonlinear susceptibility. [21]} \]
\[ 2j\beta_0 \frac{\partial \mathcal{E}(\omega - \omega_0)}{\partial z} + \nabla_i^2 \mathcal{E}(\omega - \omega_0) + (\beta^2 - \beta_0^2) \mathcal{E}(\omega - \omega_0) - \frac{1}{c^2} \mathcal{F} \left\{ \frac{\partial^2 \varepsilon_{nl} \varepsilon e^{j\omega_0 t}}{\partial t^2} \right\} = 0, \]  

(2.38)

when \( \beta \approx \beta_0 \). The value \( \beta^2 - \beta_0^2 \) is usually approximated as \( 2\beta_0 (\beta - \beta_0) \) [21]; such approximation will be avoided here. The usual Taylor expansion for \( \beta \) will be used, and \( \beta^2 \) is the term to be replaced in (2.38). Aiming at returning to the time-domain, clearly the expansions of \( \beta \) and \( \beta^2 \) are linear operators. Now those expansions are developed:

\[
\beta = \beta_0 + (\omega - \omega_0)\beta_{1i} + \frac{1}{2}(\omega - \omega_0)^2 \beta_{2i} + \frac{1}{6}(\omega - \omega_0)^3 \beta_{3i} + \frac{1}{24}(\omega - \omega_0)^4 \beta_{4i} + O \left( (\omega - \omega_0)^5 \right) \]  

(2.39)

\[
\beta^2 = \beta_0^2 + 2(\omega - \omega_0)\beta_{0i}\beta_{1i} + (\omega - \omega_0)^2 \left( \beta_{1i}^2 + \beta_{0i}\beta_{2i} \right) + (\omega - \omega_0)^3 \left( \beta_{1i}\beta_{2i} + \frac{1}{3} \beta_{0i}\beta_{3i} \right) + (\omega - \omega_0)^4 \left( \frac{1}{4} \beta_{2i}^2 + \frac{1}{3} \beta_{1i}\beta_{3i} + \frac{1}{12} \beta_{0i}\beta_{4i} \right) + O \left( (\omega - \omega_0)^5 \right) \]  

(2.40)

where

\[
\beta_{qi} = \frac{d^q \beta_i}{d\omega^q} \quad q = 1, 2, 3, \ldots, \text{ (where "i" indicates material).} \]  

(2.41)

And the approximate operator, using the inverse Fourier Transformation is:

\[
\beta^2 = \beta_0^2 - 2j\beta_{0i}\beta_{1i} \frac{\partial}{\partial t} - \left( \beta_{1i}^2 + \beta_{0i}\beta_{2i} \right) \frac{\partial^2}{\partial t^2} + j \left( \beta_{1i}\beta_{2i} + \frac{1}{3} \beta_{0i}\beta_{3i} \right) \frac{\partial^3}{\partial t^3} + \left( \frac{1}{4} \beta_{2i}^2 + \frac{1}{3} \beta_{1i}\beta_{3i} + \frac{1}{12} \beta_{0i}\beta_{4i} \right) \frac{\partial^4}{\partial t^4} \]  

(2.42)

In the case of fast and simple response time of nonlinearities, usually 2\(^{nd}\) order time derivatives are enough, but if the accuracy is to be increased, for example if the delay has a dependence on the frequency or simply when the 3\(^{rd}\) order terms are comparable to lower order terms, the 3\(^{rd}\) order time derivative should also be included; in such a case the F.E.M. problem is increased because 2\(^{nd}\) order finite elements (at least) have to be used, but as 2\(^{nd}\) order elements allow the use of 4\(^{th}\) order finite derivatives, it is advisable to include those higher order derivatives whenever 2\(^{nd}\) order finite elements are used.

In order to express everything with no explicit appearance of \( e^{j\omega_0 t} \), i.e., eliminating the carrier or high frequency beating, the nonlinear term is calculated here:

\[
-\frac{1}{c^2} \mathcal{F} \left\{ \frac{\partial^2 \varepsilon_{nl} \varepsilon e^{j\omega_0 t}}{\partial t^2} \right\} = \frac{1}{c^2} \omega^2 \varepsilon_{nl} \mathcal{E}(\omega - \omega_0) \]  

(2.43)
Now it is possible to apply the Inverse Fourier Transformation to (2.38), using all the considerations already made:

\[
\begin{align*}
2j\beta_0 \frac{\partial \psi}{\partial z} + \nabla_i^2 \psi + (\beta_0^2 - \beta_0) \psi - 2j\beta_0 \beta_1 \frac{\partial \psi}{\partial t} - (\beta_1^2 + \beta_0 \beta_2) \frac{\partial^2 \psi}{\partial t^2} + j \left( \beta_1 \beta_2 + \frac{1}{3} \beta_0 \beta_3 \right) \frac{\partial^3 \psi}{\partial t^3} \\
+ \left( \frac{1}{4} \beta_2^2 + \frac{1}{3} \beta_1 \beta_3 + \frac{1}{12} \beta_0 \beta_4 \right) \frac{\partial^4 \psi}{\partial t^4} = \frac{1}{c^2} \left( \frac{\partial^2 \varepsilon_{nl} \psi}{\partial t^2} + 2j\omega_0 \frac{\partial \varepsilon_{nl} \psi}{\partial t} - \omega_0^2 \varepsilon_{nl} \psi \right) .
\end{align*}
\] (2.46)

If the internal product is defined as

\[\langle f, g \rangle = \int \int_{\Delta} fg^* d\Delta,\]

and recalling that 3\textsuperscript{rd} and 4\textsuperscript{th} order time derivatives could be needed to improve accuracy, the decision whether to use them or not, should be made on the basis of relative values of the terms \(\left( \beta_1 \beta_2 + \frac{1}{3} \beta_0 \beta_3 \right) (\Delta \omega)^3\) and \(\left( \frac{1}{4} \beta_2^2 + \frac{1}{3} \beta_1 \beta_3 + \frac{1}{12} \beta_0 \beta_4 \right) (\Delta \omega)^4\) when compared to \((\beta_1^2 + \beta_0 \beta_2) (\Delta \omega)^2\), given some maximum value \(\Delta \omega\).

The existence of 3\textsuperscript{rd} and 4\textsuperscript{th} order time derivatives under the FEM sets the need for expressions dealing with \(\langle \psi, \frac{\partial^2 \psi}{\partial t^2} \rangle\) and \(\langle \psi, \frac{\partial^4 \psi}{\partial t^4} \rangle\); these expressions are given in Appendix A.

Renaming some of the parameters, and introducing relaxation by replacing the instantaneous nonlinearity by a delayed nonlinear permittivity \((\delta)\), it is possible to build a new set of equations that represent the situation.

At this level, the modeling of the nonlinearity is altered by introducing the Debye equation for a delayed permittivity so the delay is accounted by an external relation. Additionally, derivatives of \(\delta \psi\) are approximated to \(\delta\) times the derivatives of \(\psi\) (slow time variation of \(\delta\)). The paraxial problem of propagation along the \(z\) axis, considering a slab waveguide analyzed in the time-domain, and relaxation in the nonlinear term is then represented by the equations:

\[
\begin{align*}
\left( \left( \frac{\beta_0 \beta_1}{\beta_0} \right) \frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial z} \right) - \frac{j}{2\beta_0} \frac{\partial^2 \psi}{\partial z^2} - \frac{j(\beta_2 \beta_0 + \beta_0^2)}{2\beta_0} \frac{\partial^2 \psi}{\partial t^2} + \frac{j}{2\beta_0} \left( \beta_0^2 - (\varepsilon_{ii} + \delta) k_0^2 \right) \psi &= 0, \\
\left[ \text{Debye equation}\right]: \hspace{2cm} \tau_i \frac{\partial \delta}{\partial t} + \delta - \alpha_i \psi \psi^* &= 0,
\end{align*}
\] (2.47) (2.48)
where \( k_0 = \frac{2\pi}{\lambda_0}, \beta_{0i} = \sqrt{\varepsilon_i}k_0 \) and \( \delta \) represent the nonlinear part of the relative permittivity. When relaxation time is assumed \( \tau_i \neq 0 \) for some of the materials that constitute the structure under study, the nonlinear response becomes delayed. By using some coordinate transformation, it is possible to analyze the problem in the local time domain, and eventually reduce the size of the transformed equation (2.47). As any input signal travels at the group velocity when dispersion is low, it is very convenient to define a new coordinate system of reference where time is locally measured in a time-frame moving at a speed closer to the group velocity of the main beam. With such choice of coordinates, the analysis of results is of much more practical interest. In fact, by defining:

\[
\begin{align*}
t &= \frac{y}{a} + \left( \frac{\beta_0 \beta_{1N}}{\beta_0} \right) Z, \\
z &= Z,
\end{align*}
\]  

all the variables are measured in a reference frame moving at the speed \( \frac{\beta_0 \beta_{1N}}{\beta_0} \).

So now the coordinate transformation is:

\[
\begin{align*}
\frac{\partial}{\partial t} &= a \frac{\partial}{\partial y}, \\
\frac{\partial}{\partial z} &= -a \left( \frac{\beta_0 \beta_{1N}}{\beta_0} \right) \frac{\partial}{\partial y} + \frac{\partial}{\partial \tau}.
\end{align*}
\]  

When \( Z \) is replaced by \( z \), the transformed equations are:

\[
\begin{align*}
\frac{\partial \psi}{\partial z} - \frac{j}{2\beta_0} \frac{\partial^2 \psi}{\partial x^2} - \frac{j}{2\beta_0} \left( \beta_0 \beta_{1i} + \beta_{1i}^2 \right) \frac{\partial^2 \psi}{\partial y^2} + \frac{j}{2\beta_0} \left( \beta_0^2 - (\varepsilon_i + \delta) \beta_0^2 \right) \psi &= \frac{a \left( \beta_0 \beta_{1N} - \beta_0 \beta_{1i} \right)}{\beta_0} \frac{\partial \psi}{\partial y}, \\
\tau_i a \frac{\partial \delta}{\partial y} + \delta &= \alpha_i \psi \psi^*.
\end{align*}
\]  

It is worth mentioning that \( y \) represents a length-scaled measure of local time. The constant \( a \) is arbitrary, but it is useful to choose it near the group velocity of the main beam.

The two previous equations are rewritten in a convenient single matrix equation where \( \psi \) and \( \delta \) form an equivalent vector field:

\[
\begin{bmatrix}
L_t - \frac{j \beta_0^2 \psi}{\beta_0^2} \\
-\alpha_i \psi^* \tau_i a \frac{\partial}{\partial y} + 1
\end{bmatrix}
\begin{bmatrix}
\psi \\
\delta
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
0
\end{bmatrix},
\]  

(2.55)
where

\[
\mathcal{L}_t = \frac{\partial}{\partial z} - \frac{j}{2\beta_0} \frac{\partial^2}{\partial x^2} - \frac{ja^2(\beta_{2i}\beta_{0i} + \beta_{1i}^2)}{2\beta_0} \frac{\partial^2}{\partial y^2} + \frac{j}{2\beta_0} \left( \beta_0^2 - \varepsilon_{li} k_0^2 \right) \frac{\partial}{\partial y} - a \frac{(\beta_{0N}\beta_{1N} - \beta_{0i}\beta_{1i})}{\beta_0} \frac{\partial}{\partial y}.
\]

(2.56)

A different way can be explored by employing a perturbation method for (2.54). In fact, if the delay is fast enough, \( a\tau_i \) is negligible so the zero order approximation is trivially the non-delayed permittivity. An equivalent result can be obtained by expanding the integral operator in Taylor series, or if the Debye equation is integrated and then its solution is developed and approximated by using integration by parts. The expression for such approximation is:

\[
\delta_0 = \alpha_i \psi^* \quad (2.57)
\]

\[
\delta_{n+1} = \alpha_i \psi^* - \tau_i a \frac{\partial \delta_n}{\partial y} \quad (2.58)
\]

Using the expansion (2.58) only until the second order term, \( \delta_2 \) can be substituted into (2.53) and a single equation describes the optical beam propagation:

\[
\frac{\partial^2}{\partial z^2} \psi - \frac{ja^2(\beta_{2i}\beta_{0i} + \beta_{1i}^2)}{2\beta_0} \frac{\partial^2}{\partial y^2} + \frac{j}{2\beta_0} \left( \beta_0^2 - \varepsilon_{li} k_0^2 \right) \psi = \frac{\partial}{\partial y} \left( \beta_{0N}\beta_{1N} - \beta_{0i}\beta_{1i} \right) \frac{\partial \psi}{\partial y} + \frac{k_0^2 \alpha_i}{2\beta_0} \left( \psi \psi^* - \tau_i a \frac{\partial (\psi \psi^*)}{\partial y} + (\tau_i a)^2 \frac{\partial^2 (\psi \psi^*)}{\partial y^2} \right). \quad (2.59)
\]

2.1.9 Time Domain and Noninstantaneous response (Non-Paraxial approximation)

If the perturbation method is employed for the Debye equation, the formulation for the Non-Paraxial approximation can be applied, keeping the problem restricted to \( 2N \times 2N \) sizes. In such a case, the equations should be (2.59) or (2.28) and (2.29). In that way,

\[
\mathcal{L} = \frac{\partial^2}{\partial x^2} + a^2(\beta_{2i}\beta_{0i} + \beta_{1i}^2) \frac{\partial^2}{\partial y^2} - \left( \beta_0^2 - \varepsilon_{li} k_0^2 \right) + 2ja \left( \beta_{0N}\beta_{1N} - \beta_{0i}\beta_{1i} \right) \frac{\partial}{\partial y}, \quad (2.60)
\]

\[
\mathcal{N} = -k_0^2 \alpha_i \left( \psi \psi^* - \tau_i a \frac{\partial (\psi \psi^*)}{\partial y} + (\tau_i a)^2 \frac{\partial^2 (\psi \psi^*)}{\partial y^2} \right), \quad (2.61)
\]

can also be represented by (2.30).
2.1.10 Pumping and First Order Dispersion

An interesting problem to analyze makes use of two excitations, pump and signal, that work at different frequencies. A simple situation includes only slow response time of the linear behaviour, and instantaneous response of the nonlinearity.

The paraxial problem of propagation along the z axis, considering slabs analyzed in the time-domain, signal pumping and relaxation only through first order dispersion is represented by the following set of equations [23], [24]:

\[
\left( \frac{\beta_{0is}\beta_{1is}}{\beta_{0s}} \frac{\partial E_s}{\partial t} + \frac{\partial E_s}{\partial z} \right) - \frac{j}{2\beta_{0s}} \frac{\partial^2 E_s}{\partial x^2} + \frac{j}{2\beta_{0s}} \left( \frac{\beta^2_{0s} - (\varepsilon_{ii} + \alpha_s|E_s|^2 + 2\alpha_i|E_p|^2) k_{0s}^2}{2\beta_{0s}} \right) E_s = 0, 
\]

\[
\left( \frac{\beta_{0ip}\beta_{1ip}}{\beta_{0p}} \frac{\partial E_p}{\partial t} + \frac{\partial E_p}{\partial z} \right) - \frac{j}{2\beta_{0p}} \frac{\partial^2 E_p}{\partial x^2} + \frac{j}{2\beta_{0p}} \left( \frac{\beta^2_{0p} - (\varepsilon_{ii} + \alpha_i|E_p|^2 + 2\alpha_i|E_s|^2) k_{0p}^2}{2\beta_{0p}} \right) E_p = 0, 
\]

(2.62)

(2.63)

where \( k_{0s} = \frac{2\pi}{\lambda_{0s}}, \beta_{0s} = \sqrt{\varepsilon_{ii}}k_{0s} \) and \( k_{0p} = \frac{2\pi}{\lambda_{0p}}, \beta_{0p} = \sqrt{\varepsilon_{ii}}k_{0p} \). By using some coordinate transformation, it is possible to analyze the problem in the local time domain, and eventually reduce the size of the transformed (2.62) and (2.63). In fact, by defining a local time, travelling with the signal (not the pump):

\[
t = \frac{y}{a} + \left( \frac{\beta_{0N}\beta_{1N}}{\beta_{0s}} \right) Z, 
\]

\[
z = Z. 
\]

(2.64)

(2.65)

So now the coordinate transformation is:

\[
\frac{\partial}{\partial t} = a \frac{\partial}{\partial y}, 
\]

\[
\frac{\partial}{\partial z} = -a \left( \frac{\beta_{0N}\beta_{1N}}{\beta_{0s}} \right) \frac{\partial}{\partial y} + \frac{\partial}{\partial Z}. 
\]

(2.66)

(2.67)

When Z is replaced by z, the transformed equations now are:

\[
\frac{\partial E_s}{\partial z} - \frac{j}{2\beta_{0s}} \frac{\partial^2 E_s}{\partial x^2} + \frac{j}{2\beta_{0s}} \left( \frac{\beta^2_{0s} - (\varepsilon_{ii} + \alpha_s|E_s|^2 + 2\alpha_i|E_p|^2) k_{0s}^2}{2\beta_{0s}} \right) E_s = a \left( \frac{\beta_{0N}\beta_{1N}}{\beta_{0s}} - \frac{\beta_{0is}\beta_{1is}}{\beta_{0s}} \right) \frac{\partial E_s}{\partial y}, 
\]

(2.68)

\[
\frac{\partial E_p}{\partial z} - \frac{j}{2\beta_{0p}} \frac{\partial^2 E_p}{\partial x^2} + \frac{j}{2\beta_{0p}} \left( \frac{\beta^2_{0p} - (\varepsilon_{ii} + \alpha_i|E_p|^2 + 2\alpha_i|E_s|^2) k_{0p}^2}{2\beta_{0p}} \right) E_p = a \left( \frac{\beta_{0N}\beta_{1N}}{\beta_{0s}} - \frac{\beta_{0ip}\beta_{1ip}}{\beta_{0p}} \right) \frac{\partial E_p}{\partial y}. 
\]

(2.69)
As in the previous problem of time-domain analysis, \( y \) represents a length-scaled measure of local time.

The formulation introduced here is analyzed for stationary solutions and stability in section 2.2.6.

2.2 Methods of Solution

2.2.1 Overview

A numerical approach is the only one that can give a solution for the general case of the Helmholtz equation and the GNSE. So the following choice is to decide how is the domain going to be discretized. One possible approach is using Fourier analysis [25], [26], but this means that a dense matrix should be solved for a relatively simple domain. Even having enough computer resources to solve the propagation problem, if the domain has nonuniform refractive index, Fourier analysis turns to be very complex and even more inefficient. Another approach is to discretize the domain employing simple shape functions for describing the fields, this is the Finite Element Method. The main advantages of this method are the option of using an irregular or even an adapted mesh to discretize the domain, and the feature of leading to a sparse matrix which means that very efficient techniques can be used for solving the matrix problem [16].

2.2.1.1 Theta and Crank-Nicolson methods

Crank-Nicolson/Galerkin stands for a combination of two methods: Galerkin for the weak formulation in the transverse coordinates, considering application of internal product, and Crank-Nicolson [27] for describing propagation along \( z \) and/or time. As the problem is nonlinear, the formulation does not define completely the algorithm, so some choices will have to be made.

The following is the description of the implementation of the method and some variations
The Crank-Nicolson algorithm for the problem:

$$\frac{\partial F}{\partial z} = G(z)$$

(2.70)

consists of using the central difference approximation for the left hand side of (2.70). That is, to approximate (2.70) by:

$$\frac{F(z + \Delta z) - F(z)}{\Delta z} \approx G(z + \theta \Delta z)$$

(2.71)

with

$$F(z + \theta \Delta z) \approx \theta F(z) + (1 - \theta)F(z + \Delta z)$$

(2.72)

and

$$\theta = \frac{1}{2}$$

(2.73)

These relations have been defined for the linear formulation of the problem, but when nonlinear terms appear, other expressions should be defined. For example, if the nonlinear term is a product of the field by a function of the field $\mathcal{E} f(\mathcal{E})$, the corresponding approximation could be:

- $$(1/2)(\mathcal{E}(z + \Delta z) f(\mathcal{E}(z + \Delta z)) + \mathcal{E}(z) f(\mathcal{E}(z)))$$
- $$(1/2) (\mathcal{E}(z + \Delta z) + \mathcal{E}(z)) (f(\mathcal{E}(z + \Delta z)) + f(\mathcal{E}(z)))$$
- $$(1/2) (\mathcal{E}(z + \Delta z) q(\mathcal{E}(z + \Delta z)) + \mathcal{E}(z) q(\mathcal{E}(z))) \left( \frac{f(\mathcal{E}(z + \Delta z))}{q(\mathcal{E}(z + \Delta z))} + \frac{f(\mathcal{E}(z))}{q(\mathcal{E}(z))} \right)$$

Where $q(\mathcal{E})$ is assumed to be any function that ensures $q(\mathcal{E}) \neq 0$ for any plausible value of $\mathcal{E}$.

