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Nonlinear self-focus of pulsed-wave beams in Kerr media

Judkins, Justin Boyd, M.S.

The University of Arizona, 1992

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NONLINEAR SELF-FOCUS OF
PULSED-WAVE BEAMS IN
KERR MEDIA

by

Justin Boyd Judkins

A Thesis Submitted to the Faculty of the
DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING
In Partial Fulfillment of the Requirements
For the Degree of
MASTER OF SCIENCE
WITH A MAJOR IN ELECTRICAL ENGINEERING
In the Graduate College
THE UNIVERSITY OF ARIZONA

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ABSTRACT

A modified finite-difference time-domain method for solving Maxwell's equations in nonlinear media is presented. This method allows for a finite response time to be incorporated in the medium, physically creating dispersion and absorption mechanisms. Our technique models electromagnetic fields in two space dimensions and time and encompasses both the TE_z and TM_z set of decoupled field equations. Aspects of an ultra-short pulsed Gaussian beam are studied in a variety of linear and nonlinear environments to demonstrate that the methods developed here can be used efficaciously in the modeling of pulses in complex problem space geometries even when nonlinearities are present.

CHAPTER 1

INTRODUCTION

Since the late 60's, sources have been available that are capable of producing high power, highly focused energy at optical frequencies. By pulsing a laser, for instance, an instantaneous power output of more than 100 kW focused to a spot size smaller than $100\text{ }\mu\text{m}$ can be achieved (an intensity of $\sim 10^{15}\text{ W/m}^2$). In this regime, materials often do not respond normally. Indeed, properties such as the intensity dependence of the refractive index occur and play a key role in producing some very unusual effects. It then becomes a nontrivial task to include these properties in any conventional electromagnetic or optical modeling technique. However, it is of great interest and practical importance to know how a pulse behaves in this environment. In particular, the characterization of the behavior of short pulses of "light" (just one or two optical cycles) in nonlinear media is especially important in a number of areas including: high bit rate fiber optic communication lines, high speed switching in an all-optical computer (in case there ever is such a thing), and catastrophic self-focusing of pulses in the bulk media of linear devices operated at high intensities. Envelope and paraxial approximations abound but it is the intent of this author to present another, in many ways more useful, approach to modeling high power focused pulses of electromagnetic energy in nonlinear media.

With the philosophy that difficult problems just require bigger computers, we go after the most computationally flexible method we know of to model fields in nonlinear media, the vector finite-difference time-domain technique. This approach affords us the means to fully and directly describe each individual field component, every aspect of the medium everywhere in space, and each and every nuance of a nonlinear simulation as it occurs in time. Other systems, while they are convenient

for certain specific applications, are not as versatile since they all omit some aspect of the physics, usually the transverse field components. Remember that superposition applies to *linear* media only because the field components are coupled by nonlinear media. The vector approach, however, is a complete electromagnetic model and can be coupled with just about any physical medium model. Because summing the responses for each frequency in the pulse to get the total medium response is not allowed, a frequency domain approach is invalid and a time domain model is required. From a computational standpoint, vector time-domain modeling can be expensive and with the addition of dispersion, especially nonlinear dispersion, it can be very expensive. In the past, approaches that were this computationally intensive would consume enormous amounts of computer time and were seldom considered. However, due to advancements in computer technology, the demand for time and size for these simulations has entered into the realm of legitimacy. We are therefore justified in making copious use of various high performance machines to simulate nonlinear electromagnetic phenomena by the approach presented in this thesis.

The second chapter sets this research in motion by presenting a short study of ultra-short pulsed Gaussian beams in freespace. We introduce in this chapter the method of applying linear system theory to the paraxial beam approximation for a beam with Gaussian taper in order to characterize the linear aspects of such a beam. Chapter 3 deals with the development of the vector finite-difference time-domain technique for two dimensional space. We first derive numerical equivalents to Maxwell's equations that can be solved on a finite grid and second, discuss the launching of pulses into the finite-difference simulation volume. Chapter 4 deals in depth with the nonlinear self-focus phenomenon. The nonlinear medium differential equation is written in a finite-difference form and added to the linear set of difference equations to produce the complete nonlinear modeling tool. We then use this tool to

model self-focusing of pulsed Gaussian beams in bulk media in order to gain a better understanding of the self-focusing phenomenon. In chapter 5 we take advantage of this tool to model more complicated geometries containing nonlinear parts. The main idea behind the devices we are modeling is their use of the nonlinearities to produce the desired effects. As a challenge, various devices for the switching of ultrashort pulses are designed and modeled with varying degrees of success. Finally, in chapter 6 we summarize the research and discuss some possible avenues for future research.