It has been shown [28] that if instead of setting $\theta = \frac{1}{2}$, the value of $\theta$ is given a value greater than 0.5 and smaller than 1.0, solutions to the differential equation will converge always, but this result is restricted to linear media. And even for that simple case, a value of $\theta > 0.5$ would make the solution smoother by introducing an artificial damping.

The choice made for the Crank-Nicolson Method on the basis of the approximation for the product, will certainly determine convergence [29].
2.2.1.2 Analysis of CN approximation for the Nonlinear Term

The Nonlinear wave equations have a term that when using the Crank-Nicolson approach needs a special definition in order to solve the problem. That term is actually the product of the electric field by a function of the electric field. Defining \( x \) as the variable representing the electric field and \( f(x) \) as the nonlinearity, the problem may be expressed by:

Given two points \( x \) and \( y = x + \Delta x \), find the best approximation of \( x \cdot f(x) \) evaluated at \( x + \frac{\Delta x}{2} \), if the approximation is defined by:

\[
I = x \cdot g(x) \frac{f(x)}{g(x)}
\]  

(2.74)

The idea is to find the best choice for \( g(x) \) that makes \( (xg(x)) \cdot \left( \frac{f(x)}{g(x)} \right) \) closer to \( (x_0 + \frac{\Delta x}{2})f(x_0 + \frac{\Delta x}{2}) \). Assuming that \( g(x) \) admits a variation \( h(x) \), i.e., \( h(x) \) must be zero at the extremes of the interval \( (x, x + \Delta x) \) and evaluating (2.74):

\[
I = \frac{(x + \Delta x)g(x + \Delta x) + xg(x)}{2} \frac{f(x + \Delta x) + f(x)}{g(x + \Delta x) + f(x)}
\]  

(2.75)

\[
I + \delta I = \frac{(x + \Delta x)(g(x + \Delta x) + h(x + \Delta x)) + x(g(x) + h(x))}{2} \frac{f(x + \Delta x) + f(x)}{g(x + \Delta x) + h(x + \Delta x) + g(x)}
\]  

(2.76)

And after some simple manipulation:

\[
\delta I = \frac{1}{4} \left( \frac{h(x + \Delta x)g(x) - h(x)g(x + \Delta x)}{g^2(x) + g(x)h(x)} \right) \frac{(x + \Delta x)f(x)}{g^2(x) + g(x)h(x)} - \frac{x f(x + \Delta x)}{g^2(x + \Delta x) + g(x + \Delta x)h(x + \Delta x)}
\]  

(2.77)

Equation (2.77) should be valid for any value of \( \Delta x \), in particular if it approaches zero, so taking that limit:

\[
\delta I = \frac{1}{4} \left( \frac{f(x)g(x)}{g^2(x) + g(x)h(x)} \right)^2 \frac{d}{dx} \left[ \frac{x (g^2(x) + g(x)h(x))}{f(x)} \right] \frac{d}{dx} \left[ \frac{h(x)}{g(x)} \right]
\]  

(2.78)

Admissibility of \( h(x) \) means that \( h(x) \) must be zero at both extremes of the interval, condition that is not satisfied if

\[
h(x) = Ag(x),
\]
so the only possibility for optimizing $I\ (\delta I = 0)$ is to set the other derivative in (2.78) equal to zero. The latter implies:

$$\frac{x (g^2(x) + g(x)h(x))}{f(x)} = a^2$$

(2.79)

The arbitrary constant $a$ can be set to any value that gives a nontrivial solution, in particular to 1. As at the extremes $h(\cdot)$ is zero, the new expression for $g(x)$ is:

$$g(x) = a \sqrt{\frac{f(x)}{x}}$$

(2.80)

Now assuming that the problem to be solved is:

$$Lx = xf(x)$$

(2.81)

Under the Crank-Nicolson approximation, and applying (2.80), equation (2.81) is transformed to:

$$L_f x_{n+1} + L_2 x_n =$$

$$\left( f(x_{n+1}) + \sqrt{f(x_n) f(x_{n+1})} \right) \frac{x_{n+1}}{4} + \left( f(x_n) + \sqrt{f(x_n) f(x_{n+1})} \right) \frac{x_n}{4}.$$  \tag{2.82}

From (2.82) it is easy to obtain:

$$L_f x_{n+1}^{(j+1)} + L_2 x_n^{(j)} =$$

$$\left( f(x_{n+1}^{(j)}) + \sqrt{f(x_n^{(j)}) f(x_{n+1}^{(j)})} \right) \frac{x_{n+1}^{(j)}}{4} + \left( f(x_n^{(j)}) + \sqrt{f(x_n^{(j)}) f(x_{n+1}^{(j)})} \right) \frac{x_n^{(j)}}{4},$$

(2.83)

the "slowest":

$$L_f x_{n+1}^{(j)} + L_2 x_n^{(j)} =$$

$$\left\{ \left( f(x_{n+1}^{(j)}) + \sqrt{f(x_n^{(j)}) f(x_{n+1}^{(j)})} \right) \frac{x_{n+1}^{(j)}}{4} \right\} + f(x_n^{(j)}) + \sqrt{f(x_n^{(j)}) f(x_{n+1}^{(j)})} \frac{x_n^{(j)}}{4},$$

(2.84)

the "fastest":

$$L_f x_{n+1}^{(j+1)} + L_2 x_n^{(j+1)} =$$

$$\left\{ f(x_{n+1}^{(j)}) + \sqrt{f(x_n^{(j)}) f(x_{n+1}^{(j)})} \frac{x_{n+1}^{(j)}}{4} + \left( f(x_n^{(j)}) + \sqrt{f(x_n^{(j)}) f(x_{n+1}^{(j)})} \right) \frac{x_n^{(j)}}{4} \right\} \frac{x_{n+1}^{(j+1)}}{4},$$

(2.85)
among other iteration schemes.

But this is not the end, it is not clear which iteration schemes will converge; as Galerkin method applied to (2.85) creates a matrix problem, convergence criteria should be applied to it. The conclusions drawn here are implemented in all the computer programs and tested in the next chapters.

2.2.1.3 Finite Element Method

This method needs some decisions to be made; one is to decide the shape of the finite elements, another one is to decide the order of the basis functions to be employed. As sparsity plays a main role in this decision, the first attempt will be to get the simplest matrices; this means for the present case that the elements are going to be triangles and the shape functions, linear.

2.2.2 Paraxial approximation

2.2.2.1 Propagation

Crank-Nicolson method is to be applied to (2.24), so (2.70), (2.72), (2.73) should be applied, but two choices are going to be used:

1. (2.72) just as appears applied to $\mathcal{E}$
2. (2.72) applied to the product $\varepsilon_r(\mathcal{E})\mathcal{E}$.

In any case, the z-discretized Schrödinger Equation may be written as:

$$-\nabla_z^2 \mathcal{E}_e^{(n+1)} + p\mathcal{E}_e^{(n+1)} = -\left(-\nabla_z^2 \mathcal{E}_e^{(n)} + q\mathcal{E}_e^{(n)}\right)$$  \hspace{1cm} (2.86)

In (2.86), functions $p$ and $q$ are expressed by:

$$p = \begin{cases} 
\beta_0^2 + 4j\frac{\delta\varepsilon}{\Delta z} - \frac{1}{2}k_0^2(\sigma_{r}^{(n+1)}(e) + \varepsilon_r^{(n)}(e)) & \text{case (1)} \\
\beta_0^2 + 4j\frac{\delta\varepsilon}{\Delta z} - k_0^2\varepsilon_r^{(n+1)}(e) & \text{case (2)}
\end{cases}$$  \hspace{1cm} (2.87)
2: Physical background and formulations

\[
q = \begin{cases} 
\beta_0^2 - 4j \frac{\partial^2}{\partial z^2} - \frac{1}{2} k_0^2 \left( \varepsilon_{(n+1)}^{(e)}(e) + \varepsilon_r^{(n)}(e) \right) & \text{case (1)} \\
\beta_0^2 - 4j \frac{\partial^2}{\partial z^2} - k_0^2 \varepsilon_z^{(n)}(e) & \text{case (2)}
\end{cases}
\quad (2.88)
\]

Now the Galerkin method will be applied to (2.86) using the following definition for the internal product:

\[
\langle f(x, y), g(x, y) \rangle = \int \int_{R_{xy}} f(x, y) \cdot g^*(x, y) \cdot dx \cdot dy
\quad (2.89)
\]

The region \( R_{xy} \) for this development will be the elementary triangle. For each triangle three basis functions \( \varphi_{i,e} \) \( (i = 1, 2, 3 \text{ and } e = 1, \cdots, n) \) are defined, so if \( f(x, y) \) is replaced by \( \varphi_{j,e} \) and the internal product already defined applied to (2.86), the equation may be expressed in terms of the pairs \((i, e)\):

\[
\sum_{e=1}^{M} \sum_{i=1}^{j=3} \left\{ -\langle \varphi_{i,e}, \nabla_i^2 \mathcal{E}_e^{(n+1)} \rangle + \langle \varphi_{i,e}, p_{e}^{(n+1)} \mathcal{E}_e^{(n+1)} \rangle \right\} = \\
- \sum_{e=1}^{M} \sum_{i=1}^{j=3} \left\{ -\langle \varphi_{i,e}, \nabla_i^2 \mathcal{E}_e^{(n)} \rangle + \langle \varphi_{i,e}, q_{e}^{(n)} \mathcal{E}_e^{(n)} \rangle \right\}.
\quad (2.90)
\]

Using Green’s First Identity (See Appendix A), equation (2.90) is transformed into:

\[
\sum_{e=1}^{M} \sum_{i=1}^{j=3} \left\{ \langle \nabla_i \varphi_{i,e}, \nabla_i \mathcal{E}_e^{(n+1)} \rangle + \langle \varphi_{i,e}, p_{e}^{(n+1)} \mathcal{E}_e^{(n+1)} \rangle - \oint_{\Gamma_e} \varphi_{i,e} \nabla_i \mathcal{E}_e^{(n+1)} \cdot \hat{n} dl \right\} = \\
- \sum_{e=1}^{M} \sum_{i=1}^{j=3} \left\{ \langle \nabla_i \varphi_{i,e}, \nabla_i \mathcal{E}_e^{(n)} \rangle + \langle \varphi_{i,e}, q_{e}^{(n)} \mathcal{E}_e^{(n)} \rangle - \oint_{\Gamma_e} \varphi_{i,e} \nabla_i \mathcal{E}_e^{(n)} \cdot \hat{n} dl \right\}.
\quad (2.91)
\]

At this stage, it is convenient to write \( \mathcal{E}_e^{(n+1)} \) and \( \mathcal{E}_e^{(n)} \) in terms of the basis functions of the FEM. If the mesh that defines the elements is unchanged during propagation, and \( j = 1, 2, 3 \) are the local nodes of the element, then the \( \mathcal{E}_e^{(n)} \) field may be expressed as:

\[
\mathcal{E}_e^{(n)} = \sum_{j=1}^{j=3} \eta_{j,e} \varphi_{j,e}
\quad (2.92)
\]

Replacing (2.92) into (2.91), assuming that \( e \) is a particular element and rearranging terms:

\[
\sum_{e=1}^{M} \sum_{j=1}^{j=3} \left\{ \langle \nabla_i \varphi_{i,e}, \nabla_i \varphi_{j,e} \rangle + \langle \varphi_{i,e} p_{e}^{(n+1)}(e), \varphi_{j,e} \rangle - \oint_{\Gamma_e} \varphi_{i,e} \nabla_i \varphi_{j,e} \cdot \hat{n} dl \right\} \eta_{j,e}^{(n+1)} = \\
- \sum_{e=1}^{M} \sum_{j=1}^{j=3} \left\{ \langle \nabla_i \varphi_{i,e}, \nabla_i \varphi_{j,e} \rangle + \langle \varphi_{i,e} q_{e}^{(n)}(e), \varphi_{j,e} \rangle - \oint_{\Gamma_e} \varphi_{i,e} \nabla_i \varphi_{j,e} \cdot \hat{n} dl \right\} \eta_{j,e}^{(n)}
\quad (2.93)
\]
Clearly for the particular element \( e \), (2.93) is a matrix operation over the column vector \( r_e \). However, the operation already defined is expressed in terms of local node numbering and the field values there rely on boundary conditions which are responsible for the field values at the neighbouring elements (the set of equations defined by (2.93) are coupled to themselves), so adding over all the elements, (2.93) becomes a matrix problem with the same number of nodes as unknowns, before applying boundary conditions. \( \Gamma_{xy} \) is the line that surrounds the boundaries of the domain \( R_{xy} \); and it replaces the other equations due to the cancelling of pairs of equal functions line-integrated in opposite directions. Equation (2.93) with a suitable index replacement for \( j \) and \( e \) represents an \( N \times N \) assembly of \( 3 \times 3 \) matrices operated over the \( \eta \) column-vector of \( M \) rows.

**Line Integral** The Galerkin method is a weak formulation [30] because it makes use of an internal product that works as a screen for some pseudo-solutions of the problem. The way of recognizing those pseudo-solutions is to find "Natural Boundary Conditions" implicit to the method, by using a variational approach. And once found, use the variational approach that is consistent with "Physical Boundary Conditions" [31].

Defining the functional:

\[
F = \langle \mathcal{L} \xi_y, \xi_y \rangle, \\
F + \delta F = \langle \mathcal{L} \xi_y, \xi_y \rangle + \langle \mathcal{L} \delta \xi_y, \xi_y \rangle + \langle \mathcal{L} \xi_y, \delta \xi_y \rangle + O_2(\xi), \\
\delta F = \frac{\langle \mathcal{L} \xi_y, \delta \xi_y \rangle + \langle \mathcal{L} \delta \xi_y, \xi_y \rangle + O_2(\xi)}{A}. \\
\]

Now taking \( \mathcal{L} \) as a **Helmholtz Operator**:

\[
A = \int (\nabla_i^2 + k_c^2) \xi_y \delta \xi_y^* dS, \\
B = \int (\nabla_i^2 + k_c^2) \xi_y \delta \xi_y^* dS, \\
B = \int \nabla_i^2 \delta \xi_y \xi_y^* dS + \int k_c^2 \xi_y \xi_y^* dS. \\
\]

Again, using the Green’s First Identity,

\[
B = \int \delta \xi_y \nabla_i^2 \xi_y^* dS + \oint \left( \xi_y^* \frac{\partial \delta \xi_y}{\partial n} - \delta \xi_y \frac{\partial \xi_y^*}{\partial n} \right) dl + \int k_c^2 \xi_y \xi_y^* dS, \\
B = \int (\nabla_i^2 + k_c^2) \xi_y^* \delta \xi_y dS + \oint \left( \xi_y^* \frac{\partial \delta \xi_y}{\partial n} - \delta \xi_y \frac{\partial \xi_y^*}{\partial n} \right) dl. \\
\]
Solution of the variational problem is found when \( \delta F = 0 \) which implies:

\[
\mathcal{L}\mathcal{E}_y = 0, \quad \mathcal{L}\mathcal{E}_y^* = 0 \quad \text{and} \quad \oint \left( \mathcal{E}_y^* \frac{\partial \mathcal{E}_y}{\partial n} - \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} \right) dl = 0. \quad (2.102)
\]

As the last condition does not answer the question, a modified functional is defined as:

\[
G = F + h \oint \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl, \quad (2.103)
\]

\[
\delta G = A + B + h \oint \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl + h \oint \delta \mathcal{E}_y \frac{\partial \mathcal{E}_y}{\partial n} dl, \quad (2.104)
\]

\[
= (h + 1) \oint \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl + h \oint \delta \mathcal{E}_y \frac{\partial \mathcal{E}_y}{\partial n} dl - \oint \delta \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl. \quad (2.105)
\]

Now, defining a new functional in the same way:

\[
I = G + k \oint \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl, \quad (2.106)
\]

\[
\delta I = \delta G + k \oint \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl + k \oint \delta \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl, \quad (2.107)
\]

\[
= (h + 1) \oint \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl + (k - 1) \oint \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl + h \oint \delta \mathcal{E}_y \frac{\partial \mathcal{E}_y}{\partial n} dl + k \oint \delta \mathcal{E}_y \frac{\partial \mathcal{E}_y^*}{\partial n} dl. \quad (2.108)
\]

Physical boundary conditions of special interest are magnetic and metallic walls, but these two cases are not easily identified through this approach. Any pair of \((h, k)\) values does not represent well this kind of restriction. This result means that simulations must be done taking a large enough domain so the electric field is negligible near the conflictive boundaries; the other boundaries will be modelled properly. This provision allows the method to eliminate the line integral from (2.93), technique that corresponds to the so-called “Transparent Boundary Conditions” (TBC) [32].

**Local and Global Matrices** Two sparse matrices can be defined for this problem. In order to solve it numerically, it is necessary to calculate the internal products for each local element:

\[
\langle \nabla_t \varphi_i, \nabla_t \varphi_j \rangle = \int \int_{\Delta_e} \nabla_t \varphi_i \cdot \nabla_t \varphi_j \, dxdy, \quad (2.109)
\]

\[
\langle \varphi_i e^{(n+1)}, \varphi_j e \rangle = 2A_e \int_0^1 \int_{L_1}^{1-L_1} \varphi_i e \varphi_j e^{(n+1)} dL_2 dL_1, \quad (2.110)
\]

\[
\langle \varphi_i e^{(n+1)}, \varphi_j e \rangle = 2A_e \int_0^1 \int_{L_1}^{1-L_1} \varphi_i e \varphi_j e^{(n)} dL_2 dL_1, \quad (2.111)
\]
Expressions 2.110 and 2.111 make use of local coordinates for ease of evaluation, but they also need a numerical integration in order to improve the estimate of $p$ and $q$ when used for those integrals. The scheme of numerical integration [33] makes use of the corners, the points on the mid sides and the centroid. Labelling the corners as 11, 12 and 13, the middle points of each side as 23, 21 and 22, and the centroid as 33, the nonlinear part of (2.110) and (2.111) can be rewritten as:

$$m_{i,j}^{(n)} = \langle \varphi_i e p_{nl}^{(n+1)}, \varphi_j e \rangle$$

$$= 2A_e \left\{ \sum_{l=1}^{3} \sum_{m=1}^{3} \varphi_i e(l,m) \varphi_j e(l,m) p_{nl}^{(n+1)}(l,m) W(l,m) \right\}$$

$$\omega_{i,j}^{(n)} = \langle \varphi_i e q_{nl}^{(n)}, \varphi_j e \rangle$$

$$= 2A_e \left\{ \sum_{l=1}^{3} \sum_{m=1}^{3} \varphi_i e(l,m) \varphi_j e(l,m) q_{nl}^{(n)}(l,m) W(l,m) \right\}$$