CHAPTER 2

PROPAGATION CHARACTERISTICS OF PULSED WAVE GAUSSIAN BEAMS

The behavior of PG (pulsed Gaussian) beams in nonlinear media deviates significantly from conventional CW (continuous wave) linear theory. A better understanding of PG beams in the linear regime is therefore essential to our successful analysis in the nonlinear regime. The propagation characteristics of the beam generated by driving an aperture with an ultra-short, time-limited (hence, ultra-wide frequency bandwidth) signal whose amplitude is weighted as a Gaussian across the aperture will be derived in Sec. 1. Particular attention will be given to the case involving a Gaussian time signal. An approximate form of the resulting pulsed Gaussian beam field will be derived in Sec. 2. It will be shown that the beam intensity and beam energy have different diffraction lengths and rates of beam spread in the far field. The conclusions of Sec. 2 are supported with numerical simulations as described in Sec. 3. In particular, a study of the spatial and temporal behavior of a femtosecond pulsed Gaussian beam is provided.

1. PG Gaussian beam field

As modern science expands its horizons in the development of stable, repeatable pulsed sources of signals in the 10^{-12} to 10^{-15} second regimes, we are quickly approaching the realization of electromagnetic energy devices and their applications in those regimes. The need for understanding the characteristics of the beams generated by these millimeter wave and optical pulsed-sources is important for the successful engineering of those applications. Most conventional sources can be classified as being CW (continuous wave or monochromatic) or having narrow bandwidths (quasi-monochromatic). The characteristics of the Gaussian beams resulting from these sources are well known and can be found in a variety of textbooks [1] [2].

However, as the bandwidths of the pulses increase, their properties can no longer be characterized by those CW results. It is the purpose of this chapter to derive and characterize ultra-short (time-limited), hence, ultra-wide frequency bandwidth PG beams. Comparisons with the results predicted for general systems of this type [3] will be made.

We begin the analysis of a Gaussian beam by considering a circular aperture of radius a in the plane $z = 0$. We assume that this aperture is driven everywhere with the Gaussian time signal:

$$F(t) = e^{-p t^2}, \quad (2.1)$$

with a spatial Gaussian taper e^{-r^2/ω^2} . The field is assumed to propagate from the initial aperture into the half-space $z > 0$, which is taken to be a dispersionless, lossless, linear medium. To simplify the analysis, we assume that the radius of the aperture is sufficiently larger than the initial waist w_0 of this pulsed beam to remove any edge effects from the discussion.

Since the system is linear, this initial field will evolve into a pulsed electromagnetic Gaussian beam that is propagating in free space. We can thus use standard linear system theory and known representations for a CW Gaussian beam to derive an expression for the resulting pulsed beam in the desired half-space. In particular, we use the well-known frequency domain representation of the amplitude of a linearly polarized electric field (polarized in a direction orthogonal to the direction of propagation) of an azimuthally symmetric, zeroth order, Gaussian beam in a homogeneous media. Assuming that the propagation direction is along the z -axis, this field has the form [1]:

$$\tilde{E}(r, \phi, z, \omega) = E_0 \frac{w_0}{w(z)} \exp \left\{ -i[kz - \eta(z)] - r^2 \left[\frac{1}{w^2(z)} + \frac{ik}{2R(z)} \right] \right\} \quad (2.2)$$

where the waist, radius of curvature, phase term and diffraction length parameters are given by the expressions

$$w^2(z) = w_0^2 \left[1 + \left(\frac{\lambda z}{\pi w_0^2} \right)^2 \right] = w_0^2 \left(1 + \frac{z^2}{z_0^2} \right) \quad (2.3)$$

$$R(z) = z \left[1 + \left(\frac{\pi w_0^2}{\lambda z} \right)^2 \right] = z \left(1 + \frac{z_0^2}{z^2} \right) \quad (2.4)$$

$$\eta(z) = \tan^{-1} \left(\frac{\lambda z}{\pi w_0^2} \right) = \tan^{-1} \left(\frac{z}{z_0} \right) \quad (2.5)$$

$$z_0 \equiv \frac{\pi w_0^2}{\lambda} = \left(\frac{w_0^2}{2c} \right) \omega. \quad (2.6)$$

The rate of beam spread (beam spread angle) in the far field where $z \gg z_0$ follows from the waist expression (2.3):

$$\theta_{\text{CW}} = \tan^{-1} \left[\frac{w(z)}{\sqrt{2} z} \right] \approx \tan^{-1} \left(\frac{\lambda}{\sqrt{2} \pi w_0} \right) \approx \sqrt{2} \left(\frac{\lambda}{2 \pi w_0} \right) \quad (2.7)$$

In contrast to its usual definition as the radius at which the electric field amplitude has decreased to $1/e$ of its value on the axis, we have taken this angle to be defined as the radius at which the electric field intensity has decreased to $1/e$ of its value on the axis. Note that the same angle would have been obtained from the energy profile in this CW case. The usual definition results in (2.7) without the $1/\sqrt{2}$ factor.