For the linear part of (2.110) and (2.111) the following definitions apply:

$$t_{i,j} = \langle \varphi_i e p_l^{(n+1)}, \varphi_j e \rangle,$$

$$t'_{i,j} = \langle \varphi_i e q_l^{(n)}, \varphi_j e \rangle,$$

For example, $p_{nl}$, $q_{nl}$, $p_l$ and $q_l$ may be defined as:

$$p_l = \beta_0^2 + 4j \frac{\beta_0}{\Delta z},$$

$$p_{nl} = p - p_l,$$

$$q_l = \beta_0^2 + 4j \frac{\beta_0}{\Delta z},$$

$$q_{nl} = q - q_l.$$

The weights for the numerically evaluated integral are defined by:

$$W(1,1) = W(1,2) = W(1,3) = \frac{1}{20},$$

$$W(2,1) = W(2,2) = W(2,3) = \frac{2}{15},$$

$$W(3,3) = \frac{9}{20},$$

$$W(3,1) = W(3,2) = 0.$$
For the local matrix \( m_{ij}^{(n+1)} \):

\[
\begin{align*}
 m_{11,e}^{(n+1)} &= A_e \left( \frac{1}{20} p_{33,e,nl}^{(n+1)} + \frac{1}{30} p_{22,e,nl}^{(n+1)} + \frac{1}{30} p_{23,e,nl}^{(n+1)} + \frac{1}{20} p_{11,e,nl}^{(n+1)} \right), \\
 m_{22,e}^{(n+1)} &= A_e \left( \frac{1}{20} p_{33,e,nl}^{(n+1)} + \frac{1}{30} p_{22,e,nl}^{(n+1)} + \frac{1}{30} p_{23,e,nl}^{(n+1)} + \frac{1}{20} p_{12,e,nl}^{(n+1)} \right), \\
 m_{33,e}^{(n+1)} &= A_e \left( \frac{1}{20} p_{33,e,nl}^{(n+1)} + \frac{1}{30} p_{23,e,nl}^{(n+1)} + \frac{1}{30} p_{21,e,nl}^{(n+1)} + \frac{1}{20} p_{13,e,nl}^{(n+1)} \right), \\
 m_{12,e}^{(n+1)} &= A_e \left( \frac{1}{20} p_{33,e,nl}^{(n+1)} + \frac{1}{30} p_{21,e,nl}^{(n+1)} \right), \\
 m_{13,e}^{(n+1)} &= A_e \left( \frac{1}{20} p_{33,e,nl}^{(n+1)} + \frac{1}{30} p_{22,e,nl}^{(n+1)} \right), \\
 m_{23,e}^{(n+1)} &= A_e \left( \frac{1}{20} p_{33,e,nl}^{(n+1)} + \frac{1}{30} p_{22,e,nl}^{(n+1)} \right).
\end{align*}
\]

Changing both \( m \) and \( p_{nl}^{(n+1)} \) by \( w \) and \( q_{nl}^{(n)} \) respectively, another local matrix is calculated. A slightly different way is to use the following relations:

\[
q^{(n)} - p^{(n+1)} = -8 j A_e \frac{\beta_0}{\Delta z}
\]

\[
w_{ij}^{(n)} = m_{ij}^{(n+1)} - \frac{2}{3} j A_e \frac{\beta_0}{\Delta z} \quad \text{for } i \neq j
\]

In order to calculate matrices defined by (2.109), it is convenient to use cartesian coordinates. The basis functions are defined as:

\[
\varphi_{ie} = \left( \frac{1}{2 A_e} \right) (a_{ie} + b_{ie} x + c_{ie} y)
\]

So the differential operator \( \nabla_{\varphi} \) applied to (2.137) gives:

\[
\begin{align*}
\nabla_{\varphi} \varphi_{1e} &= \left( \frac{1}{2 A_e} \right) ((y_2 - y_3) \ddot{x} + (x_3 - x_2) \ddot{y}) \\
\nabla_{\varphi} \varphi_{2e} &= \left( \frac{1}{2 A_e} \right) ((y_3 - y_1) \ddot{x} + (x_1 - x_3) \ddot{y}) \\
\nabla_{\varphi} \varphi_{3e} &= \left( \frac{1}{2 A_e} \right) ((y_1 - y_2) \ddot{x} + (x_2 - x_1) \ddot{y})
\end{align*}
\]

It is clear that \( |2 A_e \nabla_{\varphi} \varphi_{i}| \) is exactly the length of the opposite side to local node \( i \). The vector \( \nabla_{\varphi} \varphi_{i} \) is orthogonal to that side. This means that angles subtended by these vectors will be the same angles subtended by the respective orthogonal sides. Internal products of
the vectors can be easily calculated, calling \( l_{ij} \) the length of the side between local nodes \( i \) and \( j \); \( \alpha_i \) the angle of the triangle at node \( i \), and \( s_{ij} \) the internal product \( (\nabla_i \varphi_i, \nabla_j \varphi_j) \):

\[
\begin{align*}
l_{23} & = \frac{\sin \alpha_1}{\sin \alpha_2} \\
l_{23} & = \frac{\sin \alpha_1}{\sin \alpha_3} \\
\end{align*}
\] (2.142)

\[
\alpha_1 + \alpha_2 + \alpha_3 = \pi
\] (2.144)

\[
A_e = \frac{1}{2} l_{31} l_{12} \sin \alpha_1
\] (2.145)

\[
A_e = \frac{1}{2} l_{23} l_{12} \sin \alpha_2
\] (2.146)

\[
A_e = \frac{1}{2} l_{31} l_{23} \sin \alpha_3
\] (2.147)

and

\[
S_{11} = \frac{l_{23}^2}{4 \frac{1}{2} l_{31} l_{12} \sin \alpha_1} = \frac{l_{23} l_{23}}{2 l_{31} l_{12} \sin \alpha_1} = \frac{1}{2} \frac{\sin \alpha_1 \sin \alpha_1}{\sin \alpha_2 \sin \alpha_3 \sin \alpha_1} = \frac{1}{2} (\text{ctg} \alpha_2 + \text{ctg} \alpha_3)
\] (2.148)

\[
s_{22} = \frac{1}{2} (\text{ctg} \alpha_1 + \text{ctg} \alpha_2)
\] (2.149)

\[
s_{33} = \frac{1}{2} (\text{ctg} \alpha_1 + \text{ctg} \alpha_2)
\] (2.150)

and

\[
s_{12} = -\frac{l_{23} l_{31} \cos \alpha_3}{4 A_e} = -\frac{l_{13} l_{23} \cos \alpha_3}{2 l_{13} l_{23} \sin \alpha_3} = -\frac{1}{2} \text{ctg} \alpha_3
\] (2.151)

\[
s_{23} = -\frac{1}{2} \text{ctg} \alpha_1
\] (2.152)

\[
s_{13} = -\frac{1}{2} \text{ctg} \alpha_2
\] (2.153)

\[
s_{ij} = s_{ji}
\] (2.154)

The same values may be written also as:

\[
s_{ij} = \frac{1}{4 A_e} (b_i b_j e + c_i c_j e)
\] (2.155)
where:

\[
\begin{align*}
    b_{ie} &= y_{l2e} - y_{l1e} \\
    c_{ie} &= x_{l1e} - x_{l2e}
\end{align*}
\]  (2.156)

and,

\[
\begin{align*}
    I1(i) &= 1 + \text{mod}(i, 3) \\
    I2(i) &= 1 + \text{mod}(i + 1, 3)
\end{align*}
\]  (2.158)

Sometimes it will be necessary to include the line integral that appears in (2.93). The analysis begins with a triangle which has two nodes \(i\) and \(j\) on the boundary line. Clearly, on that line \(\varphi_{k,e} = 0\) and:

\[
I_{ij} = \int_{l_{ij}} \varphi_{i,e} \nabla_t \varphi_{j,e} \cdot dl
\]  (2.160)

is the line integral over the segment \(l_{xy}\). Calling \(I_{i,jx}\) and \(I_{i,jy}\) the integrals over horizontal and vertical segments, it follows that:

\[
I_{i,jx} = \int_{x_i}^{x_j} \varphi_{i,e} \nabla_t \varphi_{j,e} \cdot \hat{y} dx
\]  (2.161)

\[
= -\frac{1}{2A} \int_{x_i}^{x_j} \varphi_{i,e} c_{j,e} dx
\]

\[
= -\left( \frac{1}{2A} \right)^2 \int_{x_i}^{x_j} \left( a_{i,e} + b_{i,e}x + c_{i,e}y \right) c_{j,e} dx
\]

\[
= -\left( \frac{1}{2A} \right)^2 \left\{ \frac{a_{i,e} + b_{i,e} \left( \frac{x_j + x_i}{2} \right) + c_{i,e}y}{A} \right\} (x_j - x_i) c_{j,e}
\]  (2.162)

The last expression can be simplified noticing that the \(A\) factor is \(\varphi_{i,e}\) evaluated at the centre point of line \(l_{ij}\). And for this first order basis functions, that value is \(\frac{1}{2}\). Therefore:

\[
I_{i,jx} = -\left( \frac{1}{4A} \right)^2 (x_j - x_i) c_{j,e}
\]

\[
= -\left( \frac{1}{4A} \right)^2 (x_j - x_i) (x_k - x_l)
\]  (2.163)

\(k\) is the node opposite to the side used as integration path. This result shows that only the simplified scheme that neglects the line integral gives origin to a symmetrical matrix problem, but for the general case, \(I_{i,jx} \neq I_{j,i}x\). Application to a vertical boundary line is
straightforward from (2.163). Because of the double sign change, both in the normal vector and on the integration direction, the same result is valid for upper and lower boundary lines as well as for right and left boundary lines.

**Iteration Schemes** With all the relevant global matrices already defined, the numerical problem becomes a matrix problem, and for the cases defined in (2.87) and (2.88), it is possible to write:

\[
\begin{align*}
\{[L_p] + [N^{(n+1)}]\} u^{(n+1)} &= -\{[L_q] + [N^{(n)}]\} u^{(n)} \\
\end{align*}
\]

(2.164)

for case (1). But for case (2), two options are sketched:

\[
\begin{align*}
\{[L_p] + \frac{1}{2} [N^{(n+1)} + N^{(n)}]\} u^{(n+1)} &= -\{[L_q] + \frac{1}{2} [N^{(n+1)} + N^{(n)}]\} u^{(n)} \\
\end{align*}
\]

(2.165)

and

\[
\begin{align*}
[L_p] u^{(n+1)} &= -[L_q] u^{(n)} + \frac{1}{2} [N^{(n+1)} + N^{(n)}] [u^{(n+1)} + u^{(n)}] \\
\end{align*}
\]

(2.166)

Calling \( u^{(n+1)} = u_j \) and \( u^{(n)} = u_0 = u_0^{(n+1)} \) and in a similar way for \( N \), where \( j \) indicates number of iterations, three iteration schemes may be developed:

\[
\begin{align*}
\{[L_p] + [N_{j-1}]\} u_j &= -\{[L_q] + [N_0]\} u_0 \\
\{[L_p] + \frac{1}{2} [N_{j-1} + N_0]\} u_j &= -\{[L_q] + \frac{1}{2} [N_{j-1} + N_0]\} u_0 \\
[L_p] u_j &= -[L_q] u_0 + \frac{1}{2} [N_{j-1} + N_0] [u_{j-1} + u_0] \\
\end{align*}
\]

(2.167, 2.168, 2.169)

These three schemes of iteration have different convergence ratios and in order to converge they will take different number of iterations. Besides that, the computer implementation of each scheme also has its own differences in terms of work for each iteration, which in practical terms means CPU time. Further discussions of these aspects will appear in section 3.1.6.

### 2.2.2.2 Modal Equation

On propagation, it is said that a mode is settled when fluctuations on the longitudinal axis vanish. In mathematical terms that means partial derivatives respect to the longitudinal
variable \((z)\) should be removed from the propagation equation. It is important to notice that there will be no difference between this modal equation and the one related to the non-paraxial case. Calling \([A], [L]\) and \([N]\) the matrices that represent the assemblies of local matrices associated to a scalar multiplier, the Laplacian and the nonlinearity, respectively, the eigenvalue problem (or modal equation) for a locally invariant nonlinearity is:

\[
\left\{-[L] + k_0^2 [N]\right\} v_q = \chi_q^2 [A] v_q, \quad (2.170)
\]

When linear modes are sought, annihilating \(N\) is required. According to (2.170), \((v_q, \chi_q^2)\) is the eigenvector-eigenvalue pair. If \(\chi_q^2 \leq 0\) then the associated mode is an evanescent mode; on the other hand, if \(\chi_q^2 > 0\) then the related mode is a guided mode.

### 2.2.2.3 Stability

The modal procedure for stability [34], [35] is to be employed here for the analysis. Using the same convention as in the description of the modal equation, and applying the \(\theta\)-method the resulting matrix equation is:

\[
\begin{align*}
\left\{2j\beta_0 [A] + \theta \Delta z \left([L] + \beta_0^2 [A] - k_0^2 [N]\right)\right\} u^{(n+1)} &= \\
\left\{2j\beta_0 [A] + (\theta - 1) \Delta z \left([L] + \beta_0^2 [A] - k_0^2 [N]\right)\right\} u^{(n)}.
\end{align*}
\]

(2.171)

Now expressing \(u^{(n+1)}\) and \(u^{(n)}\) in terms of the local modes yielded by (2.170) the following relations hold:

\[
\begin{align*}
u^{(n+1)} &= \sum_{i=1}^{M} \xi_i^{(n+1)} v_i, \\
u^{(n)} &= \sum_{i=1}^{M} \xi_i^{(n)} v_i. \quad (2.172)
\end{align*}
\]

Now, in order to have stability, \(\xi_i^{(n+1)} = \rho \xi_i^{(n)}\) and \(|\rho| \leq 1.\) Replacing all these relations into (2.171) the amplification factor \(\rho\) is given by:

\[
\rho = \frac{2j\beta_0 + (\theta - 1) \Delta z (\beta_0^2 - \chi_i^2)}{2j\beta_0 + \theta \Delta z (\beta_0^2 - \chi_i^2)}. \quad (2.174)
\]

Defining \(h = \frac{\theta \Delta z (\beta_0^2 - \chi_i^2)}{2j\beta_0},\) \(\rho\) can be made unitary and unconditionally stable even when the spectrum (defined by \(h\)) varies, by choosing \(\theta = \frac{1}{2}.\) A different choice of \(\theta,\) even for a narrow spectrum gives either attenuation or amplification. An illustration of this behaviour is shown in Fig. 2.1.
2.2.3 Non-Paraxial approximation for 2D+z

2.2.3.1 Propagation

Recurring to Crank-Nicolson Method, the operators matrix equation is:

\[
\begin{bmatrix}
1 & -\frac{\Delta z}{2} \\
-\frac{\Delta z}{2} (L + \mathcal{N}^{(n+1)}) & 1 - j\beta_0 \Delta z
\end{bmatrix}
\begin{bmatrix}
\mathcal{E}^{(n+1)} \\
\mathcal{F}^{(n+1)}
\end{bmatrix}
= 
\begin{bmatrix}
\frac{\Delta z}{2} (L + \mathcal{N}^{(n)}) & \frac{\Delta z}{2} \\
1 + j\beta_0 \Delta z
\end{bmatrix}
\begin{bmatrix}
\mathcal{E}^{(n)} \\
\mathcal{F}^{(n)}
\end{bmatrix}.
\] (2.175)

At this point it is clear that for small nonlinearities, stability is guaranteed because the iterative procedure is unitary. Lastly, applying Green’s First Identity [37] and then FEM,
a global matrix equation represents this nonparaxial approximation:

\[
\begin{bmatrix}
[U] & -\frac{\Delta z}{2} [U] \\
-\frac{\Delta z}{2} (\{\mathcal{L}\} + [\mathcal{N}^{(n)}]) & (1 - j\beta_0 \Delta z) [U]
\end{bmatrix}
\begin{bmatrix}
\eta_{j+1}^{(n+1)} \\
\phi_{j+1}^{(n+1)}
\end{bmatrix}
= \begin{bmatrix}
\frac{\Delta z}{2} [U] \\
\frac{\Delta z}{2} (\{\mathcal{L}\} + [\mathcal{N}^{(n)}]) & (1 + j\beta_0 \Delta z) [U]
\end{bmatrix}
\begin{bmatrix}
\eta^{(n)} \\
\phi^{(n)}
\end{bmatrix},
\tag{2.176}
\]

where:

\[
\mathcal{S}_e = \sum_{i=1}^{i=3} \phi_i \varphi_{i,e},
\tag{2.177}
\]

\[
\mathcal{E}_e = \sum_{i=1}^{i=3} \eta_i \varphi_{i,e}.
\tag{2.178}
\]

In order to implement this method, the local matrices for each operator are:

\[
[U] = \frac{A_e}{12}
\begin{bmatrix}
2 & 1 & 1 \\
1 & 2 & 1 \\
1 & 1 & 2
\end{bmatrix}
\tag{2.179}
\]

\[
\{\mathcal{L}\}_{ij} = \frac{b_i b_j + c_i c_j}{4A_e} + (\beta_0^2 - k_0^2 \varepsilon_{ij}) \{U\}_{ij},
\tag{2.180}
\]

\[
\{\mathcal{N}\}_{ij} = -k_0^2 \varepsilon_{nij} \{U\}_{ij}.
\tag{2.181}
\]

As usual, this local matrices are assembled into global matrices, by converting the local nodes indices to global nodes indices.

### 2.2.3.2 Modal Equation

The search for stationary solutions, in this case electromagnetic waves whose envelopes are independent of the propagation coordinate, gives the same modal equation as the paraxial analysis because partial derivatives with respect to the z-coordinate disappear from eqs. (2.24) and (2.28), leading to the same equation (2.170) that is an eigenvalue problem. When the numerical solution of the matrix equation for stationary modes is sought, methods like inverse iteration, forward iteration both with or without shift, etc. [38] can be successfully applied in most of the problems, ensuring very fast and reliable results, both for the linear and nonlinear cases.
2.2.3.3 Stability

Calling:

\[
\{A\}_{ij} = \langle \varphi_i, \varphi_j \rangle, \quad (2.182)
\]
\[
\{L\}_{ij} = \langle \nabla_t \varphi_i, \nabla_t \varphi_j \rangle, \quad (2.183)
\]
\[
\{N\}_{ij} = \langle \epsilon_j \varphi_i, \varphi_j \rangle. \quad (2.184)
\]

Assuming that both "fields" can be expressed as a linear combination of the local modes, then:

\[
E = \sum e_i u_i, \quad (2.185)
\]
\[
F = \sum f_i u_i. \quad (2.186)
\]

Where \(u_i\) is the eigenvector associated to the eigenvalue \(\chi_i\). As the modes are orthogonal vectors, each eigenvalue leads to two equations:

\[
A \left( \frac{\partial f_i}{\partial z} - 2j \beta_0 \frac{\partial e_i}{\partial z} \right) = A \left( \beta_0^2 - \chi_i^2 \right) e_i, \quad (2.187)
\]
\[
A \left( \frac{\partial e_i}{\partial z} - f_i \right) = 0. \quad (2.188)
\]

As \(A\) is certainly non-singular, the following equations hold:

\[
\frac{\partial f_i}{\partial z} - 2j \beta_0 \frac{\partial e_i}{\partial z} = \left( \beta_0^2 - \chi_i^2 \right) e_i, \quad (2.189)
\]
\[
\frac{\partial e_i}{\partial z} = f_i. \quad (2.190)
\]

And the \(\theta\)-method is introduced by:

\[
e_i = \theta_1 e_n + (1 - \theta_1) e_{n+1}, \quad (2.191)
\]
\[
f_i = \theta_2 f_n + (1 - \theta_2) f_{n+1}. \quad (2.192)
\]

Defining a strong amplification factor \(\rho\) (strong in the sense that it is the same one for both \(e\) and \(f\)) by:

\[
\begin{bmatrix}
e_{n+1} \\
f_{n+1}
\end{bmatrix} = \rho \begin{bmatrix}
e_n \\
f_n
\end{bmatrix}, \quad (2.193)
\]
combining all the equations conveniently, and defining $p = \beta_0 \Delta z$ and $q = \chi_1 \Delta z$, a second degree equation for $\rho$ allows discriminating stable from non-stable cases:

$$\rho^2 z_2 - \rho z_1 + z_0 = 0,$$  \hfill (2.194)

where:

$$x_0 = 1 - (p^2 - q^2)(1 - \theta_1)(1 - \theta_2),$$  \hfill (2.195)

$$y_0 = -2p(1 - \theta_2),$$  \hfill (2.196)

$$x_1 = 2 + (p^2 - q^2)(\theta_1 + \theta_2 - 2\theta_1\theta_2),$$  \hfill (2.197)

$$y_1 = -2p(2\theta_2 - 1),$$  \hfill (2.198)

$$x_2 = 1 - (p^2 - q^2)\theta_1\theta_2,$$  \hfill (2.199)

$$y_2 = 2p\theta_2,$$  \hfill (2.200)

$$|z_m| = \sqrt{x_m^2 + y_m^2},$$  \hfill (2.201)

$$\phi_m = \cos^{-1} \frac{x_m}{R_m}, \quad m = 1, 2,$$  \hfill (2.202)

$$A = x_1^2 - y_1^2,$$  \hfill (2.203)

$$B = 2x_1y_1,$$  \hfill (2.204)

$$C = x_2y_0 - y_2y_0,$$  \hfill (2.205)

$$D = x_2y_0 + y_0y_2,$$  \hfill (2.206)

$$E = 4(AC - BD),$$  \hfill (2.207)

$$F = 4(BC + AD),$$  \hfill (2.208)

$$G = \sqrt{(|z_1|^4 - E^2 + F^2},$$  \hfill (2.209)

$$H = \sqrt{(A - 4C)^2 + (B - 4D)^2},$$  \hfill (2.210)

$$\psi = \cos^{-1} \frac{|z_1|^4 - E}{G}. $$  \hfill (2.211)

And the two solutions of (2.194) can be expressed as:

$$|\rho_1| = \frac{|z_1|^2 + H + G \cos \left( \frac{\psi}{2} \right)}{4|z_2|^2},$$  \hfill (2.212)

$$|\rho_2| = \frac{|z_1|^2 + H - G \cos \left( \frac{\psi}{2} \right)}{4|z_2|^2}. $$  \hfill (2.213)
For stability, \(|\rho| \leq 1\), and to avoid damping, unitarity is sought. Making both solutions with exactly the same modulus, gives the following condition:

\[ F = 0. \quad (2.214) \]

By simple inspection, \(\theta_2 = \theta_1 = \frac{1}{2}\) makes the formulation unconditionally unitary and stable. So again Crank–Nicolson method guarantees better performance for the simulations.