When the driving function has a Gaussian time history, it also has a Gaussian spectrum. In particular, the temporal Fourier transform of the initial pulse (2.1) is

$$\tilde{F}(\omega) = \left(\frac{\pi}{p}\right)^{1/2} e^{-\omega^2/4p} . \quad (2.8)$$

Therefore, the resulting beam field in the region $z > 0$ is the inverse Fourier transform of the product of the spectral fields (2.2) and (2.8):

$$E(r, \phi, z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{E}(r, \phi, z, \omega) \tilde{F}(\omega) e^{+i\omega t} d\omega . \quad (2.9)$$

The intensity of the beam at the field point (r, ϕ, z) is determined by squaring the electric field (2.9); the energy is obtained by integrating the intensity over all time. This discussion is extended in a straightforward manner to Gaussian beam modes of any order and symmetry.

2. Analytical characterization of PG beams

An approximate form of the field expression (2.2) is readily obtained so that a similar form can be derived from (2.9) analytically. When $z \ll z_0$, one has from Eq. (2.3) that the waist $w(z) \simeq w_0$. The approximation for the electric field at an observation point near the initial surface for a particular angular frequency ω then becomes

$$\tilde{E}(r, \phi, z, \omega) \approx E_0 e^{-ikz} e^{-r^2/w_0^2} \quad (z \ll z_0) . \quad (2.10)$$

Thus, the CW beam retains essentially a Gaussian shape in any transverse plane; its amplitude remains constant along the z -axis. However, as the distance away from the aperture increases, the waist (2.3) becomes more dependent on z . In fact, for $z \gg z_0$ Eq.(2.3) becomes

$$w(z) \simeq w_0 \left(\frac{z}{z_0} \right), \quad (2.11)$$

and the resulting approximation for the frequency domain field far away from the initial $z = 0$ plane is

$$\begin{aligned} \tilde{E}(r, \phi, z, \omega) &\approx E_0 \frac{z_0}{z} \exp \left\{ -i \left[kz - \frac{\pi}{2} \right] - r^2 \left[\left(\frac{z_0}{w_0 z} \right)^2 + \frac{ik}{2z} \right] \right\} \\ &= i E_0 \frac{w_0^2}{2cz} \omega \exp \left[-i \omega \left(\frac{z}{c} + \frac{r^2}{2cz} \right) - \omega^2 \left(\frac{w_0 r}{2cz} \right)^2 \right] \quad (z \gg z_0). \end{aligned} \quad (2.12)$$

While an analytical expression for (2.9) is not directly available, it can be reasonably approximated by using (2.8), (2.10) and (2.12), and performing the inverse transforms analytically. With Eq. (3.323.2) of Ref. 4, one obtains near the aperture

$$E(r, \phi, z, t) \approx E_0 e^{-r^2/w_0^2} e^{-p(z/c-t)^2}, \quad (2.13)$$

and far from the aperture

$$\begin{aligned} E(r, \phi, z, t) &\approx \frac{E_0}{2\pi} \left(\frac{\pi}{p} \right)^{1/2} \frac{w_0^2}{2cz} \int_{-\infty}^{\infty} i\omega \exp \left\{ -\omega^2 \left[\frac{1}{4p} + \left(\frac{w_0 r}{2cz} \right)^2 \right] \right\} \exp \left\{ -i \omega \left[\left(\frac{z}{c} - t \right) + \frac{r^2}{2cz} \right] \right\} d\omega \\ &= \frac{E_0}{2\pi} \left(\frac{\pi}{p} \right)^{1/2} \frac{w_0^2}{2cz} \partial_t \left[\int_{-\infty}^{\infty} \exp \left\{ -\omega^2 \left[\frac{1}{4p} + \left(\frac{w_0 r}{2cz} \right)^2 \right] \right\} \exp \left\{ -i \omega \left[\left(\frac{z}{c} - t \right) + \frac{r^2}{2cz} \right] \right\} d\omega \right] \\ &= E_0 \frac{p w_0^2}{c z} \left[\frac{1}{1 + p \left(\frac{w_0 r}{cz} \right)^2} \right]^{3/2} \left(\frac{z}{c} - t + \frac{r^2}{2cz} \right) \exp \left[-p \frac{\left(\frac{z}{c} - t + \frac{r^2}{2cz} \right)^2}{1 + p \left(\frac{w_0 r}{cz} \right)^2} \right]. \end{aligned} \quad (2.14)$$

Thus the initial pulsed beam retains its form near the aperture and acquires a time derivative form that decays as z^{-1} far from it. The specification of the diffraction length of this field (distance to the near-to-far-field boundary) will be given below.

The time derivative behavior far from the aperture represented by (2.14) is expected from the radiation process. Recall that the field away from the aperture can be treated as arising from a set of equivalent electric and magnetic sources in the aperture; i.e., if $\hat{n}_{ap}$ is the normal to the aperture in the direction of propagation, the equivalent (dipole) current sources in the aperture may be formed from the tangential electric and magnetic fields there: $\mathbf{J}_{ap} = \hat{n} \times \mathbf{H}_{ap}$ and $\mathbf{M}_{ap} = -\hat{n} \times \mathbf{E}_{ap}$. In the very near field of the aperture rather than the individual dipole sources, the electromagnetic field is dominated by the induction fields of these current sources; those fields are directly related to the tangential electric and magnetic fields in the aperture so that $\mathbf{E}_{near} \propto \mathbf{E}_{ap}$ and $\mathbf{H}_{near} \propto \mathbf{H}_{ap}$. One then expects, as shown above, that the initial field is recovered near the aperture, modulo a phase term. The radiated (far field) electric field can be simply connected to the aperture field; it is related to a time derivative of the electric vector potential which in turn is proportional to the aperture electric current density: $\mathbf{E}_{far} \propto -\partial_t \mathbf{A}_e \propto \partial_t \mathbf{J}_{ap}$. However, the fields in and near the aperture are dominated by the TEM-like property that they are nearly translationally invariant along the propagation direction. This means: $\partial_{ct} Z_0 \mathbf{H}_{near} \sim \partial_z (\hat{n}_{ap} \times \mathbf{E}_{near})$ and, hence, $Z_0 \mathbf{H}_{near} \sim \hat{n}_{ap} \times \mathbf{E}_{near}$ so that $\mathbf{J}_{ap} \propto \mathbf{H}_{ap} \propto \mathbf{E}_{ap}$. These near and far field arguments then give $\mathbf{E}_{far} \propto \partial_t \mathbf{E}_{ap}$. Thus, as the field evolves from the near to the far field region, it acquires the observed time derivative behavior.

The intensity of the beam field in the near and far field regions is readily obtained as the absolute square of the electric fields (2.13) and (2.14). One obtains for the near field

$$\mathcal{I}(r, \phi, z, t) \approx |E(r, \phi, z, t)|^2 = |E_0|^2 e^{-2r^2/w_0^2} e^{-2p(z/c-t)^2}, \quad (2.15)$$

and for the far field

$$\mathcal{I}(r, \phi, z, t) \approx E_0^2 \left(\frac{p w_0^2}{c z} \right)^2 \left[\frac{1}{1 + p \left(\frac{w_0 r}{c z} \right)^2} \right]^3 \left(\frac{z}{c} - t + \frac{r^2}{2c z} \right)^2 \exp \left[-2p \frac{\left(\frac{z}{c} - t + \frac{r^2}{2c z} \right)^2}{1 + p \left(\frac{w_0 r}{c z} \right)^2} \right]. \quad (2.16)$$

Because the intensity depends on time, (2.16) has limited usefulness as a cogent beam quantity. A more descriptive quantity is the maximum of the intensity in time: $\mathcal{I}_{\max} = \max_t \mathcal{I}$. It allows one to associate a pattern (transverse spatial distribution) with the intensity. Setting the partial with respect to time of the electric fields (2.13) and (2.14) to zero, one finds that the maxima of the electric field in the near field are located at the time $t_{\max} = z/c$ and in the far field at the time

$$t_{\max} = \frac{z}{c} + \frac{r^2}{2c z} \pm \left[\frac{1}{2p} + \frac{w_0^2 r^2}{2 c^2 z^2} \right]^{1/2}, \quad (2.17)$$

so that the maximum intensity received at an observation point in the near field is

$$\mathcal{I}_{\max}(r, \phi, z) = E_0^2 e^{-2r^2/w_0^2}, \quad (2.18)$$

and in the far field

$$\mathcal{I}_{\max}(r, \phi, z) \approx \frac{1}{2e} E_0^2 \left[\frac{w_0^2}{c z} \right]^2 p \left[1 + p \left(\frac{w_0 r}{c z} \right)^2 \right]^{-2}. \quad (2.19)$$

Consequently, the ratio of the maximum intensity along the axis of propagation to the maximum intensity on axis at the aperture $z = 0$ is

$$\Gamma_{\text{int},\parallel}(r=0, \phi, z) \stackrel{\text{def}}{=} \frac{\mathcal{I}_{\text{max}}(r=0, \phi, z)}{\mathcal{I}_{\text{max}}(r=0, \phi, z=0)} = \begin{cases} 1.0 & (\text{near field}) \\ \frac{p}{2e} \left(\frac{w_0^2}{zc} \right)^2 & (\text{far field}) . \end{cases} \quad (2.20)$$

Similarly, the ratio of the maximum intensity at a point in a plane orthogonal to the axis of propagation to its value on that axis will be

$$\Gamma_{\text{int},\perp}(r, \phi, z) = \frac{\mathcal{I}_{\text{max}}(r, \phi, z)}{\mathcal{I}_{\text{max}}(r=0, \phi, z)} = \begin{cases} e^{-2r^2/w_0^2} & (\text{near field}) \\ \left[1 + p \frac{w_0^2 r^2}{c^2 z^2} \right]^{-2} & (\text{far field}) . \end{cases} \quad (2.21)$$

The maximum intensity profile remains the same in the near field but begins to spread in the far field. One can thus define a beam spread in the far field for the maximum intensity θ_{int} in terms of the far field ratio (2.21). In particular, let R_{int} be the value of the ratio (2.21) in the far field at which the beam spread is taken. With this quantity, one then has

$$\theta_{\text{int}} \stackrel{\text{def}}{=} \frac{r}{z} = \left[(R_{\text{int}}^{-1/2} - 1) \frac{c^2}{p w_0^2} \right]^{1/2} . \quad (2.22)$$

A standard choice of the evaluation point of the beam spread ratio would be the $1/e$ intensity point, i.e., taking $R_{\text{int}} = 1/e$.