### 2.2.4 Time Domain (Paraxial approximation)

#### 2.2.4.1 Propagation

It is possible to write a convenient matrix formulation:

\[
\begin{bmatrix}
\frac{\partial}{\partial x} + 2\mathcal{S} - \frac{j k_0^2 \mathcal{E}}{2\beta_0} \\
-\alpha_i \mathcal{E}^* - \tau_\alpha \frac{\partial}{\partial y} + 1
\end{bmatrix}
\begin{bmatrix}
\mathcal{E} \\
\delta
\end{bmatrix}
= \begin{bmatrix}
0 \\
0
\end{bmatrix}. \quad (2.215)
\]

So as a first approximation, a Crank–Nicolson based discretization over \(z\) will be applied to (2.215). The resulting matrix equation is:

\[
\begin{bmatrix}
\mathcal{S} + \frac{1}{\Delta z} & B \\
A & D
\end{bmatrix}
\begin{bmatrix}
\mathcal{E}^{(n+1)} \\
\delta^{(n+1)}
\end{bmatrix}
= \begin{bmatrix}
-S + \frac{1}{\Delta z} & -B \\
-A & -D
\end{bmatrix}
\begin{bmatrix}
\mathcal{E}^{(n)} \\
\delta^{(n)}
\end{bmatrix}. \quad (2.216)
\]

Equations (2.215) and (2.216), make use of:

\[
S = \frac{j}{4\beta_0} \left( \beta_0^2 - \varepsilon_{11} k_0^2 \right) - \frac{j}{4\beta_0} \frac{\partial^2}{\partial x^2} - \frac{j(\beta_2 \beta_0 + \beta_{11})a^2}{4\beta_0} \frac{\partial^2}{\partial y^2} - \frac{a(\beta_0 \beta_{11} - \beta_0 \beta_{11})}{2\beta_0} \frac{\partial}{\partial y}, \quad (2.217)
\]

\[
B = \frac{j k_0^2 \left( \mathcal{E}^{(n+1)} + \mathcal{E}^{(n)} \right)}{8 \beta_0}, \quad (2.218)
\]

\[
A = - \frac{\alpha_i \left( \mathcal{E}^{(n+1)} + \mathcal{E}^{(n)} \right)}{4}, \quad (2.219)
\]

\[
D = \frac{1}{2} + \frac{\tau_\alpha}{\delta} \frac{\partial}{\partial y}. \quad (2.220)
\]

The next stage is to complete the method by using a set of basis functions. As first order finite elements keep simplicity and allow reliable results, this method is to be applied here. When applying Green’s First Identity and then FEM, (2.216) can be rewritten as:

\[
([L_L] + [N]) \mathbf{F}^{(n+1)} = ([L_R] - [N]) \mathbf{F}^{(n)}, \quad (2.221)
\]
provided that:

\[ \mathcal{E}_e = \sum_{j=1}^{j=3} \eta_{je} \varphi_{je} \quad (2.222) \]

\[ \delta_e = \sum_{j=1}^{j=3} \xi_{je} \varphi_{je} \quad (2.223) \]

where \([L_L]\) and \([L_R]\) are linear and diagonal matrix operators. \([N]\) is a nonlinear matrix operator where the diagonal is empty. \(\mathbf{F}^{(n)}\) is a vector composed of \(\eta^{(n)}\) and \(\xi^{(n)}\). By denoting \(q\) the iteration index, the nonlinear matrices will be calculated for index \(q\) when \((n+1)\) appears, but \(\mathbf{F}^{(n+1)}\) will refer to index \(q+1\). Each element of the matrices in (2.221) generates a 3 x 3 matrix. For the sake of programming simplicity, the following relations are introduced:

\[ \mathcal{U}_L = \frac{A_x}{12 \Delta z} \left( 1 + \frac{j \Delta z (\beta_0^2 - \beta_1^2)}{4 \beta_0^3} \right) [T] + \frac{j \Delta z}{16 A_x} [M] + \frac{a (\beta_0 N \beta_1 N - \beta_0 \beta_1 L)}{12 \beta_0^3} [H] \quad (2.224) \]

\[ \mathcal{U}_R = \frac{A_x}{12 \Delta z} \left( 1 - \frac{j \Delta z (\beta_0^2 - \beta_1^2)}{4 \beta_0^3} \right) [T] - \frac{j \Delta z}{16 A_x} [M] + \frac{a (\beta_0 N \beta_1 N - \beta_0 \beta_1 L)}{12 \beta_0^3} [H] \quad (2.225) \]

\[ \mathcal{L}_L = - \frac{A_x}{24} [T] + \frac{j \delta_a}{12} [H] \quad (2.226) \]

\[ \mathcal{L}_R = - \frac{A_x}{24} [T] - \frac{j \delta_a}{12} [H] \quad (2.227) \]

\[ \mathcal{N}_D = \frac{36 \alpha_a (\gamma^{(n+1)} + \eta^{(n)})}{48} [T] \quad (2.228) \]

\[ \mathcal{N}_U = - \frac{jk_x A_x (\gamma^{(n+1)} + \eta^{(n)})}{96 \beta_0} [T] \quad (2.229) \]

And the matrices are defined by:

\[ [T] = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \quad (2.230) \]

\[ \{ m_{rs} \} = \frac{b_r b_s}{\beta_0} + \frac{(\beta_2 s \beta_0 s + \beta_1^2 s) a^2 c_r c_s}{\beta_0} \quad (2.231) \]

\[ \{ h_{rs} \} = c_s \quad (2.232) \]

The global matrices defined in (2.221) are now:

\[ [L_L] = \begin{bmatrix} \mathcal{U}_L & 0 \\ 0 & \mathcal{L}_L \end{bmatrix} \quad (2.233) \]

\[ [L_R] = \begin{bmatrix} \mathcal{U}_R & 0 \\ 0 & \mathcal{L}_R \end{bmatrix} \quad (2.234) \]
2: Physical background and formulations

\[
[N] = \begin{bmatrix}
0 & N_U \\
N_D & 0
\end{bmatrix}
\] (2.235)

\[
(2.236)
\]

The factor \( a \) is defined in terms of \( \beta_1 \), and it should be of the order of \( 1/\beta_1 N \). Clearly “\( a \)” dimensions are in [m/s].

As for the alternative formulation that makes use of second order approximations for the delayed permittivity (2.59), the inclusion of the Crank–Nicolson method leads to the following matrix equation:

\[
\left( [U_L] + [D_{n+1/2}] \right) \eta^{(n+1)} = \left( [U_R] - [D_{n+1/2}] \right) \eta^{(n)},
\]

(2.237)

where \([U_L,R]\) have already been defined in (2.224) and (2.225) and in order to find \([D_{n+1/2}]\), it is necessary to compute the following internal products:

- \( \langle \varphi_i e_i, \varphi_j e_j | \eta_j |^2 \rangle \),
- \( \langle \varphi_i e_i, \varphi_j e_j \frac{\partial \varphi_j e_j}{\partial y} | \eta_j |^2 \rangle \),
- \( \langle \varphi_i e_i, \varphi_j e_j \frac{\partial^2 \varphi_j e_j}{\partial y^2} | \eta_j |^2 \rangle \).

Taking the nonlinear part of (2.237), applying the Crank-Nicolson method, one of the Green identities, and assuming transparent boundary conditions and finally introducing the FEM, the local matrix that represents the nonlinearity can be calculated using the results of Appendix B. Its elements are given by:

\[
\{D\}_{ii} = -j \frac{k_0^2 \alpha_i}{480 \beta_0} \left( 8 A_e - 6 \alpha \tau c_i - 20 \left( \frac{a \tau c_i}{A_e} \right)^2 \right) |\eta_i|^2, \quad (2.238)
\]

\[
\{D\}_{ij} = -j \frac{k_0^2 \alpha_j}{480 \beta_0} \left( 2 A_e - 2 a \tau c_j - (10 c_i c_j + 5 c_i^2) \left( \frac{a \tau c_j}{A_e} \right)^2 \right) |\eta_j|^2, \quad \text{for } i \neq j. \quad (2.239)
\]

This second formulation has the advantage of reducing the size of the matrix problem but underestimates the influence of the nonlinearity whenever the nonlinear response times are large.
2.2.4.2 Modal Equation

Assuming that (2.53) admits stationary solutions and considering the fact that when searching for modes, transverse variations are assumed to disappear, (2.53) is transformed into:

\[
\frac{\partial^2 \mathcal{E}}{\partial x^2} + a^2(\beta_{2i}\beta_{0i} + \beta_{1i}^2) \frac{\partial^2 \mathcal{E}}{\partial y^2} - (\beta_0^2 - (\varepsilon_{ii} + \delta)k_0^2)\mathcal{E} = 2ja(\beta_{0N}\beta_{1N} - \beta_{0i}\beta_{1i}) \frac{\partial \mathcal{E}}{\partial y}. \tag{2.240}
\]

Debye equation (2.48) along with (2.240) represent the exact modal equation for (2.53). The discretized equation, generated by applying the FEM, makes use of the matrices already defined in (2.224) to (2.235).

A good choice of mode makes use of second order approximations for the delayed permittivity, that reduce the problem of searching modes to a single scalar equation that can be represented through a discretization of \( N \) nodes into a \( N \times N \) matrix problem, instead of the \( 2N \times 2N \) problem. The nonlinear modes found through this short-cut keep the shape both in local time \( (y) \) and in the transverse coordinate \( (x) \). These stationary solutions are then called "bullets" [39] or also "time and space solitons" [40]. The equation they satisfy when the approximations are used is:

\[
\frac{\partial^2 u_i}{\partial x^2} + a^2(\beta_{2i}\beta_{0i} + \beta_{1i}^2) \frac{\partial^2 u_i}{\partial y^2} + (\chi_i^2 - (\varepsilon_{ii} + \delta_2(u_i))u_i = -2aj(\beta_{0N}\beta_{1N} - \beta_{0i}\beta_{1i}) \frac{\partial u_i}{\partial y}, \tag{2.241}
\]

where \( \delta_2(u_i) \) is an explicit function of the eigenmode \( u_i \) and the related eigenvalue is \( \chi_i \).

Another kind of stationary solutions appear if time variations are neglected; in such a case the modes are given by:

\[
\frac{\partial^2 u_i}{\partial x^2} + (\xi_i^2 - (\varepsilon_{ii} + \alpha_i|u_i|^2))u_i = 0, \tag{2.242}
\]

where the eigenmodes are characterized by \( u_i \) and \( \xi_i \).

The nonlinear solution gives a spatial soliton, and the linear solution (neglecting the nonlinear term) gives just simple linear modes. When either of the solutions is obtained, a
suitable user-defined time envelope is applied to the eigenvector found, and subsequently used as the input for the simulation.

### 2.2.4.3 Stability

When analyzing the stability of this problem, it becomes clear that "local" stationary solutions are represented by the same kind of equation as the 2D+\(z\) paraxial case, so it is clear that the stability is reached when Crank-Nicolson method is applied. The same conclusion applies to the formulation that includes the perturbed approximation of \(\delta\).

### 2.2.5 Time Domain (Perturbed Debye equation and Non-paraxiality)

#### 2.2.5.1 Propagation

Starting from equation (2.59) which models time domain behaviour restricted to fast response times of the material nonlinearities and recurring to Crank-Nicolson Method for the propagation coordinate (\(z\)), the operator matrix equation is discretized as:

\[
\begin{bmatrix}
1 & -\frac{\Delta z}{2} \\
-\frac{\Delta z}{2} \left( L + N^{(n+1)} \right) & 1 - j\beta_0 \Delta z
\end{bmatrix}
\begin{bmatrix}
E^{(n+1)} \\
F^{(n+1)}
\end{bmatrix} =
\begin{bmatrix}
1 & \frac{\Delta z}{2} \\
\frac{\Delta z}{2} \left( L + N^{(n)} \right) & 1 + j\beta_0 \Delta z
\end{bmatrix}
\begin{bmatrix}
E^{(n)} \\
F^{(n)}
\end{bmatrix}.
\]  

(2.243)

At this point it is clear that for small nonlinearities, stability is guaranteed because the iterative procedure is unitary. Lastly, applying Green's First Identity and then FEM for the discretization of the transverse domain, the global matrix equation that represents this nonparaxial approximation is:

\[
\begin{bmatrix}
\mathcal{U} & -\frac{\Delta z}{2} \mathcal{U} \\
-\frac{\Delta z}{2} \left( \mathcal{L} + N_j^{(n+1)} \right) & (1 - j\beta_0 \Delta z) \mathcal{U}
\end{bmatrix}
\begin{bmatrix}
\eta_j^{(n+1)} \\
\phi_j^{(n+1)}
\end{bmatrix} =
\begin{bmatrix}
\mathcal{U} & \frac{\Delta z}{2} \mathcal{U} \\
\frac{\Delta z}{2} \left( \mathcal{L} + N^{(n)} \right) & (1 + j\beta_0 \Delta z) \mathcal{U}
\end{bmatrix}
\begin{bmatrix}
\eta^{(n)} \\
\phi^{(n)}
\end{bmatrix}.
\]  

(2.244)
2. Physical background and formulations

when:

\[ J = \sum_{i=1}^{3} \phi_{ie} \varphi_{ie}, \quad (2.245) \]

\[ E = \sum_{i=1}^{3} \eta_{ie} \varphi_{ie}. \quad (2.246) \]

In order to implement this method, the local matrices for each operator are provided:

\[ [U] = \frac{A_e}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \quad (2.247) \]

\[ \{\mathcal{L}\}_{ij} = \frac{a^2}{8A_e} (b_i b_j + c_i c_j (\beta_2 j \beta_0 j + \beta_1 j)) - \frac{\beta_0^2 - k_0^2 \varepsilon_{ij}}{2} \{\mathcal{U}\}_{ij} + \frac{a_j c_j}{6} (\beta_0 N \beta_1 N - \beta_0 j \beta_1 j), \quad (2.248) \]

\[ \{\mathcal{N}\}_{ij} = -\frac{k_0^2 \alpha_j}{240} \eta_j |\eta_j|^2 Y_{ij}, \quad (2.249) \]

where

\[ Y_{jj} = 8A_e - 6a \tau_j c_j - 20 \left( \frac{a \tau_j c_j}{A_e} \right)^2, \quad (2.250) \]

\[ Y_{ij} = 2A_e - 2a \tau_j c_j - (10c_i c_j + 5c_j^2) \left( \frac{a \tau_j c_j}{A_e} \right)^2, \text{ for } i \neq j. \quad (2.251) \]

As usual, these local matrices are assembled into global matrices, by converting the local nodal indices to global nodal indices.

2.2.5.2 Modal Equation

As the paraxial and non-paraxial equations for the propagation have the same terms except for the partial derivatives with respect to \( z \), the propagation coordinate, both models share the same modal equations (2.241) for the so-called bullets and (2.242) for the time independent set of stationary solutions. The associated matrix problems can be solved by using the vector iteration methods described by Bathe and Wilson [38], ensuring fast and reliable solutions for the numerical problem.
2.2.5.3 Stability

It is clear that the stability analysis is exactly the same as for the non-paraxial formulation applied to the $2D + z$ problem, so again the Crank–Nicolson method ensures stability.

2.2.6 Pumping and First Order Dispersion

2.2.6.1 Propagation

Recalling equations (2.68) and (2.69) that describe propagation in Kerr-like media where pumping induces another nonlinearity and where time harmonic behaviour is of interest, if the Crank-Nicolson and then FEM are used, then the following system of equations should be solved:

$$
\begin{align*}
\left( \begin{bmatrix} [L_{sl}] & 0 \\ 0 & [L_{pl}] \end{bmatrix} + \begin{bmatrix} [N_{sl}] & [N_{sr}] \\ [N_{pl}] & [N_{pr}] \end{bmatrix} \right) \begin{bmatrix} \eta_{s}^{(n+1)} \\ \eta_{p}^{(n+1)} \end{bmatrix} &= \left( \begin{bmatrix} [L_{sr}] & 0 \\ 0 & [L_{pr}] \end{bmatrix} - \begin{bmatrix} [N_{sl}] & [N_{sr}] \\ [N_{pl}] & [N_{pr}] \end{bmatrix} \right) \begin{bmatrix} \eta_{s}^{(n)} \\ \eta_{p}^{(n)} \end{bmatrix}
\end{align*}
$$

Equation 2.252, makes use of the definitions:

$$
[L_{sl}] = \frac{A_e}{12 \Delta z} \left( 1 + \frac{j \Delta z (\beta_{0s}^2 - \varepsilon_{1j} k_0^2)}{4 \beta_{0s}} \right) [T] + \frac{j}{16 A_e} [M_s] - \frac{a}{12} \left( \frac{\beta_{0N} \beta_{1N}}{\beta_{0s}} - \frac{\beta_{0js} \beta_{1js}}{\beta_{0s}} \right) [H], \tag{2.253}
$$

$$
[L_{pl}] = \frac{A_e}{12 \Delta z} \left( 1 + \frac{j \Delta z (\beta_{0p}^2 - \varepsilon_{1j} k_0^2)}{4 \beta_{0p}} \right) [T] + \frac{j}{16 A_e} [M_p] - \frac{a}{12} \left( \frac{\beta_{0N} \beta_{1N}}{\beta_{0p}} - \frac{\beta_{0jp} \beta_{1jp}}{\beta_{0p}} \right) [H], \tag{2.254}
$$

$$
[L_{sr}] = \frac{A_e}{12 \Delta z} \left( 1 - \frac{j \Delta z (\beta_{0s}^2 - \varepsilon_{1j} k_0^2)}{4 \beta_{0s}} \right) [T] - \frac{j}{16 A_e} [M_s] + \frac{a}{12} \left( \frac{\beta_{0N} \beta_{1N}}{\beta_{0s}} - \frac{\beta_{0js} \beta_{1js}}{\beta_{0s}} \right) [H], \tag{2.255}
$$

$$
[L_{pr}] = \frac{A_e}{12 \Delta z} \left( 1 - \frac{j \Delta z (\beta_{0p}^2 - \varepsilon_{1j} k_0^2)}{4 \beta_{0p}} \right) [T] - \frac{j}{16 A_e} [M_p] + \frac{a}{12} \left( \frac{\beta_{0N} \beta_{1N}}{\beta_{0p}} - \frac{\beta_{0jp} \beta_{1jp}}{\beta_{0p}} \right) [H], \tag{2.256}
$$

$$
[N_{sr}] = \frac{j k_0^2 A_e \alpha_2}{48 \beta_{0s}} \left( \eta_{s}^{*(n+1)} \eta_{s}^{(n+1)} + \eta_{p}^{*(n)} \eta_{s}^{(n)} \right) [T], \tag{2.257}
$$

$$
[N_{pl}] = - \left( \frac{\beta_{0s}}{\beta_{0p}} \right) \left( \frac{k_0^2}{k_0^2} \right) [N_{sr}], \tag{2.258}
$$
The matrices are defined by:

\[
[T] = \begin{bmatrix}
2 & 1 & 1 \\
1 & 2 & 1 \\
1 & 1 & 2 \\
\end{bmatrix}
\]  \hspace{1cm} (2.261)

\[
\{m_{ru}\}_s = \frac{b_r b_u}{\beta_{0s}} 
\]  \hspace{1cm} (2.262)

\[
\{m_{ru}\}_p = \frac{b_r b_u}{\beta_{0p}} 
\]  \hspace{1cm} (2.263)

\[
\{h_{ru}\} = c_u 
\]  \hspace{1cm} (2.264)

The factor \(a\) is defined in terms of \(\beta_1\), and it should be of the order of \(1/\beta_{1N}\). Clearly, the dimensions of \(a\) are in \([m/s]\).