On the other hand, the energy at a field point (r, ϕ, z) is determined simply by integrating the intensities (2.15) and (2.16) over all time. With Eqs. (3.463.6) and (3.463.8) of Ref. 4, one obtains in the near field

$$\mathcal{E}(r, \phi, z) \approx \int_{-\infty}^{\infty} |E_0|^2 e^{-2r^2/w_0^2} e^{-2p(z/c-t)^2} dt = |E_0|^2 e^{-2r^2/w_0^2} \left(\frac{\pi}{2p} \right)^{1/2} , \quad (2.23)$$

and in the far field

$$\begin{aligned}\mathcal{E}(r, \phi, z) &\approx \frac{E_0^2 \left[p w_0^2 / (cz) \right]^2}{\left\{ 1 + p \left[w_0 r / (cz) \right]^2 \right\}^3} \int_{-\infty}^{\infty} \left(\frac{z}{c} - t + \frac{r^2}{2cz} \right)^2 \exp \left[-2p \frac{\left(\frac{z}{c} - t + \frac{r^2}{2cz} \right)^2}{1 + p \left(\frac{w_0 r}{cz} \right)^2} \right] dt \\ &= E_0^2 \left(\frac{w_0^2}{2cz} \right)^2 \left(\frac{\pi}{2} p \right)^{1/2} \left[1 + p \left(\frac{w_0 r}{cz} \right)^2 \right]^{-3/2}.\end{aligned}\quad (2.24)$$

Consequently, the ratio of the energy along the axis of propagation to the energy on axis at the aperture $z = 0$ is

$$\Gamma_{\text{enrg}, \parallel} (r = 0, \phi, z) \stackrel{\text{def}}{=} \frac{\mathcal{E}(r = 0, \phi, z)}{\mathcal{E}(r = 0, \phi, z = 0)} = \begin{cases} 1.0 & \text{(near field)} \\ p \left(\frac{w_0^2}{2cz} \right)^2 & \text{(far field)} \end{cases} \quad (2.25)$$

Similarly, the ratio of the energy at a point in a plane orthogonal to the axis of propagation to its value on that axis is

$$\Gamma_{\text{enrg}, \perp} (r, \phi, z) = \frac{\mathcal{E}(r, \phi, z)}{\mathcal{E}(r = 0, \phi, z)} = \begin{cases} e^{-2r^2/w_0^2} & \text{(near field)} \\ \left[1 + p \frac{w_0^2 r^2}{c^2 z^2} \right]^{-3/2} & \text{(far field)} \end{cases} \quad (2.26)$$

The energy profile remains the same in the near field but begins to spread in the far field. One can thus define a beam spread in the far field for the energy θ_{enrg} in terms of the far field ratio (2.26). In particular, let R_{enrg} be the value of the ratio (2.26) in the far field at which the beam spread is taken. With this quantity, one then has

$$\theta_{\text{enrg}} \stackrel{\text{def}}{=} \frac{r}{z} = \left[(R_{\text{enrg}}^{-2/3} - 1) \frac{c^2}{p w_0^2} \right]^{1/2}. \quad (2.27)$$

A standard choice of the evaluation point of the beam spread ratio would be the $1/e$ energy point, i.e., taking $R_{\text{enrg}} = 1/e$.

Now, we would like to characterize the far field maximum intensity and energy parameters in terms of the effective frequency associated with the radiated field that was introduced in Ref. 3. This effective frequency was obtained from analytical bounds on the rate of energy decay along the direction of propagation of the beam generated by an arbitrary array driven with a general spatially distributed set of time signals: $\mathcal{F}(\mathbf{r}, t)$, taking into account the time derivative effect that results from the propagation of the beam from the near to the far field. For the case under consideration the initial time signal distribution is: $\mathcal{F}(\mathbf{r}, t) = E_0 \exp(-r^2/w_0^2) F(t)$; and the associated effective frequency is defined as

$$\omega_{\text{rad}}^2 \stackrel{\text{def}}{=} \frac{\int_A dS \int_{-\infty}^{\infty} dt |\partial_t \mathcal{F}(\mathbf{r}, t)|^2}{\int_A dS \int_{-\infty}^{\infty} dt |\mathcal{F}(\mathbf{r}, t)|^2} = \frac{\int_{-\infty}^{\infty} dt |\partial_t F(t)|^2}{\int_{-\infty}^{\infty} dt |F(t)|^2} = p. \quad (2.28)$$

This effective frequency ω_{rad} is a measure of the spectral energies radiated into the medium in our model. It is a ratio of the aperture-weighted accumulation of the contributions to the energy spectrum of the field away from the aperture and the aperture-weighted accumulation of the energy spectra of the signals driven into the aperture. It is a very useful quantity since it characterizes *by a single frequency value* all of the ultra-wide bandwidth components contained in all of the signals radiated by the aperture. We now rewrite the far field intensity and energy relations in terms of this effective frequency ω_{rad} , its corresponding wavelength λ_{rad} , and the associated diffraction length L_{rad} :

$$\lambda_{\text{rad}} = \frac{2\pi c}{\omega_{\text{rad}}} = \frac{2\pi c}{\sqrt{p}} \quad (2.29)$$

$$L_{rad} = \frac{\pi w_0^2}{\lambda_{rad}}. \quad (2.30)$$

In particular, one finds in the far field

$$\Gamma_{\text{int},\parallel}(r=0, \phi, z) = \frac{2}{e} \left(\frac{\pi w_0^2}{\lambda_{rad} z} \right)^2 = \frac{2}{e} \left(\frac{L_{rad}}{z} \right)^2 \equiv \left(\frac{L_{\text{int}}}{z} \right)^2 \quad (2.31)$$

$$\theta_{\text{int}} = (R_{\text{int}}^{-1/2} - 1)^{1/2} \frac{\lambda_{rad}}{2 \pi w_0} \quad (2.32)$$

$$\Gamma_{\text{enrg},\parallel}(r=0, \phi, z) = \left(\frac{\pi w_0^2}{\lambda_{rad} z} \right)^2 = \left(\frac{L_{rad}}{z} \right)^2 \equiv \left(\frac{L_{\text{enrg}}}{z} \right)^2 \quad (2.33)$$

$$\theta_{\text{enrg}} = (R_{\text{enrg}}^{-2/3} - 1)^{1/2} \frac{\lambda_{rad}}{2 \pi w_0}. \quad (2.34)$$

Thus one readily observes that the diffraction lengths and the rate of beam spreading in the far field are different for the maximum intensity and the energy. Quantitatively, the diffraction lengths for the maximum intensity and energy satisfy

$$\frac{L_{\text{int}}}{L_{\text{enrg}}} = \left(\frac{2}{e} \right)^{1/2} = 0.858, \quad (2.35)$$

and the rates of beam spread, taking the $1/e$ roll-off point, satisfy:

$$\frac{\theta_{\text{int}}}{\theta_{\text{enrg}}} = \left(\frac{R_{\text{int}}^{-1/2} - 1}{R_{\text{enrg}}^{-2/3} - 1} \right)^{1/2} = 0.827. \quad (2.36)$$

Although the diffraction lengths are only slightly different, the rates of spreading of the intensity and energy in the far field are significantly different, particularly if one were to consider the spot size ramifications at large distances from the aperture. The differences, as explained in Ref. 3, result from the fact that the maximum

intensity is a point quantity that depends on the bandwidth and the energy is an average quantity that, hence, depends on an average frequency value. We also note that if the aperture were driven with a CW signal corresponding to the effective frequency: $\omega_{CW} = \omega_{rad}$, a comparison of (2.7) with (2.32) and (2.34) reveals that the ultra-wide bandwidth beam has energy and intensity profiles in the far field that are narrower than that CW case: e.g., $\theta_{int}/\theta_{CW} = [(e^{+1/2} - 1)/2]^{1/2} = 0.570$. Situations where these differences could be designed to be much larger than they are in this simple, but important example were discussed in Ref. 3.

3. Numerical simulations

The situation we have modeled in Sec. 2 could occur, at least to a first order approximation, when a optical fiber is terminated and a linearly polarized, Gaussian space-time pulse that is traveling in this waveguide is launched into free space. We will choose for discussion purposes the parameter values $w_0 = 2.5 \mu m$, $a = 5.0 \mu m$, and $p = 1.90 \times 10^{30}$. These values correspond to launching a Gaussian pulse from a fiberoptic waveguide whose core radius is $5.0 \mu m$. This pulse has a $1.45 fs$ full-width between its $1/e$ amplitude points; its Fourier spectrum has a $1/e$ roll-off point at the frequency $f_{1/e} = 4.39 \times 10^{14} Hz$ or radian frequency $\omega_{1/e} = 2.76 \times 10^{15} rad/sec$, which corresponds to the wavelength $\lambda_{1/e} = 0.683 \mu m$. The pulse has a maximum amplitude of 0.018 at $r = 5.0 \mu m$, the edge of the aperture, which is small enough for our purposes here. No other aspects of the fiber need be considered. The initial pulse's time history is plotted versus time in Fig. (2.2), and its Fourier spectrum is plotted versus radial frequency in Fig. (2.3). The effective frequency of this pulse is $f_{rad} = 2.19 \times 10^{14} Hz$ or $\omega_{rad} = 1.38 \times 10^{15} rad/sec$, which corresponds to the wavelength $\lambda_{rad} = 1.367 \mu m$. An analogous situation, but scaled down to THz frequencies, arises in the large aperture, photoconductive switch, ps / THz sources [13]-[15].