2.2.6.2 Modal Equation

By defining:

\[
[L_s] = \frac{j A_e (\beta_{0s}^2 - \epsilon_{lj} k_{0s}^2)}{48 \beta_{0s}^3} [T] + \frac{j}{16 A_e} [M_s] - \frac{a}{12} \left( \frac{\beta_{0N} \beta_{1N}}{\beta_{0s}} - \frac{\beta_{0s} \beta_{1js}}{\beta_{0s}} \right) [H],
\]  \hspace{1cm} (2.265)

\[
[L_{pl}] = \frac{j A_e \Delta x (\beta_{0p}^2 - \epsilon_{lj} k_{0p}^2)}{48 \beta_{0p}^3} [T] + \frac{j}{16 A_e} [M_p] - \frac{a}{12} \left( \frac{\beta_{0N} \beta_{1N}}{\beta_{0s}} - \frac{\beta_{0p} \beta_{1jp}}{\beta_{0p}} \right) [H],
\]  \hspace{1cm} (2.266)

it is clear that for "local" modes or linear modes, the eigenvalue problem for the signal can be isolated, and only then, the eigenvalue problem for the pump can be solved. In any case, the general formulation of the eigenvalue problem is:

\[
\begin{pmatrix}
[L_s] & 0 \\
0 & [L_p]
\end{pmatrix}
+ \begin{pmatrix}
[N_{sl}] & [N_{sr}] \\
[N_{pl}] & [N_{pr}]
\end{pmatrix}
\begin{bmatrix}
\eta_s^{(n+1)} \\
\eta_p^{(n+1)}
\end{bmatrix} = 0,
\]  \hspace{1cm} (2.267)

where the nonlinear matrices have already been defined.
2.2.6.3 Stability

As in the analysis of the time-domain formulation, when considering local modes for the signal, the stability analysis is bound to be the same as for the paraxial problem, and the eigenvalue problem for the pump becomes dependent of the signal, but keeps the same form as the paraxial formulation, so again the Crank-Nicolson method ensures stability.

2.2.7 Split-Operator/Galerkin Method

The Split-Operator Method [41], [42], [43], [44], is a combination of two methods, Crank-Nicolson /Galerkin for some linear part of the equation, and a formal analytic solution for the nonlinear part of the equation. For the paraxial approximation and slab waveguides it has been reported [45] that its implementation results in a drastic reduction in execution time. The last referred work goes further on the approximation by reducing the nonlinear split part of the operator to a vector operation instead of a matrix operation. More about this subject is discussed in the following sections.

2.2.7.1 Paraxial Formulation

The following is a short development of the method. Assuming that $\mathcal{L}$ is a linear differential operator not dependent of $z$, $u$ is a function of the coordinates, $\mathcal{N}$ is a nonlinear operator that depends on the coordinates and explicitly on the function $u$. Then if the equation to be solved is:

$$\frac{\partial u}{\partial z} = \mathcal{L}(x, y) \ u(x, y, z) + \mathcal{N}(x, y, u) \ u(x, y, z)$$

(2.268)

Formally, it is possible to write:

$$u(x, y, z_0 + \Delta z) = e^{(\mathcal{L} \Delta z + \mathcal{N} \Delta z)} u(x, y, z_0)$$

(2.269)

Now assuming that $\mathcal{L} \mathcal{N} \simeq \mathcal{N} \mathcal{L}$, the exponential expression may be separated in two, and (2.269) becomes [21]:

$$u(x, y, z_0 + \Delta z) = e^{(\mathcal{L} \Delta z)} e^{(\mathcal{N} \Delta z)} u(x, y, z_0) + \mathcal{O}(x, y, \Delta z, u)$$

(2.270)
Now, defining:

\[ u(x, y, z_0 + \Delta z) = e^{(N \Delta z)} u(x, y, z_0 + \Delta z) \]  \hspace{1cm} (2.271)
\[ v(x, y, z_0 + \Delta z) = e^{(L \Delta z)} v(x, y, z_0) \]  \hspace{1cm} (2.272)

And (2.272) is evaluated by solving the equivalent equation:

\[ \frac{\partial v}{\partial z} = L(x, y) v(x, y, z) \]  \hspace{1cm} (2.273)

Solution of (2.271) and (2.273) constitute what is called the Split-Operator Method. The last equation is solved using the proper Crank–Nicolson/Galerkin Method. Improvements in accuracy over this method can be reached by splitting the nonlinear operator into two and then use one to premultiply and the other one to postmultiply the linear operator. The price of this improvement is speed of the algorithm, that forces a further analysis on the error before trying this approximation. In fact, the approximation error for the split operator technique can be expressed by:

\[ \epsilon_1 = |LN - NL| \frac{(\Delta z)^2}{2} \]  \hspace{1cm} (2.274)

If the symmetrized operator is developed, then the approximation error becomes:

\[ \epsilon_2 = |L^2 N + N L^2 - 2LNCL + 4NLNL - 2NLNL - 2NLNL| \frac{(\Delta z)^3}{24} \]  \hspace{1cm} (2.275)

It is important to realize that both errors (\( \epsilon_1 \) and \( \epsilon_2 \)) become zero if \( L \) and \( N \) commute, i.e.: \( LN = NL \). It is important to notice that (2.271) admits another approximation, that is to consider the exponential term as a scalar value, where \( N \) is replaced by the corresponding nonlinear scalar, this is exactly the method developed in [45].

### 2.2.7.2 Non-paraxial Formulation

Taking (2.30), and applying FEM, the problem may be written as:

\[ \frac{\partial}{\partial z} \begin{bmatrix} \eta \\ \phi \end{bmatrix} = \begin{bmatrix} [0] & [U] \\ [L] + [N] & 2j\beta [U] \end{bmatrix} \begin{bmatrix} \eta \\ \phi \end{bmatrix}, \]  \hspace{1cm} (2.276)

and formally the solution may be expressed as:

\[ \begin{bmatrix} \eta^{(n+1)} \\ \phi^{(n+1)} \end{bmatrix} = e^{[Q] \Delta z} \begin{bmatrix} \eta^{(n)} \\ \phi^{(n)} \end{bmatrix}, \]  \hspace{1cm} (2.277)
but following Silberberg [39], a symmetrization is applied, which is second order accurate in $\Delta z$ accordingly to (2.275). The new approximation is written as:

$$
\begin{bmatrix}
\eta^{(n+1)} \\
\phi^{(n+1)}
\end{bmatrix} =
\begin{bmatrix}
\mu^{(n)} \\
\nu^{(n)}
\end{bmatrix}
\begin{bmatrix}
\rho^{(n)} \\
\sigma^{(n)}
\end{bmatrix}
\begin{bmatrix}
\eta^{(n)} \\
\phi^{(n)}
\end{bmatrix}
\begin{bmatrix}
\rho^{(n+1)} \\
\sigma^{(n+1)}
\end{bmatrix}.
\tag{2.278}
$$

Now, setting:

$$
\begin{bmatrix}
\rho^{(n)} \\
\sigma^{(n)}
\end{bmatrix} =
\begin{bmatrix}
\eta^{(n)} \\
\phi^{(n)}
\end{bmatrix},
\tag{2.279}
$$

the equivalent differential equation is written and then C-N is applied to the linear split problem:

$$
\begin{bmatrix}
\rho^{(n+1)} - \rho^{(n)} \\
\sigma^{(n+1)} - \sigma^{(n)}
\end{bmatrix} =
\frac{\Delta z}{4}
\begin{bmatrix}
[0] & [U] \\
[L] & 2j\beta[U]
\end{bmatrix}
\begin{bmatrix}
\rho^{(n+1)} + \rho^{(n)} \\
\sigma^{(n+1)} + \sigma^{(n)}
\end{bmatrix}.
\tag{2.280}
$$

The next stage is to generate $\nu^{(n)}$ and $\mu^{(n)}$, which is done by applying the nonlinear expression; it is important to notice that:

$$
\begin{bmatrix}
Q_N
\end{bmatrix}_i = [0], \text{ for } i \geq 2.
\tag{2.281}
$$

So, the transformation is:

$$
\begin{bmatrix}
\nu_{j+1}^{(n)} \\
\mu_{j+1}^{(n)}
\end{bmatrix} =
\begin{bmatrix}
[I] & 0 \\
\Delta z [N_{j+1}] & [I]
\end{bmatrix}
\begin{bmatrix}
\rho^{(n+1)} \\
\sigma^{(n+1)}
\end{bmatrix},
\tag{2.282}
$$

and iterations might be necessary to give consistency to the procedure, because:

$$
[N_{j+1}] = \mathcal{N}
\left(
\begin{bmatrix}
\frac{\rho^{(n+1)} + \nu^{(n)}}{2} \\
\frac{\sigma^{(n+1)} + \mu^{(n)}}{2}
\end{bmatrix}
\right).
\tag{2.283}
$$

The last equation to solve is:

$$
\begin{bmatrix}
\nu^{(n+1)} - \nu^{(n)} \\
\mu^{(n+1)} - \mu^{(n)}
\end{bmatrix} =
\frac{\Delta z}{4}
\begin{bmatrix}
[0] & [U] \\
[L] & 2j\beta[U]
\end{bmatrix}
\begin{bmatrix}
\nu^{(n+1)} + \nu^{(n)} \\
\mu^{(n+1)} + \mu^{(n)}
\end{bmatrix}.
\tag{2.284}
$$
The solution now is given by:

\[ \begin{bmatrix}
\eta^{(n+1)} \\
\phi^{(n+1)}
\end{bmatrix} = \begin{bmatrix}
\nu^{(n+1)} \\
\mu^{(n+1)}
\end{bmatrix}. \tag{2.285} \]

Clear advantages of this method are:

- Equation (2.280) has a simple solution, and it is unitary and stable,
- Equation (2.284) has the same characteristics as (2.280),
- The procedure defined by (2.281) requires only one level of recursion,
- Iterations on the nonlinearity are straightforward and exclude the need of solving another matrix problem,
- Both simultaneous linear systems of equations are defined by the same linear matrix, so every procedure of solving a matrix is very fast (except the first one).
Chapter 3

Analysis in Steady State

3.1 Practical Structures under Paraxial Approximation

In order to reach the goals defined earlier, a program is described next. The first test will be done for the linear case and later on further complexities will be included. Certainly the simplest formulations will also have to be of interest. Since propagation problems for slab waveguides have already been well covered, the starting point considers propagation along one spatial coordinate for a 2D cross section structure. Also, all the problems will be treated using a scalar approximation.

3.1.1 Validation

The first test made against previously published results, considers beam propagation in rib waveguides and couplers [9]. This problem looks very attractive as a first test because it allows to verify the linear behaviour before starting simulations in nonlinear media. As all the main results given in [9] come in terms of contour plots, special attention will be given to local maxima and local minima for those plots, which will be compared with the results obtained through the simulation of the programs based on the developments made in the previous chapter. Power plots are also included with the aim of testing the stability and accuracy of the program.
Other differences for this simulation are:

- Size of the domain
- Discretization of the domain (about $2 \times 1800$ nodes here, vs. about 65000 nodes in [9])
- Modes generated by different procedures than in [9]
- Different $z$-step (up to $\frac{1}{50}$ freespaced wavelength here vs $\frac{1}{8}$ freespaced wavelength used in [9]).

3.1.1.1 Evolution of Overfilling Gaussian Input through a rib structure

The first simulation is executed on a rib-shaped structure made of two linear materials and surrounded by air. The rib structure together with its dimensions and composition is shown schematically in Fig. 3.1. The excitation overfills the main part of the rib at $z = 0$ the shape of the excitation is given by a Gaussian beam defined by:

$$E_y(x, y, 0) = e^{-\left(\frac{x^2+(y-0.55)^2}{\lambda^2}\right)}$$  \hspace{1cm} (3.1)

distances are measured in metres and electric field in [V/m].

The nature of the material above the rib is not explicitly defined in the reference. Here it is assumed to be air, supposition that could lead to some inaccuracies when the results
of the reference and the validations are faced to each other. Anyway, as the strongest permittivity is inside the rib, guiding results should be similar.

The values for the relative linear permittivities are those of reference [9]:

\[
\begin{align*}
\varepsilon_{\text{sub}} &= 11.1556 \text{ \it in the substrate} \\
\varepsilon_{\text{rib}} &= 11.8336 \text{ \it in the rib} \\
\varepsilon_{\text{air}} &= 1.0.
\end{align*}
\]

Plots shown on Fig. 3.2 are directly comparable with Fig. 3 of [9]. The results obtained using the finite element method explained, in the previous chapter, are clearly closer to the results shown after using paraxial analysis with iterative Lanczos reduction [9].

![Figure 3.2: Contour plot at 0, 1 and 2 [µm]](image)

The structure analyzed and the mesh used are shown in Fig. 3.3. The mesh considered is one half of the full structure because symmetric behaviour is expected.

Radiation during the initial steps make the total power to be reduced (Fig. 3.4) nearly to 92% after 0.073 µm of propagation along the z-axis, effect that can be justified by the fact that although the mesh was adapted, initial settling of the input to the structure makes that each element of the mesh increases the error in the approximations.
After settling down, the power is kept constant and power fluctuations during propagation are negligible.

Figure 3.4: Power evolution plot
3.1.1.2 Evolution of Embedded Gaussian Input through a rib structure

A further validation is performed on the same structure but employing an embedded excitation. In terms of mismatching, as the input is closer to the mode, this situation is less demanding because the mesh keeps its level of adaptiveness to the electric field. The input beam keeps nearly all the power confined inside the rib. Its envelope is given by:

\[ E_y(x, y, 0) = e^{-\left(\frac{x^2 + (y - 0.55)^2}{0.72}\right)} \]

where all distances are measured in metres and electric field in [V/m]. Values for the permittivities are the same used in the previous example.

The structure analyzed and the mesh used are shown in Fig. 3.5, taking advantage of the symmetry.

![Figure 3.5: Basic and final (3654 elements and 1866 nodes) meshes on the structure](image)

Figs. 3.6 to 3.8 are directly comparable with Fig. 2 of [9]. The results obtained by using our program based on finite elements and Crank-Nicolson/Galerkin methods are clearly very similar to those displayed in [9], specially the number and apparent location of the local maxima.
Fig. 3.9 shows that for the Crank-Nicolson/Galerkin method power fluctuations are negligible. Results show clear similarities with those presented in [9]. Even though the approximation here is scalar and paraxial and in [9] is scalar but both paraxial and non-paraxial, the plots show almost exactly the same location for local maxima, both on the x-y plane and on the distance of propagation. Again, as in the previous example, some mismatching between the field distribution and the mesh at the initial stages of propagation alters the calculated value of propagated power, but then it stays almost unchanged. As this time the excitation is completely inside the rib-region, nearly all the modes are guided (not ra-
diation modes) and mismatching between field and mesh is effectively reduced, resulting in conservation of calculated power.

3.1.1.3 Evolution of a single waveguide mode through a rib coupler

Validation of the linear part of the program can also be achieved by testing the behaviour of a coupling device. In fact, in these kind of tests, shapes can be compared and what is
even more important, coupling length. The structure of the coupler rib to be used for this test is shown schematically in Fig. 3.10. The media are characterized through the following

\[ \varepsilon_{\text{sub}} = 11.2896 \quad \text{in the substrate} \]
\[ \varepsilon_{\text{rib}} = 11.8336 \quad \text{in the ribs} \]
\[ \varepsilon_{\text{air}} = 1.0 \]

The envelope of the input beam is given by:

\[ \mathcal{C} = \varepsilon_0 e^{-\left(\frac{(x+2.5)^2}{4.5} + \frac{(y-0.4)^2}{0.72}\right)} \]  

(3.3)

The structure analyzed is shown in Fig. 3.11 and the mesh used is displayed in Fig. 3.12.

For the coupling length, the predicted value is \( L_{\text{pred}} = 785 \, \mu m \) [9] and the result obtained from the power plot (Fig. 3.13) is about \( L_{\text{FEM}} = 800 \, \mu m \). From the same plot the error on the last measurement can be estimated around 50 \( \mu m \), so further analysis is necessary to have a better estimate of the coupling length otherwise the disagreement can be misleadingly taken as higher than expected.

Total power and transfer of power are shown in Fig. 3.13. It can be seen that total power is practically unchanged through all the propagating distance, the other curve shows the steady transfer of power, with very little fluctuations that break the expected symmetry of the graph due to the presence of other modes with lower powers and different coupling lengths.
Figures 3.11 and 3.12 show the basic and actual mesh and structure, respectively. Figures 3.14 to 3.24 show similar results to those in Fig. 4 of [9]. Marking a slight difference from the simulations done by Ratowsky et al. [9], the simulations made here were done with a Gaussian beam instead of a proper mode of the single rib-structure. Indeed this induces some fluctuations in the power transfer graph, but should not make big differences.
in the measurement of coupling length. From the contour plots, it is rather clear that $L_{FEM} = 775 \, \mu m$, when power disappears from the launching side. At this point the differences between $L_{pred}$ and $L_{FEM}$ are of the order of 1.5%. This very small disagreement (bearing in mind that the simulation made with the FEM uses a gaussian beam which is a superposition of modes) comes to confirm the reliability of the method. On the other hand, very small fluctuations of the total power indicate high stability, which is of capital importance for the extension of the method to structures showing nonlinear behaviour.
Figure 3.15: Contour plot at $z = 77.5 \mu m$

Figure 3.16: Contour plot at $z = 155 \mu m$

Figure 3.17: Contour plot at $z = 232.5 \mu m$
Figure 3.18: Contour plot at $z = 310[\mu m]$

Figure 3.19: Contour plot at $z = 387.5[\mu m]$

Figure 3.20: Contour plot at $z = 465[\mu m]$
Figure 3.21: Contour plot at \( z = 542.5[\mu m] \)

Figure 3.22: Contour plot at \( z = 620[\mu m] \)

Figure 3.23: Contour plot at \( z = 697.5[\mu m] \)
3.1.2 Nonlinear Switch

Every time a modal analysis is applied to nonlinear structures used as switches, a question remains unanswered: whether the modes will propagate over a reasonable distance or whether they will appear as an asymptotic result of doubtful practical value. Propagation analysis can and will lead to the answer to the latter question by eventually measuring the distance needed for the settling down of the mode.

The example analyzed here deals with a very simple structure proposed by Li et al. in [46]. This is the first time that switching properties of nonlinear strip optical structures have been analyzed numerically in propagation using both the Crank-Nicolson/Galerkin and the Split-Operator methods along with finite elements.

The simulation considers a linear strip over a nonlinear substrate and covered by a linear cladding. The structure is shown schematically in Fig. 3.25.

All the plots for this simulation have been generated using the Crank-Nicolson/Galerkin method described in the previous chapter. The simulation makes use of a longitudinal step of $\lambda_0/20$, where $\lambda_0 = 0.515 \mu m$. The excitation is provided using a linear mode that is injected to the strip. It has been reported by Li et al. [46] that after applying modal analysis, switching eventually appears from the linear strip to the nonlinear cladding. Previously published results for this structure [46] contain no prediction about the propagation distance.
Figure 3.25: Strip-based Switch Structure. $\varepsilon_{l,cl} = \varepsilon_{l,sub} = 2.2500$, $\varepsilon_{l,at} = 2.4010$ mWry,..., $G = 6.37726 \cdot 10^{-12}$ [m²/V²], as in reference [46].

from a modal analysis, neither they give a prediction about dynamic behaviour in the cross section. Propagation analysis can give results for these two aspects. Fig. 3.26 shows how the beam of the electric field evolves from its initial position to the new position when switching happens. Fig. 3.27 shows that once the beam has been switched, its location remains unchanged for a very long distance.