We have developed a numerical simulator to calculate Eq. (2.9) directly to check our predictions. The waves that are generated by the simulator are visualized with PV-WAVE, a commercial software system for plotting and displaying images. Eq. (2.9) is also implemented using the prepackaged FFT routine provided with PV-WAVE. The FFT routine is used in two places within the program. It is used first to produce a spectrum of the initial driving pulse F . The FFT routine is used again to calculate the inverse Fourier transform in Eq. (2.9). This approach makes the program more versatile since it allows for an arbitrary driving pulse.

A systematic numerical investigation was undertaken with the simulator to study the evolution of the pulsed Gaussian beam as it propagates away from the initial aperture, i.e., as time (or distance) increases. Several standard sampling criteria on the window size T and the number of time samples N associated with FFT routines were readily met with the values $T = 25 \text{ fs}$ and $N = 512$ samples.

Contour plots of the Gaussian pulse beam field that were created with our simulator are shown in Figs. (2.4a) - (2.4d). Each picture was generated by constructing the time signals received at a set of radial positions in a plane perpendicular to the propagation axis at a specified distance from the initial aperture. There are 32 radial positions in each figure; this was the minimal number of radial time signals needed to produce a smooth surface plot. The total radial distance in each plot is $7.5 \mu\text{m}$, the total time record is 25.0 fs . The distances from the aperture represented by Figs. (2.4a) - (2.4d) are respectively, $15.0 \mu\text{m}$, $30.0 \mu\text{m}$, $45.0 \mu\text{m}$, and $60.0 \mu\text{m}$. Because the axial coordinate is fixed and the wave is calculated in time, the image is reversed from what one might expect. The form of these pictures is analogous to what a detector array would "see" if it were placed in a plane perpendicular to the axis of propagation and sampled the pulsed beam as it went by.

The time derivative behavior expected from (2.14) is apparent in the figures; the pulse is completely in the far field in Figs. (2.4a) - (2.4d) ($L_{rad} = 14.36 \mu m$). To illustrate this behavior more clearly, the on-axis signal $E(r = 0, \phi, z, t)$ is graphed versus time in Figs. (2.5a) - (2.5d) for the z locations $z = 0.0 \mu m$, $2.0 \mu m$, $4.0 \mu m$, and $16.0 \mu m$. This sequence clearly demonstrates the evolution of the initial Gaussian pulse into its first derivative form as the beam propagates further from the aperture.

The results of Eq. (2.7) for the CW beam energy and intensity spread at the CW frequency $\omega_{CW} = \omega_{rad}$ are plotted in Fig. (2.6). Recall that the initial waist (distance from the core centerline to the $1/e$ field magnitude) is $2.5 \mu m$. The $1/e$ beam spread curves for the intensity and energy of the pulsed Gaussian beam obtained directly from Eq. (2.9) are given by, respectively, dash-triple-dot and dash-dot curves in Fig. (2.7). Similarly, the $1/e$ beam spread curves for the intensity and energy of the pulsed Gaussian beam predicted from Eqs. (2.32) and (2.34) are shown in Fig. (2.8). They begin at $z = 50.0 \mu m$, well into the far field. The solid curve in Fig. (2.8) is the beam spread curves of the corresponding CW Gaussian beam. Asymptotes to the numerically obtained curves in Fig. (2.7) allow us to calculate accurately the pulsed Gaussian beam spread rates. We find from Fig. (2.7) the values $\theta_{int} = 4.04^\circ$ and $\theta_{enrg} = 4.84^\circ$. The predicted values are, respectively, 4.02° and 4.87° . The agreement improves for larger distances away from the aperture. Comparing Fig. (2.6) with Figs. (2.7) and (2.8), one sees that the pulsed Gaussian beam diffracts more slowly than the corresponding CW beam.

Figure (2.9) shows the values of the pulsed beam's maximum intensity and energy in the plane $z = 200.0 \mu m$. As indicated by a comparison of Eqs. (2.21) and (2.26), the profile of the maximum intensity of the pulsed beam is narrower than the corresponding beam energy profile.

Figure (2.1), Diffraction affects the higher order coherence properties of a beam generated by a UWB pulse-driven aperture more slowly than its lower orders. The envelopes of the energy distribution in a pulsed beam as detected by a zero and one time derivative measurement system are defined by their diffraction lengths and the rate of spread of the beam in the region beyond their diffraction lengths.

Figure (2.2), The initial aperture is excited with a Gaussian pulse tapered with a Gaussian envelope. The time history of the initial Gaussian pulse.

Figure (2.3), The initial aperture is excited with a Gaussian pulse tapered with a Gaussian envelope. The Fourier spectrum of the initial Gaussian pulse.