Figure 3.26: Evolution of the optical beam along the waveguide. Projections on the x=0 plane are shown for values of z from 0 to 12 μm.

For this study, the fundamental linear mode of the structure has been adopted as the
input beam with different power levels and then propagated down the optical waveguide for long distances. Results of this simulation show clearly that for low input powers (below the critical power $P_c$, the beam is kept trapped in the linear strip, as it has been shown by modal analysis of the same structure [47], [46]. If that critical power is exceeded, the beam is sharpened, but still inside the nonlinear substrate, where it remains confined at some distance from the interface for the rest of the distance of propagation. Fig. 3.28 show the beam at the input and after the switching has been settled. It should be noticed that the graphs for Fig. 3.28 use different length scales.

Fig. 3.29 displays switching distance as a function of power of the input beam showing roughly the expected behaviour. Moreover, according to Li et al. [46] the curve should have a vertical asymptote at the critical power $P_c = 0.086 \text{ mW}$ and a horizontal one at some positive distance.

In principle, it could have been possible to get a relation between power of the input beam and distance to the interface, but results show that differences between these distances are of the order of the size of minimum triangles at the interface. This suggests that if such
Figure 3.28: Transverse distribution of the $E_y$ field of the input beam and of the switched beam at a distance of 40 free-space wavelengths (20.6 $\mu m$) from the excitation plane.

Figure 3.29: Switching distance as a function of the power of the input beam.
a relation is sought, then a new mesh should be adapted keeping a high density of nodes on the neighbourhood of the interface between the strip and the substrate. If these results are compared with what is obtained from the analysis in $1D + z$ simulations for Kerr-like media, it is remarkable the fact that solitons are found as the solution to slab-waveguides but not for $2D + z$ simulations. This difference is explained by considering that in $2D + z$ simulations, power is spread on an extra dimension, thus compensating the increase in local electric filed intensity due to the Kerr permittivity. A second effect that can be used to obtain some advantage is the fact that once the switching has settled, the main beam is constrained to a much smaller spot, a situation that could be used for reducing crosstalk.

3.1.3 Nonlinear Coupler

A directional coupler permits transfer of power between two structures, and if nonlinearity is present, the coupling could be controlled or switched, by means of the input power. The structure analyzed is perhaps the simplest form of nonlinear coupler, and consists of two equal buried nonlinear guides immersed in a linear medium. As a symmetric result is expected, only one half of the domain is analyzed, and some of the calculations will take into account what happens on the symmetry line. Fig. 3.30 shows the basic mesh used to analyze the lower part of the structure. The values for relative permittivities are:

\[
\begin{align*}
\varepsilon_{cl} & = 2.2801 \quad \text{cladding} \\
\varepsilon_{co,ld} & = 2.30432 \quad \text{core} \\
\varepsilon_{cp,ld} & = 3.1 \cdot 10^{-13} \, [m^2 V^{-2}] \quad \text{core}. \\
\end{align*}
\]

This simulation is made using a gaussian beam as the envelope for the excitation. The shape of the excitation is given by:

\[
\exp\left(-2 \left(\frac{(x + 6.0)^2 + y^2}{9}\right)\right)
\]

and its amplitude adjusted accordingly to the desired input power. The free-space wavelength is $\lambda_0 = 1.532 \mu m$. 
Fig. 3.31 shows how the electric field on the symmetry line varies through the propagating distance. The overall coupling effect is clearly seen, but more reassuring of the good behaviour are the results for power evolution (that include not only the fields on the symmetry line), which are displayed in Fig. 3.32. The dynamic nature of the coupling is observed both in Figs. 3.31 and 3.32, where power is transferred from one arm to the other, but suffering from fluctuations explained by the spreading and further focusing of the field during propagation, in the case of electric field evolution, and the presence of other modal components in the case of the power evolution.

Figs. 3.33 and 3.34 describe exactly the same phenomenon, but for the approximation cases explained in section 2.2.2.1, with power totally preserved in only one of the cases. Then, according to these results, as total power is conserved at a higher degree, transfer of power is much more reliable for (2.168).

Fluctuations of total power for the Split Operator method shown in Fig. 3.35 cannot be attributed to initial radiation, because total power is not conserved and the only possible interpretation of the results is that this method is not reliable for simulating media involving fairly high nonlinearities when three spatial coordinates are taken into account.
Program results show clearly that for small power (below 1 [mW]), enough coupling is achieved, but for high power (near or above 10 [mW]), most of the power is bounded to the launching side of the structure. Switching is found in these nonlinear device, these time this effect can be used for controlling the output by changing its input power.

Again, the behaviour of the solution methods for the Schrödinger equation shows that for strong nonlinearities (or strong excitations), the Split Operator method does not preserve power and hence stability is lost. On the other hand, the current formulation of the Crank-Nicolson/Galerkin method shows power conservation and stability. At this point it is worth to point out that similar conclusions were found using a slightly different version of the Split Operator method when it was applied to the structure mentioned in Section 3.1.2.
Figure 3.32: Comparison of power in one guide of a buried guide coupler, calculated over two complete cycles with the CN method (2.168) and SOM. Total input power in the coupler = 1 mW. © IEEE, 1995 [36]

Figure 3.33: Total power in the coupler and power in the excitation arm calculated with the CN method based on (2.168) for total input of 10 mW. ©IEEE, 1995 [36]
3.1.4 Three-state Nonlinear Coupler

An interesting device designed to route or split power according to the input power is proposed here. The structure consists basically of two square cross-section channels with a rectangular section channel between them, all embedded in a linear material. All three channels have a Kerr type nonlinearity. The input considered is the fundamental mode of one square channel exciting the left square channel. The purpose of this simulation is to find levels of power for each state and also the sensitivity to power variations. The structure is shown schematically in Fig. 3.36.

The parameters that define the structure are:

\[
\begin{align*}
\varepsilon_{sub} &= 2.2801, \\
\varepsilon_{ch} &= 2.304324, \\
\alpha_{ch} &= 3.1 \times 10^{-13} m^2/V^2.
\end{align*}
\]

The materials used are:

\[
\{ \text{SiO}_2 \text{ based materials} \}.
\]

Figure 3.34: Total power in the coupler and power in the excitation arm calculated with the CN method based on (2.167) for total input of 10 mW. Small fluctuations are visible. © IEEE, 1995 [36]
Figure 3.35: Power in the buried guide coupler calculated with the CN method (2.168) and SOM. The SOM fails to conserve power for total input power of 10 mW. ©IEEE, 1995 [36]

Several levels of input power are used to simulate propagation. As the behaviour of the beam during propagation should be the same on both the upper and lower half of the structure, symmetry is used. That is an advantage in terms of execution time for the simulation or alternatively an advantage in accuracy because more nodes can be used for the discretization of the cross-section. In order to have a better description of the fields in the cross-section, the distribution of the nodes of the domain should be strongly dependent
of the power density. In order to obtain a good distribution of the nodes, it is assumed that the distribution of power is nearly gaussian and that distribution is employed to adapt a mesh. The resultant mesh consists of 1088 nodes and 2070 triangles (elements) and is shown schematically in Fig. 3.37.

Figure 3.37: Coupler: 1088 nodes, 2070 elements

The dimensions of the middle channel are chosen small enough to introduce no significant effect during propagation, apart from some fluctuations of the main mode. As an example, the evolution on the horizontal upper border is shown in Fig. 3.38 for many values of the longitudinal coordinate when $P_{in} = 0.020 \text{ mW}$. 

A more useful plot, in the sense that it allows quantitative predictions of the coupling effect must include absolute total powers, situation that is seen in Fig. 3.39. In fact, despite more simulations are required for optimum design, the range of power for such a device should be restricted between 0.05 $mW$ and 0.08 $mW$, so it is implied that the ranges of output powers for discrimination should be set above 0.045 $mW$ and below 0.02 $mW$ for the coupled channel, and above 0.06 $mW$ and below 0.015 $mW$ for the launching channel.

It is likely that suppressing that narrow channel, the curves showing transfer of power would become clear than here. The plots for a wide range of powers are shown in Fig. 3.40.
Figure 3.38: Evolution of the Electric Field on the symmetry line

Figure 3.39: Design curves: Absolute Output Power vs. Total Input Power

It is clear that given a fixed length for this structure and according with the input power, this device can be used for driving the output at a particular location of the cross-section. One possible practical application could be in a ternary logic system. Small input power gives output power on one side, high input power gives output power on the other side and "half power" at the input gives output power equally split on both sides. Another possible use could be in a more complex system where some lumped probes can be coupled only
at some prescribed length, so output power then is selectively routed out of the device, according to the input power. As no significant trapping in the middle channel is found, further experiments could be done by changing either its dimensions or its materials.

3.1.5 Wavelength Multiplexor/De-multiplexor

A useful application of 1D + z simulation that is excited by two different beams featuring different wavelengths is analyzed next. The model combines the propagation method described in section 2.1.6, but restricted to only one transverse dimension, and the model introduced by Federighi et al. in [24]. The purpose of this example is to design a wavelength selective device that can route its output according to its input signal wavelength. Assuming slowly varying amplitudes, for planar waveguides, the propagation of pump and signal transverse electric field can be described using the following coupled differential equations [24]:

\[ -2j\beta_p k_{op} \frac{\partial \psi_p}{\partial z} = \frac{\partial^2 \psi_p}{\partial y^2} + k_{op}^2 (\epsilon_{xp} - \beta_p^2) \psi_p, \]

\[ -2j\beta_s k_{os} \frac{\partial \psi_s}{\partial z} = \frac{\partial^2 \psi_s}{\partial y^2} + k_{os}^2 (\epsilon_{xs} - \beta_s^2) \psi_s, \]

where \( \psi_{p,s} \) are the slowly varying amplitudes of pump and signal electric fields \( E_{xp,s} \), \( k_{op,s} \) are the free-space wavenumbers, \( \beta_{p,s} \) the effective propagation constants and \( \epsilon_{xp,s} \) the nonlinear
complex permittivities.

The imaginary parts of $\epsilon_{\text{xp,a}}$ and the resonant nonlinear index contributions can be computed locally in the active region once the populations of the $\text{Er}^{3+}$ and $\text{Yb}^{3+}$ levels involved in the transitions are known. These values depend on the local value of the fields, and can be obtained by resorting to the steady-state-rate equation and conservation laws described in [24]:

$$\frac{\partial n_1}{\partial t} = -W_{12}n_1 - W_{13}n_1 + A_{21}n_2 + W_{21}n_2 + C_{\text{up}}n_2^2 - C_{\text{cr}}n_1n_4 = 0,$$  \hspace{1cm} (3.6)

$$\frac{\partial n_2}{\partial t} = W_{12}n_1 - A_{21}n_2 - W_{21}n_2 + A_{32}n_3 - 2C_{\text{up}}n_2^2 + 2C_{\text{cr}}n_1n_4 = 0,$$  \hspace{1cm} (3.7)

$$\frac{\partial n_3}{\partial t} = W_{13}n_1 - A_{32}n_3 + A_{43}n_4 - 2C_{\text{up}}n_3^2 + C_{\text{cr}}n_1n_6 = 0,$$  \hspace{1cm} (3.8)

$$n_1 + n_2 + n_3 + n_4 = N_{\text{Er}},$$  \hspace{1cm} (3.9)

$$\frac{\partial n_5}{\partial t} = -W_{56}n_5 + A_{65}n_6 + W_{65}n_6 + C_{\text{cr}}n_1n_6 = 0,$$  \hspace{1cm} (3.10)

$$n_5 + n_6 = N_{\text{Yb}}.$$  \hspace{1cm} (3.11)

After some approximations, the nonlinear coefficients are expressed as [24]:

$$C_{\text{up}} = \frac{4\pi}{3} \frac{R_0^6}{R_{\text{Er/Er}}^3 \tau_{21}},$$  \hspace{1cm} (3.12)

$$\tau_{21} = 1/A_{21},$$  \hspace{1cm} (3.13)

$$C_{\text{cr}} = \frac{4\pi}{3} \frac{R_0^6}{R_{\text{Yb/Er}}^3 \tau_{65}},$$  \hspace{1cm} (3.14)

Other assumptions lead to:

$$R_0^6 = \frac{9}{16\pi^2} \frac{C_{\text{up}}\tau_{21}}{N_{\text{Er}}},$$  \hspace{1cm} (3.15)

so $C_{\text{up}}$ is expressed as proportional to $N_{\text{Er}}$. Also the model described by Federighi et al. [24] includes a wavelength independent Kerr coefficient ($\alpha$) and self-phase, cross-phase modulations at pump signal wavelengths.

The values of the coefficients $W_{ij}$ are directly related to the shapeline of the Er/Yb line-spectra $g(\lambda)$ here represented by the absorption and emission cross-sections $\sigma_{ij(ab|em)}$, and to the intensity of the electric field. That relation is explained and described in [48] as:

$$W_{12} = \frac{\sigma_{12 ab}|E_s|^2}{h\nu_s},$$  \hspace{1cm} (3.16)
\[ W_{21} = \frac{\sigma_{21} \text{em} |E_s|^2}{h \nu_s}, \quad (3.17) \]
\[ W_{13} = \frac{\sigma_{13} \text{em} |E_p|^2}{h \nu_p}, \quad (3.18) \]
\[ W_{31} \approx 0, \quad (3.19) \]
\[ W_{56} = \frac{\sigma_{56} \text{em} |E_p|^2}{h \nu_p}, \quad (3.20) \]
\[ W_{65} = \frac{\sigma_{65} \text{em} |E_p|^2}{h \nu_p}, \quad (3.21) \]

This model is noise free, because spontaneous emission has been omitted.

The nonlinear permittivities depend on the values obtained by solving the rate-equations and on the local value of the electric field. These values were introduced by Fleming et al. [19] and Pantell et al. in [49], and are expressed by:

\[ \epsilon_{xp} = [n_t + \frac{\Delta \lambda_p}{\delta \lambda_{56}} \lambda_p (\sigma_{Y65} N_5 - \sigma_{Y65} N_6)]^2 + \alpha (|\psi_p|^2 + 2|\psi_s|^2) \]
\[ + j [\frac{\pi \lambda_p}{2\pi} (\sigma_{Er13} N_1 + \sigma_{Y65} N_3)], \quad (3.22) \]
\[ \epsilon_{xs} = [n_t + \frac{\Delta \lambda_s}{\delta \lambda_{12}} \lambda_s (\sigma_{Er12} N_1 - \sigma_{Er12} N_2)]^2 + \alpha (|\psi_s|^2 + 2|\psi_p|^2) \]
\[ + j [\frac{\pi \lambda_s}{2\pi} (\sigma_{Er12} N_1 - \sigma_{Er12} N_2)], \quad (3.23) \]

where the physical inter-relation between populations and emission and absorption cross-sections are out of the scope of this work, but very well described in [19] and [49].

The solution of the system of equations (3.4, 3.5) is performed numerically by means of the SOM, which has been demonstrated to be reliable for 1D + z propagation [45]; the slowly varying amplitudes of pump and signal fields at \( z = z + \Delta z \) are obtained solving numerically two large and sparse linear systems. For each step in propagation the method also requires the numerical solution of the population rate-equations in each node of the mesh that belongs to the active region.

The coupler under analysis is made of two slab silica-waveguides whose width is 5 \( \mu m \), separated by 20 \( \mu m \) of cladding. The coupler has been chosen to be 13.3 mm long. The linear refractive permittivities are:

\[ \epsilon_{\text{core}} = 2.408704, \]
\[ \epsilon_{\text{clad}} = 2.402500, \]
\[ \alpha = 3.776 \times 10^{-18} \text{m}^2/\text{V}^2 \]

Only the arm of the coupler that receives the excitation is doped by introducing the following concentrations:

\[ N_{Er} = 2.4 \times 10^{26} \text{ions}/\text{m}^3, \]
\[ N_{Yb} = 1.0 \times 10^{27} \text{ions}/\text{m}^3, \]

where \( N_{Er} \) and \( N_{Yb} \) represent the doping concentration of \( Er^{3+} \) and \( Yb^{3+} \) respectively.

When pumping is absent, the coupling length is about 11 mm for a wavelength of \( \lambda = 1.532 \mu m \).

When the nonlinear behaviour is taken into account it is realized that there is a high absorption at the pump wavelength \( \lambda_p = 0.980 \mu m \) for dopant ions. Then in order to ensure sufficient degree of population inversion for all the coupling length, the design of the device needed several trials before deciding to use the dimensions and material properties analyzed here.

The simulations have considered constant pump and signal powers and the same pump wavelength, while the signal wavelength has been varied. Each simulation at a certain wavelength yields one signal power transfer relation that can be used for choosing the optimum operating conditions for the device. Fig. 3.41 shows the normalized signal powers in both arms as functions of propagation distance for \( \lambda_s = 1530 \text{nm} \) and \( \lambda_s = 1560 \text{nm} \). Transfer of power at 1530 nm seems to be very good and also the coupling remains very weak at 1560 nm, according to the simulations. This particular result is very interesting because hints the possibility of routing the signal power through a device based on the proposed nonlinear coupler.

The operation of this device can be explained physically because the very efficient pair-induced energy transfer from \( Er^{3+} \) to \( Yb^{3+} \), the absence of \( Er^{3+}-Er^{3+} \) ion-pairs [24] ensure a strong population inversion between \( ^4I_{15/2}, ^4I_{13/2} \) Erbium levels. In this way, the resonant nonlinearity around 1532 nm is effectively boosted while the wavelength-independent nonresonant contribution increases the likelihood of the coupling being stopped in the range of wavelengths where these two refractive index contributions have the same sign. As the resonant nonlinear contribution is expected to change sign for wavelengths symmetrically
detuned from the gain peak of Erbium (1532 nm), good coupling is expected around 1550 nm where the two nonlinear contributions have opposite sign. The results shown in Fig. 3.42 fully confirm this assumption, in fact, the normalized output power has been plotted for both arms of the coupler as a function of the input signal wavelength, and the effect of the change of sign for the nonlinearity is appreciated at its full extent. (The normalization has taken place using the signal input power).

In order to guarantee a high population in the Erbium gain bandwidth along with maximum resonant and non-resonant nonlinear permittivity contributions of the same order of magnitude, a suitable and strong value of pump power must be found. Input pump power is $P_{po} = 50 \text{ kW/m}$ and input signal power is $P_{so} = 1.0 \text{ W/m}$. Recalling the expressions (3.22) and (3.23), and assuming that the input pump power is about the value prescribed for this example, signal input power can still be changed, without affecting the significant values of $\varepsilon_{xp}$ and $\varepsilon_{xs}$: this allows to ensure that feeding the structure with two simultaneous signals of different wavelength will be equivalent to the superposition principle that appears in linear analysis, i.e., two or more input signals at similar power levels but with different wavelengths will be routed as if they were treated separately. Figs. 3.43 and 3.44 show electric field distributions at $\lambda_s = 1520 \text{ nm}$ and $\lambda_s = 1548 \text{ nm}$ respectively. Gain can
be easily observed from both plots. It is interesting to note that multiplexing can also be achieved by exciting with signal on each arm at 1520 nm and 1548 nm, respectively. In that case both outputs should find their way out through the same co-doped arm.

Finally, the decision process for the "wavelength nominal" values for the device can be
simplified by using Fig. 3.42, once the length of the device has already been chosen. As an example, Fig. 3.45 shows better why $\lambda_g = 1520 \text{ nm}$ and $\lambda_g = 1548 \text{ nm}$ were used as the recommended values for the device, given the device length previously obtained. Actually, if the following figure of merit:

$$10 \log \left| \frac{P(\lambda_1)}{P(\lambda_2)} \right|,$$

is used for finding the optimum values for the wavelengths, the figures of merit for both arms at $\lambda_s = 1520 \text{ nm}$ and $\lambda_s = 1550 \text{ nm}$ are $12.37 \text{ dB}$ and $8.88 \text{ dB}$ and at $\lambda_s = 1520 \text{ nm}$ and $\lambda_s = 1548 \text{ nm}$ are $12.08 \text{ dB}$ and $8.90 \text{ dB}$. The relevant values are the minima for each wavelength over each arm, making clear that the best choice is $\lambda_s = 1520 \text{ nm}$ and $\lambda_s = 1548 \text{ nm}$.

This important application can also be realized using the electrooptic effect and choosing the appropriate structure and materials [48] as there are strong analogies to the behaviour of $\text{Er}^{3+}$-$\text{Yb}^{3+}$ co-doped media, as it is described by Friedman et al. in [50].
3.1.6 Comparison of methods for the simulations

The methods employed for the simulations have different behaviour in terms of stability, execution time, computer memory and reliability. The assessment of these features allows to decide which method is more useful. It is clear that the implementation of the split operator method is less accurate than the Crank–Nicolson variants, see Figs. 3.46, 3.35, 3.33 and 3.34, where the SOM displays a deviation of about 1% from the expected total power value. Moreover, when high nonlinearities are present, for example in the nonlinear switch, the collapse of the SOM becomes evident. In relation to the nonlinear coupler, one big advantage of the SOM is that it can predict fairly well the propagating characteristics for the first half of the coupling length, when the input power is low. On the other hand, when power is higher, and switching on the coupler is expected, SOM again collapses, making this method unreliable for $2D + z$ propagation analysis. Added iterations to the nonlinear matrix of the SOM in an attempt to ensure convergence give no real improvement on the results.

When comparing the two variants of the Crank–Nicolson/Galerkin method as described by (2.167) and (2.168), only slight differences are observed but these may become important
Figure 3.46: Comparison of total propagated power in the buried guide coupler, calculated over two complete cycles with the CN method (2.168) and SOM. Total input power in the coupler = 1 mW. ©1995, IEEE [36]

when power is increased. In fact, (2.168) guarantees power conservation of the algorithm, therefore, transfer of power and any other parameter obtained from this variant of the method is more reliable. The only drawback observed is the higher computational cost (less than a 5% in execution time), situation that might be reversed if the structure shows a higher local power fluctuation. This last statement is demonstrated in Appendix C, but the conclusion is: whenever the condition

\[ |\psi \frac{\partial^2 \mathcal{N}}{\partial \psi^2}| \leq |\psi \frac{\partial^2 \mathcal{N}}{\partial \psi^2} + 2 \frac{\partial \mathcal{N}}{\partial \psi}| \]

is satisfied, then (2.168) guarantees better convergence than (2.169). In particular, if

\[ \mathcal{N}(\psi) = K \psi^s, \]

then (2.168) gives better performance in terms of convergence no matter the value of the real parameter \( K \), if \( s \) is a positive value.

Finally, going back to the comparison of the methods for the nonlinear coupler, a mathematical justification has been found for the differences in behaviour during propagation,
3: Analysis in... ... and this also enforces the idea that a more complex structure, or a more complex distribution of Kerr-like nonlinearity, would result in a better execution time for the method that has better convergence features. Equation (C.8) also shows that even for defocusing Kerr media, the same method is equally more convergent.
Chapter 4

Analysis in Time Domain

The development of the methods described in section 2.1.8 for the analysis of propagation
in nonlinear media in the time-domain are implemented here. In order to ensure that the results describe properly the underlying physics, it is essential to validate the methods. The validations should show the conditions that ensure that the simulations are reliable. The following sections are devoted to these validations and to one practical example of application.

4.1 Validations

4.1.1 Full Inclusion of Debye Equation

Implementing the programs that simulate propagation requires careful tests that can ensure that the results from further simulations are reliable. In order to test the different parts of the programs, validations will start considering only linear behaviour and after that tests have proved successful other effects will be studied: instantaneous nonlinearity, delays, etc.

Before starting the validations it is necessary to discuss how the parameters for the solution of the matrix problem are computed. Derivatives of the propagation constant with respect to the angular frequency are not clearly defined, but they could be obtained by
using the corresponding dispersion relation. For the linear case, the situation is very simple because both the Helmholtz equation and the paraxial equation have the same relation of dispersion when forward propagation is considered. In fact, it can be expressed as:

$$\frac{\omega}{\beta} = \frac{c}{\sqrt{\varepsilon_l}},$$

where another relation is obtained:

$$v_g = 1/\frac{\partial \beta}{\partial \omega} = \frac{c}{\sqrt{\varepsilon_l}},$$

which is the group velocity and that coincides with the phase velocity. As the permittivity is supposed to be frequency independent, the group velocity is also frequency independent, therefore:

$$\frac{\partial^2 \beta}{\partial \omega^2} = 0.$$

The situation gets more complicated if the permittivity is assumed to be frequency dependent. For that particular case, even if the problem is linear, the relations already given do not hold. In fact, the derivatives are then:

$$\frac{\partial \beta}{\partial \omega} = \frac{1}{v_p} \left( 1 + \frac{1}{2} \frac{\omega}{\varepsilon_l} \frac{\partial \varepsilon_l}{\partial \omega} \right), \quad (4.1)$$

$$\frac{\partial^2 \beta}{\partial \omega^2} = \frac{2}{\omega v_p} \left( \frac{v_p - v_g}{v_g} - \left( \frac{v_p}{v_g} \right)^2 + \frac{1}{4} \frac{\omega^2}{\varepsilon_l} \frac{\partial^2 \varepsilon_l}{\partial \omega^2} \right). \quad (4.2)$$

When Kerr–like materials are considered, the relation of dispersion changes because of the added nonlinear permittivity, no matter the delay that appears in the Debye equation. As a first approximation, the relation of dispersion can be expressed as:

$$\frac{\omega}{\beta} = \frac{c}{\sqrt{\varepsilon_l + \varepsilon_{nl}}}.$$

### 4.1.1.1 Linear validation

The linear validation is performed by using a coupler that consists of two equal slabs with linear permittivity $\varepsilon_{core} = 2.458624$, but with some dependence on the frequency, so recalling the notation $\beta_{lm} = \frac{a_n a_m}{c \omega_m^2}$, $\beta_{1\ core} = 0.521360681 \; 10^{-8} \mu s/\mu m$ and $\beta_{2\ core} = 0 \; \mu s^2/\mu m$ at the excitation frequency (note that $1/v_p\ core = 0.523028501 \; 10^{-8} \mu s/\mu m$), surrounded by a substrate with linear permittivity $\varepsilon_{subs} = 2.402500$ and frequency independent,
so \(\frac{1}{v_{p\sub}} = \frac{1}{v_{g\sub}}, \frac{1}{v_{g\sub}} = \beta_{1\sub} = 0.517024348 \times 10^{-8} \mu s/\mu m\) and also \(\beta_{2\sub} = 0 \mu s^2/\mu m\). As the linear case should be rather free of fluctuations, a long \(z\)-step can be used, and \(\Delta z = \lambda_0/5\) should be sufficient to ensure a reliable solution. Input power is not really an important parameter except for monitoring power conservation of the numerical method. The free-space wavelength is \(\lambda_0 = 1.532 \mu m\).

The coupler has been analyzed with the SOM in the \(1D + z\) domain, and its coupling length has been found to be \((670.5 \pm 5) \mu m\), reaching a maximum transferred power of nearly 91.98%.

Local time is represented by the \(y\)-coordinate which is measured in \(\mu m\). For the present simulation 1 \(\mu m\) corresponds to \(2.6 \times 10^5\) fs. A flat time-envelope of \(5 \times 10^5\) cycles reshapes the linear mode.

The problem already described was simulated over more than 2000 \(\mu m\), using an adapted mesh of 703 nodes and 1041 elements (Fig. 4.1) and the results show many important features. As expected, coupling between both arms occurs, see Figs. 4.2 to 4.3. Moreover, the coupling length obtained from Fig. 4.2 occurs at the step 2058, i.e., \(z = 630.3 \mu m\) and for next cycle of coupling, it occurs at the step 4113, i.e., \(z = 1259.9 \mu m\), which shows
high accuracy and reliability for this value.

From the data generated by the computer program it can be observed that the numerical method conserves power with an error smaller than 1 in $10^{12}$ parts. Also it is clear that transferred power, which reaches an 88.65% of its total value, having begun from 0.01% has a small but not negligible difference with the results predicted for the time independent analysis. That difference can be easily explained by the influence of the numerical introduction of higher order modes due to a sparse mesh — the difference between the mode and the projection on the set of basis function is expressed in terms of higher modes — and also because the time envelope is far away from the stationary solution, especially if the edges of that envelope have been set to zero width, and so they involve more sources of higher order modes.

Evolution of the electric field for the local time–center is displayed in Fig. 4.4, and is in very good agreement with the results obtained for power transfer. Lines are separated by $10 \lambda_0$ in the propagation direction. The first line is at $z = 10 \lambda_0$ and the last one is at $z = 430 \lambda_0$ (Coupling length was estimated to be nearly $412 \lambda_0$).

Fig. 4.3 shows that even though the pulse tends to spread in the $y$ coordinate (repre-
Figure 4.3: Space-time distribution of $E_x$. From top to bottom and left to right: $z = 0.31 \mu m$, $z = 153.2 \mu m$, $z = 306.4 \mu m$, $z = 459.6 \mu m$ and $z = 612.49 \mu m$. 
senting scaled time), the pulse is centered at the same place, which is in agreement with the selection of the local time reference. Beam formation in the coupled arm represents also good behaviour because apart from keeping its local-time position, also preserves the symmetry of the pulse. Time spreading of the pulse, which is simply a manifestation of the Gibbs' phenomenon, is appreciated here at its full extent, and can be reduced if the input beam has smoother leading and trailing edges. A comparison of the time envelopes for Fig. 4.3 is shown in Fig. 4.5, where it is clear that the reshaping of the main mode is also accompanied by ripples due to other modes. It is interesting to note that the high peak of the coupled beam envelope is compensated by the reshaping of the pulse in time, and thus keeping total power invariant.

When the simulation is repeated with the same parameters but with $\Delta z = \lambda_0/20$ and the mesh is enhanced by using 1735 nodes and 3386 elements as shown in Fig. 4.7, the method again shows total power conservation, but now the results are very much in agreement with the prediction of the SOM. Effectively, coupling length is measured as 682.74 $\mu m$ (the uncertainty is now $\Delta z$) and the full cycle of coupling is completed after 667.34 $\mu m$ more (Fig. 4.6). The values of power transfer are altered to 94.21% and 2.71% respectively. Time shaping varies too as it appears in Fig. 4.8.
For comparison purposes, space–time distributions of $E_x$ for local time at the same distances as before are provided in Fig. 4.9. Because even all the space–time distributions show improvement in terms of pulse spreading in time, the effect is more noticeable when coupling is nearly total.

Clearly, ripple has been smoothed and on the other hand, spreading of the distribution in time has been reduced, at the point where two peaks are recognized, marking nearly the same time-width of the original pulse.
When nonlinearities are present, the relation of dispersion becomes more complex because the nonlinear term has to be represented. If the nonlinearity is weak, then the permittivity can be treated as a perturbation of the linear permittivity, but if that is the case, then it is not true that variations with respect to the frequency will follow the same rule. In that situation, the conditions for having a plane wave are broken, and the valid relation of dispersion will have to include terms from transverse propagation.
Figure 4.9: Space-time distribution of $E_x$. From top to bottom and left to right: $z = 0.08\,\mu m$, $z = 153.2\,\mu m$, $z = 306.4\,\mu m$, $z = 459.6\,\mu m$ and $z = 612.8\,\mu m$. 
4.1.2 Approximated Debye Term

The reliability and accuracy of the formulation for the approximated Debye equation, is done on the same structure analyzed in section 4.1.1. This time, only the denser mesh is used and the results are compared to those obtained in the previous section.

4.1.2.1 Linear validation

The excitation used for this simulation is the same described in section 4.1.1.1.

Propagation of the field follows nearly the same pattern as in section 4.1.1, and measurements taken from the numerical simulations give also high similitude. Figure 4.10 show the electric field evolution over the cross-section at nearly 0, 1/4, 1/2, 3/4 and 1 coupling length.

The same observations made in section 4.1.1 apply here.

4.1.2.2 Nonlinear validation

The nonlinear tests for the validations use the same mesh that has been used for the linear validations, but the time-scaling used is varied here. The time-scaling used for the linear case cannot give details on the effects of both linear and nonlinear delays during propagation. The time-scaling coefficient is another feature that is tested when using small nonlinearities, short delays and small values of $a$ (as defined in section 2.1.8). Excitations for this validations consider gaussian time–envelopes.

Assuming that the power density for the excitation is $\frac{\partial P}{\partial y}$ it follows that the energy density —neglecting radiation— associated to the propagating pulse is:

$$U = \frac{\partial P}{\partial y} \frac{\lambda_0}{c} a M$$

measured in Watts due to the units of the $a$ coefficient, where $M$ is equivalent to the number of cycles for a flat time envelope (or the effective number of cycles for an arbitrary envelope when $\frac{\partial P}{\partial y}$ represents the maximum value of the power density; for the time–envelope
Figure 4.10: Space–time distribution of $E_x$. From top to bottom and left to right: $z = 0.08 \mu m$, $z = 153.2 \mu m$, $z = 306.4 \mu m$, $z = 459.6 \mu m$ and $z = 612.8 \mu m$. 
given here, the effective number of cycles is 79.79% of the value to be chosen for a flat envelope if the energy is the same. $U$ measures the total energy launched and it should be invariant with respect to the change of coordinates. Moreover, it should be constant during propagation.

Simulations of the nonlinear problem show that numerical power is not preserved during propagation, thus giving unreliable predictions. One way of overriding this problem is to impose power conservation. That imposition can be done considering that power fluctuations between steps are of the order of $1 \times 10^6$ for the simulations already done. That small power fluctuation is directly related to the intensity of the field and therefore if normalization is applied, the effect is equivalent to vary the Kerr coefficient at each step, in a figure smaller than the accuracy related to that parameter. All this holds true because the equations that describe propagation are homogeneous except for the nonlinear term. When power is normalized, the electric field is then affected by the square root of the power normalization coefficient, avoiding the collapse of the total power.

If time fluctuations due to nonlinear behaviour are of interest, it is necessary to use a different time-scaling for the $y$-coordinate. In order to check these effects, the same mesh, gaussian time-envelope and time independent excitation (in terms of $y$) are used here, but this time $1 \mu m \approx 3.248 \, fs$ or what is equivalent, $a = 3.0788 \times 10^8 \, \mu m/\mu s$. The results of this simulation are displayed in Fig. 4.11, for propagation distances of $\lambda_0$, $100\lambda_0$, $200\lambda_0$ and $300\lambda_0$.

The nonlinear effect is translated into high confinement before $L_c/4$, but then not only the confinement is clear where the peak on the launching side appears, but also on the coupling arm, where the leading and trailing time-edges of the excitation appear. Recalling that with the choice of local coordinates $y = 0$ represents the initial local time, after $200\lambda_0$ the large full beams appearing on the nonlinear strips are delayed, but the contours appearing on the central zone are not delayed. This last observation is in full agreement with the increased permittivity on the nonlinear strips and the constant permittivity on the linear central zone, that implies a reduction of the wave speed and invariance of the wave speed respectively.
Figure 4.11: Space–time distribution of $E_x$. From top to bottom and left to right: $z = 0.08 \mu m$, $z = 153.2 \mu m$, $z = 306.4 \mu m$ and $z = 459.6 \mu m$.

For a given Kerr-coefficient, a higher nonlinear delay should have less influence on the intensity of the field, so stability would be better tested when $\tau = 0$. In terms of the reliability of the perturbed method, there are some restrictions that can be formulated by working with the discretized approximation of $\delta$. One way is to use higher order finite elements to describe the third order term of $\delta$. An alternative approach is to estimate the first and second degree terms of $(\alpha \tau)$, and subsequently select an appropriate value for $\alpha$ that ensures that those terms are smaller than the $(\alpha \tau)$-independent term. This last approach is made here for the next simulations, where $\tau$ will take the values 0, 1.5 $fs$, and 3.0 $fs$.

When $\tau \neq 0$, it is important to analyze fast nonlinear interactions, i.e. delays smaller
than the period of the propagated field. For the validations here, that maximum value
is nearly $\tau = 5\; fs$, so a value of $a$ near $0.19242559\; \mu m/\mu s$ or the equivalence $1\; \mu m =
51.968\; fs$ should guarantee that the perturbation method has been well applied. With this
time-scaling, linear delays are not easily seen, but they should be spotted quite simply by
comparing the same problem when the nonlinear delays are different. The corresponding
situations are shown in Figs. 4.12 to 4.15.

![Figure 4.12: Space-time distribution of $E_x$ for $z = 153.2\; \mu m$. From top to bottom and
left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0\; fs$, $\tau = 1.5\; fs$, $\tau = 3.0\; fs$.](image)

The results displayed for $459.6\; \mu m$ of propagation distance, strongly hints that the non-
linear delay is responsible for the occurrence of a delayed peak on the excitation strip and
later at $620.46\; \mu m$ of propagation distance, that delayed peak appears on the other nonlin-
Figure 4.13: Space-time distribution of $E_z$ for $z = 306.4\,\mu m$. From top to bottom and left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0\,fs$, $\tau = 1.5\,fs$, $\tau = 3.0\,fs$.

car strip. More reassurance of the proper behaviour of the equations is found in Fig. 4.16, where the delay is expected to reduce confinement for large delays, at least when the beam is still nearly bell-shaped in time. This expected and confirmed prediction relies on the fact that the bigger the delay for beams bell-shaped in time, the smaller the correlation between the local Kerr nonlinearity and the local electric field.

The physical effects shown here demonstrate that for short delays and when switching happens after a flat time-envelope excitation in this kind of nonlinear couplers, leading and trailing edges generate a “mark” on the coupling strip. These marks have their origin in the lower intensity of the fields on both edges.
Figure 4.14: Space-time distribution of $E_x$ for $z = 459.6 \mu m$. From top to bottom and left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0 \, fs$, $\tau = 1.5 \, fs$, $\tau = 3.0 \, fs$.

After all this tests, it is rather clear that the method can be made stable, but monitored in terms of its underlying stability in power. A careful definition of the domain, and of the scaling should be always taken into account, otherwise the effect of the numerical nonlinearity could render the results useless. This time, the application of the Delaunay criterion for the mesh is relevant also in the sense that it restricts the discretization of the local-time coordinates through the $a$ coefficient. The span of the $y$ range should be defined regarding the maximum fluctuation of the permittivity index, so the delay is kept between the local-time boundaries of the mesh.
Figure 4.15: Space–time distribution of $E_x$ for $z = 620.46 \mu m$. From top to bottom and left to right: linear, $\alpha = 2.5 \times 10^{-10} (m/V)^2$ with: $\tau = 0 \text{fs}$, $\tau = 1.5 \text{fs}$, $\tau = 3.0 \text{fs}$.

4.2 Applications

The computer program that uses the method of perturbations for accounting the nonlinearity when the Debye equation holds, is very well suited to analyze problems where delays are short. As these kind of problems are of current and very high interest for short–pulse communications [51], the example analyzed in the next section deals with a possible practical application.
4. Analysis in Time Domain

Figure 4.16: Level of confinement for $\tau = 3.0\, fs$ (top curve), $\tau = 1.5\, fs$ (curve in the middle) and $\tau = 0\, fs$ (bottom curve).

4.2.1 A Nonlinear Demultiplexer

A Demultiplexer has been proposed and analyzed by Adachiara et al. in [23] using a simplified model that treats solitons as particles, and neglects many terms from the equation presented here. Pulses of gaussian space distribution and nearly flat time distribution are used for the evaluation. The structure proposed consists of two semi-infinite films of similar linear permittivity, and similar nonlinearity. The input excites the region that shows both smaller linear permittivity and nonlinear Kerr coefficient, on the same spatial location, but at different times. For a suitable excitation intensity, it is expected that all the pulses should migrate to the other region. If power is too low, then no guiding modes should appear and if the input power is too high, then the structure should behave like bulk material and if power exceeds certain level, the propagating beam would just break-up.

A train of four pulses is used here, each pulse in this simulation has a different amplitude, so the nonlinear effect should be different for each pulse. The mesh used for the analysis consists of 1819 nodes and 3555 elements, and is shown in Fig. 4.17.

The launching side is characterized by $\varepsilon_{\text{right}} = 2.458674$ and $\alpha_{\text{right}} = 2.0 \times$
and the other side is characterized by $\varepsilon_{left} = 2.458824$ and $\alpha_{left} = 2.5 \times 10^2 \ (\mu m/V)^2$. The reference value for the propagation constant is $\beta_0 = 6.38968 \ \mu m^{-1}$ and the free-space wavelength is $\lambda_0 = 1.532 \ \mu m$. The excitation beam has been shaped in space by an envelope defined by:

$$V(x) = \text{sech} \left(0.5906(x - 3.5)\right) \exp\left(j \frac{x}{10}\right),$$

and the time–envelope for the train of pulses is plotted in Fig. 4.18. Notice that the amplitudes of each pulse are 1.0, 1.2, 1.4 and 1.6, so the intensities are in the rate 1 : 1.44 : 1.96 : 2.56.

If the electric field is of high intensity, the pulses grow too much, and the beam breakup occurs. Fig. 4.19 shows this situation for a propagation distance of $z = 75 \lambda_0$. The maximum electric field intensities are in the rate: 1 : 2.13 : 2.50 : 3.96, for a propagation distance of 15 $\lambda_0$, and 1 : 2.77 : 5.05 : 10.86, for a propagation distance of 50 $\lambda_0$.

Another example of the similar situation is done here with the same structure but with higher indices. $\beta_0$ and $\lambda_0$ are the same values chosen for the previous example. The launching side is characterized by $\varepsilon_{right} = 2.458674$ and $\alpha_{right} = 2.0 \times 10^2 \ (\mu m/V)^2$ and the other side is characterized by $\varepsilon_{left} = 2.479824$ and $\alpha_{left} = 3.0 \times 10^2 \ (\mu m/V)^2$. As the mesh in the previous example was not dense enough to analyze each pulse in detail, here a single pulse is analyzed. The mesh for this structure uses 2460 elements and 1278 nodes,
and is shown schematically in Fig. 4.20. The input has the same time–envelope of one of the single pulses of the previous example, and the space–envelope is also the same, defined by \( V(x) \).

The output plotted in Fig. 4.21 shows a high peak surrounded by a crown–shape of smaller intensity peaks. The surge in intensity is also accompanied by a sharpened beam, but with total energy conservation. Also, it is seen that despite the higher index region, the pulse remains confined in the launching region. A careful search for a critical value of the beam input intensity should avoid the occurrence of this effect.

Other examples of lower intensity input —not plotted here— do not clearly support guided modes, displaying some power trapped in each region, but also showing dispersion all over the structure, which can also exist because higher order modes are introduced. In order to obtain a practical design of a demultiplexer, it is highly recommended to generate a stationary solution for the bulk material, and use that as the input for the problem. Varying the intensity of the input electric field, a relation can be built between the electric field and the final position of the beam. That relation is useful to define the separation of the inputs, in space, and the power needed to achieve such demultiplexing.
Using the same structure but with the input separated in space, it is possible to design a multiplexer. Again the output of such device should be on the region of higher indices. An alternative approach, and very important is to reverse the order of propagation, so if the same input train of pulses used for the demultiplexer were employed for the proposed...
Figure 4.21: Space-time distribution of $E_x$. From left to right: $z = \lambda_0$ and $z = 50 \lambda_0$.

multiplexer, the "output" of that reversed problem would be the input of the multiplexer. In order to achieve that, the chosen propagation step should be negative.
Chapter 5

Conclusions

5.1 General Conclusions

This thesis has described the physical and mathematical aspects of paraxial propagation in nonlinear isotropic media, a subject that is very important for the technologies applied to the practical problem of designing optical devices and systems of an increasingly demanding high speed or bandwidth.

Characterization of the main physical phenomena and their model approximations have been systematically presented and analyzed in terms of stability for small nonlinearities. The numerical models have been also converted to FEM formulations including paraxial and nonparaxial assumptions on propagation, stationary behaviour, time-domain situations, pumping and mixed situations. In particular, the paraxial stationary case has been implemented using two different approaches in two computer programs: the classical Crank–Nicolson/Galerkin and the split operator methods. It has been shown that Crank–Nicolson/Galerkin is very reliable, even for very high nonlinearities, situation that is enhanced when the novel optimization technique developed here, for improving convergence of the nonlinear term, is implemented.

Two time-domain formulations have also been implemented. The formulation based on the perturbation method for the Debye equation is fast in computer resources but limited
to either fast switching or geometric constraints. The other method, based on the proper Debye equation, is easier to apply because there are no geometrical or time constraints, but since it uses matrices of twice the dimension used with the perturbation approximation, it is less efficient in computer resources. Full operability has been achieved for the case of the perturbation method applied to the Debye equation, making careful remarks on the necessary conditions to maintain the reliability of the procedures.

During the analysis, optimization of the convergence for the nonlinear term in the nonlinear extension of the Crank–Nicolson approximation has proved to be a very useful method that goes far beyond the scope of optical propagation problems. In fact it might be extended to extract conclusions from the $\theta$–method. Its usefulness has been demonstrated with the comparison of numerical results for two variants of the usual Crank–Nicolson/Galerkin method.

The split operator method implemented here is an approximation of the rigorous split step operator and has proved to be very efficient in terms of computational resources but weak in terms of stability when the nonlinearity is fairly large in $2D + z$ analysis. That undesired behaviour is not changed when iterations are introduced.

Several applications have been developed using the most reliable of the methods. A simple rib–shaped nonlinear switch has been tested, and more than confirming predictions, a relation between position and input intensity of the field has been found. These result also hints a possible application for time–division multiplex systems, but now with the analysis in the time–domain. Apart from that, the device proves to be an interesting switch of fairly short dimensions.

A nonlinear coupler has been analyzed in order to find the “on” and “off” levels. As this structure has been tested with two different iteration methods, the results confirm what has been predicted analytically. A coupler built using channel waveguides was also tested, finding the range of electric field intensity for which it behaves as a three-state device.

A rather different example was also tested using a $1D + z$ program already available, which consisted of a co–doped coupler sought to work as a multiplexer/demultiplexer in the wavelength–domain. The methodology could be repeated for a real application, designing
a more accurate model by using a $2D + z$ computer programme.

In the time-domain, a demultiplexer useful for time division multiplexing applications was analyzed. The results show a methodology for designing the location of the outputs and also show the propagation characteristics for an excitation that is not a temporal soliton. Second order partial derivatives are not neglected like in [23], thus providing full account of very fast variations in time.

A final word on the computer implementation of the methods is that all the programmes developed here were based on the writing of many subroutines that now constitute a very useful library for new programmes. The external additions are from the Harwell Library routines [52] used for solving the matrix $A x = b$, and the NAG Library routines [53] for solving nonlinear problems of one variable and the mesh generator.

5.2 Extensions and Improvements of the Methods

The main goal during this research has been the generation of reliable and accurate methods for simulating the physical behaviour of optical propagation in nonlinear media. Attention paid to the optimization of the methods has played a secondary role, and there are modifications still being carried in the algorithms and computer programmes to improve their performance. This section mentions some of these.

The stability analysis used during this research works by trying to keep bounded—or constant if unitary stability is present—the magnitude of the effective value of the electric field in the region. The conservation of the effective electric field does not imply that power (or energy) is preserved, but it does imply that power (energy) does not collapse. A further analysis on the equations is then required in order to find out which quantities are natural invariants of the equation that models the physical behaviour. In finding those invariants, Nöther equation [54] might prove useful. From the point of view of the numerical methods, it would be attractive to study stability criteria for high nonlinearities.

As the split operator method has been tested using an approximation, it would be
interesting to see if the rigorous formulation has a better behaviour. If this is so, much time can be saved on further simulations. The rigorous split operator method using non-paraxiality can also prove to be attractive if stability is accomplished. As the formulation has been developed, its implementation might improve the computer performance.

The implementation of the double matrix formulation for the $2D + z$ analysis would lead to a solution of the nonparaxial equation. Again, the analysis of stability for high nonlinearities is highly useful to see if the results are reliable.

The perturbed Debye equation with the double matrix formulation that leads to a nonparaxial solution of $1D + z + t$ problems is very attractive and despite the geometric limitations imposed by the perturbation method, when stability is guaranteed, the results will be useful to compare with the paraxial approximation.

The analysis of pumping under instantaneous nonlinear response and first order dispersion is also of practical interest. The implementation of this application uses nearly the same structure used for the double-matrix formulation of the time-domain and paraxial analysis.

As computer performances improve with the help of technology, the full $1D + t + z$ equation including nonparaxiality could be analyzed. In that case the dimension of the matrices would be $3N \times 3N$.

Full implementation of boundary conditions to all interfaces, and comparison of the methods that neglect that influence, should be studied in order to gain more accuracy when nonlinearities are large.

Applications that can be analyzed in the future with the computer programmes already developed are couplers, switches, four channel couplers (centers located in the vertices of a square) and many more.

In the time-domain, the scope of analysis is wider, the same example provided could serve as a long study including design of the separation between pulses when nonlinear response is not instantaneous, optimization of the length of the device for a given train of
pulses, optimal design of the linear and nonlinear indices, analysis of the response for different time-shaping and space-shaping, the design of the multiplexer and another optimization for a combination of the multiplexer and its matching demultiplexer.

Not mentioned before, the analysis of structures in cylindrical geometries could prove very interesting for both paraxial and nonparaxial formulations, when radial symmetry is assumed because the time-domain analysis is then applied to a 2D + z structure.

If the generation of the nonlinear matrices, in all the problems studied, is considered, there is a clear way of improving the management of the memory resource by working with a nonlinear vector and only linear matrices. For example, from (2.249) to (2.251), a linear local matrix could be generated:

\[
\{N\}_{i,j}\eta_j = -\frac{k_0^2\alpha_j}{240}|\eta_j|^2Y_{i,j}\eta_j, \tag{5.1}
\]

so a new linear matrix is defined by:

\[
\{L_n\}_{i,j}\xi_j = -\frac{k_0^2\alpha_j}{240}Y_{i,j}\xi_j, \tag{5.2}
\]

\[
\xi_j = |\eta_j|^2\eta_j, \tag{5.3}
\]

where \(\eta_j\) means the average between the value of the electric field in the last step of propagation and the value of the electric field in the last iteration of the current step of propagation. It is clear that \(L_n\) is linear, so the programmes need to generate this matrix only once (if the cross section is invariant during the propagation). On the other hand, \(\xi_j\) requires much less calculations than the nonlinear matrix. This procedure, although not implemented yet, should not alter the results shown in this work, but they should reduce the time for simulations along with the memory required space for the data. The same kind of conclusions can be extracted for the rest of the nonlinear matrices.
Appendix A

FEM formulae—Green Integrals

Green’s First Identities for high order derivatives.

Starting with:

\[
\int_{S} \nabla \cdot (\xi \vec{A}) \, dS = \oint_{\partial(S)} \xi \vec{A} \cdot \hat{n} \, dl
\]

(A.1)

\[
\oint_{\partial(S)} \xi \vec{A} \cdot \hat{n} \, dl = \int_{S} \left( \nabla \xi \cdot \vec{A} + \xi \nabla \cdot \vec{A} \right) \, dS
\]

(A.2)

rearranging terms:

\[
\int_{S} \nabla \xi \cdot \vec{A} \, dS = -\int_{S} \nabla \cdot \vec{A} \, dS + \oint_{\partial(S)} \xi \vec{A} \cdot \hat{n} \, dl
\]

(A.3)

Equation (A.3) is known as the Green’s First Identity. This equation is used for transforming the integrals that involve one function multiplied by a partial derivative of another function. The analysis is restricted to partial derivative orders smaller than five. Starting with order four:

\[
\int \int \psi \frac{\partial^4 \phi}{\partial x^4} \, dx \, dy = - \int \int \nabla \psi \cdot \left( \frac{\partial^3 \phi}{\partial x^3} \right) \, dx \, dy + \oint \psi \frac{\partial^3 \phi}{\partial x^3} \hat{x} \cdot \hat{n} \, dl
\]

(A.4)

\[
J = \int \int \hat{x} \cdot \nabla \psi \left( \frac{\partial^3 \phi}{\partial x^3} \right) \, dx \, dy
\]

(A.5)

\[
J = \int \int \hat{x} \cdot \nabla \left( \nabla \cdot \left( \frac{\partial^2 \phi}{\partial x^2} \hat{x} \right) \right) \, dS
\]

(A.6)
A: FEM formulae–Green Integrals

\[ J = - \int \nabla \left( \frac{\partial \psi}{\partial x} \right) \cdot \frac{\partial^2 \phi}{\partial x^2} \hat{x} dS + \oint \frac{\partial \psi}{\partial x} \frac{\partial^2 \phi}{\partial x^2} \hat{x} \cdot \hat{n} dl \]  
(A.7)

\[ J = - \int \int \frac{\partial^2 \psi}{\partial x^2} \frac{\partial^2 \phi}{\partial x^2} dS + \oint \frac{\partial \psi}{\partial x} \frac{\partial^2 \phi}{\partial x^2} \hat{x} \cdot \hat{n} dl \]  
(A.8)

\[ \int \int \psi \frac{\partial^4 \phi}{\partial x^4} dS = \int \int \frac{\partial^2 \psi}{\partial x^2} \frac{\partial^2 \phi}{\partial x^2} dS + \oint \left( \psi \frac{\partial^3 \phi}{\partial x^3} - \frac{\partial \psi}{\partial x} \frac{\partial^2 \phi}{\partial x^2} \right) \hat{x} \cdot \hat{n} dl \]  
(A.10)

For the third order partial derivative, the integral can be transformed by:

\[ \int \int \psi \frac{\partial^3 \phi}{\partial x^3} dS = \int \int \nabla \cdot \left( \frac{\partial^2 \phi}{\partial x^2} \hat{x} \right) dS \]  
(A.11)

\[ = - \int \int \nabla \cdot \frac{\partial^2 \phi}{\partial x^2} \hat{x} dS + \oint \psi \frac{\partial^2 \phi}{\partial x^2} \hat{x} \cdot \hat{n} dl \]  
(A.12)

Finally the result is:

\[ \int \int \psi \frac{\partial^3 \phi}{\partial x^3} dS = - \int \int \frac{\partial \psi}{\partial x} \frac{\partial^2 \phi}{\partial x^2} dS + \oint \psi \frac{\partial^2 \phi}{\partial x^2} \hat{x} \cdot \hat{n} dl \]  
(A.13)

For the second order partial derivative, the integral is easily transformed:

\[ \int \int \psi \frac{\partial^2 \phi}{\partial x^2} dS = - \int \int \nabla \psi \cdot \frac{\partial \phi}{\partial x} \hat{x} dS + \oint \psi \frac{\partial \phi}{\partial x} \hat{x} \cdot \hat{n} dl \]  
(A.14)

\[ = - \int \int \frac{\partial \psi}{\partial x} \frac{\partial \phi}{\partial x} dS + \oint \psi \frac{\partial \phi}{\partial x} \hat{x} \cdot \hat{n} dl \]  
(A.15)
Appendix B

First order FEM: Internal Products

Internal products defined by

$$\langle \psi_i, \phi_j \rangle = \int \int \psi_i \phi_j^* dS$$

were developed in Appendix A.

The functions $\psi_i$ and $\phi_j$ are the result of linear operators applied to first order local functions of the triangular element "e", where each local function is defined by:

$$\psi_i = \frac{a_i + b_i x + c_i y}{2 A_e}.$$ 

If the line integrals appearing in Appendix A are neglected (assuming a large enough domain), after applying Green's First Identity like in Appendix A, the internal products are reduced to:

$$\langle \phi_i, \phi_j \rangle = \frac{A_e}{12} (1 + \delta_{ij}), \quad \text{(B.1)}$$

$$\langle \phi_i, \frac{\partial \phi_j}{\partial x} \rangle = \frac{b_j}{6}, \quad \text{(B.2)}$$

$$\langle \phi_i, \frac{\partial \phi_j}{\partial y} \rangle = \frac{c_j}{6}, \quad \text{(B.3)}$$

$$\langle \phi_i, \frac{\partial^2 \phi_j}{\partial x^2} \rangle = -\frac{\partial \phi_i}{\partial x} \frac{\partial \phi_j}{\partial x} = -\frac{b_i b_j}{4 A_e}, \quad \text{(B.4)}$$

$$\langle \phi_i, \frac{\partial^2 \phi_j}{\partial y^2} \rangle = -\frac{\partial \phi_i}{\partial y} \frac{\partial \phi_j}{\partial y} = -\frac{c_i c_j}{4 A_e}, \quad \text{(B.5)}$$

$$\langle \phi_i, \nabla^2 \phi_j \rangle = -\nabla \phi_i \cdot \nabla \phi_j = -\frac{b_i b_j + c_i c_j}{4 A_e}. \quad \text{(B.6)}$$
All the above expressions are useful for developing first order finite element formulations of second order partial differential equations.
Appendix C

Comparison of two approximations for the CNG Method

Representing the electric field by $x$, and defining $f(x)$ the problem may be expressed by:

Given two "points" $x_0$ and $y_0 = x_0 + \Delta x$, find the best approximation of $x \cdot f(x)$ evaluated at $x_0 + \frac{\Delta x}{2}$, if the approximation is defined by assuming that $f(x)$ is arbitrary and that two products are of interest, the following analysis applies to $p = \langle x \rangle \cdot \langle f(x) \rangle$ and $q = \langle x \cdot f(x) \rangle$, being $r = \langle x \rangle \cdot f'(x)$ the exact value. In order to know which is the best approximation for some useful cases, it will be helpful to evaluate $|p - r|$ and compare it to $|q - r|$.

\begin{align*}
|r - p| &= |r - \frac{1}{2} \left( x_0 + \frac{\Delta x}{2} \right) (f(x_0 + \Delta x) + f(x_0))|, \\
|r - q| &= |r - \frac{1}{2} \left( x_0 + \frac{\Delta x}{2} \right) (f(x_0 + \Delta x) + f(x_0)) - \frac{\Delta x}{4} (f(x_0 + \Delta x) - f(x_0))|. 
\end{align*}

(C.1)
(C.2)

So the approximated value $p$ will be better than the approximated value $q$ if $|r - p| \leq |r - q|$ for each iteration. Now rewriting (C.1) and (C.2):

\begin{align*}
|r - p| &= \frac{1}{2} \left( \frac{\Delta x}{2} \right)^2 |x_0 + \frac{\Delta x}{2}||f'(2)(x_0 + \frac{\Delta x}{2})|, \\
|r - q| &= \frac{1}{2} |x_0 + \frac{\Delta x}{2}|^2 \left| \frac{\Delta x}{2} f''(x_0 + \frac{\Delta x}{2}) + \frac{2}{x_0 + \frac{\Delta x}{2}} f'(x_0 + \frac{\Delta x}{2}) \right|. 
\end{align*}

(C.3)
(C.4)

After some cancelations, if the approximated value $p$ is assumed to be better than the
approximated value \( q \), then:

\[
|\tilde{f}^{(2)}(x_0 + \frac{\Delta x}{2})| \leq |\tilde{f}^{(2)}(x_0 + \frac{\Delta x}{2}) + \frac{\Delta x}{2} f^{(1)}(x_0 + \frac{\Delta x}{2})| \quad (C.5)
\]

All this should be valid for any size of \( \Delta x \), so if the limit is taken when \( \frac{\Delta x}{2} \to 0 \), then:

\[
\tilde{f}^{(2)}(x_0 + \frac{\Delta x}{2}) \to f^{(2)}(x),
\]

\[
\tilde{f}^{(1)}(x_0 + \frac{\Delta x}{2}) \to f^{(1)}(x).
\]

And the condition is transformed into:

\[
|xf^{(2)}(x)| \leq |xf^{(2)}(x) + 2f^{(1)}(x)|. \quad (C.8)
\]

The conclusion now is: "If convergence is sought and \( \Delta x \) is small, then (C.8) should be satisfied". The reciprocal statement is more useful and it is easy to see that when dealing with first order approximations, it really holds true.

Now as an important example, if the function

\[
f(x) = Kx^s
\]

is tested with condition (C.8), then the requirements for having better convergence with (2.168) are:

- \( K \) is a real constant that can have any real value,

- \( s \) is a real constant that can have any positive value.

The condition expressed in C.8 is of real practical interest, and can be applied to decide on the best variant for the approximation of any implicit nonlinearity, not only to electromagnetic problems. Going back to the electromagnetic problem, the last set of requirements also shows that even for defocusing Kerr media, the same method is equally more convergent.
Appendix D

Published Work


References


References


References


References


References