Figure (2.4a)

Figure (2.4a-d), The evolution of the pulsed Gaussian beam is illustrated by contour maps of this field as observed in the planes: (2.4a) $z = 15.0 \mu m$, (2.4b) $z = 30.0 \mu m$, (2.4c) $z = 45.0 \mu m$, and (2.4d) $z = 60.0 \mu m$. The transverse distance from the propagation axis is given along the vertical axis, time along the longitudinal axis.

Figure (2.4b)

Figure (2.4c)

Figure (2.4d)

Figure (2.5a)

Figure (2.5a-d), As the pulsed Gaussian beam field propagates from the initial aperture, it evolves into a time derivative of the initial field. The pulsed Gaussian beam's time signals along the propagation axis are shown at the distances: (2.5a) $z = 0.0 \mu\text{m}$, (2.5b) $z = 2.0 \mu\text{m}$, (2.5c) $z = 4.0 \mu\text{m}$, and (2.5d) $z = 16.0 \mu\text{m}$.

Figure (2.5b)

Figure (2.5c)

Figure (2.5d)

Figure (2.6), The rate of spread of the CW Gaussian beam's intensity and energy are identical. The $1/e$ -points of the beam's intensity and energy profiles are given (solid curve) versus the distance along the direction of propagation. The CW frequency is $f = f_{rad} = 2.19 \times 10^{14} \text{ Hz}$. The initial waist of the Gaussian amplitude taper is $w_0 = 2.5 \mu\text{m}$. The oblique dotted line represents the asymptote given by Eq. (2.7).

Figure (2.7), The rates of spread of the pulsed Gaussian (PG) beam's maximum intensity and energy profiles are compared. The $1/e$ -points of the maximum intensity profile (dash-triple-dot curve) and the $1/e$ -points of the energy profiles (dash-dot curve) are given versus the distance along the direction of propagation. These curves are obtained directly from numerical simulations of the beam fields defined by Eq. (2.9).

Figure (2.8), The $1/e$ -points of the maximum intensity (dash-triple-dot curve) and energy (dash-dot curve) profiles of a Gaussian beam are given versus the distance along the direction of propagation for comparison purposes. The rate of spread in the far field of the maximum intensity is generated with Eq. (2.32) for pulsed Gaussian (PG) beam field (dash-triple-dot curve). The solid curve represents the beam spread values for the corresponding CW Gaussian field with $\omega_{CW} = \omega_{rad}$. The dashed line represents the asymptote to the CW curve.

Figure (2.9), The intensity profile of the pulsed Gaussian beam in the plane $z = 200.0 \mu m$ is more narrow than its energy profile. Both profiles have been normalized to unity for this comparison.

CHAPTER 3

FDTD VECTOR MAXWELL SOLVER

In this chapter we present the FDTD (finite difference time domain) formulation of Maxwell's vector equations in two space dimensions and time. The basic advantages of this approach are presented in section 1. In section 2 Maxwell's equations are separated into TE and TM mode sets and approximated as space and time are discretized. Meshes for the numerical electric and magnetic field approximations are developed further in section 3. Section 4 then introduces the boundary conditions used throughout this research. The issues of numerical stability and discretization error are raised in sections 5 and 6. In section 7 we study launching a PG beam by considering the source from the perspective of an incident-scattered field analysis and driving it on one wall of the mesh. We show that a beam can be launched with any desired cross section and time history. The beam can also be steered to accommodate the oblique incidence simulations discussed in chapter 5. Lastly, a computer simulation for the PG beam introduced in chapter 2 is given in section 8 and comparisons are made between the two solutions.

1. Justification for the Vector FDTD technique

The vector FDTD technique has application in a wide variety of electromagnetic problems. Complex geometries, dispersion, pulses, and material nonlinearity can be accurately modeled because Maxwell's curl equations can be solved directly with this numerical approach. The fields may also have multiple dimensionality because of the vector nature of the FDTD equations. Thus, the only limits to the size and complexity of a FDTD problem become computer resources: speed and virtual memory.

The problems in this thesis involve non-oscillatory time histories, finite beams, and nonlinear dispersion. Superposition of frequencies does not apply and a frequency domain approach would therefore be challenged to model such a complicated environment. A scalar FDTD model is likewise insufficient. It is demonstrated in later chapters that the contribution of multiple coupled field components to these problems is not insignificant. On the other hand, a vector FDTD approach is a much better modeling tool because it provides all the necessary features required to accurately solve these problems.

Although simple, vector FDTD numerical solutions are computationally intensive. They tend to require a great deal of processor time, and because each field component and each time dependent material parameter must be solved for independently, the memory requirements are in some cases enormous. Therefore, with this technique a high performance computer is essential in solving realistic problems in reasonable time frames. The research being presented required generous use of two 4-processor machines, a CRAY Y-MP/432 and a ConvexOS/240. While the Convex with its 128 megaword RAM was big enough to process very large problems, it was found to be somewhat limited by its relatively slow speed. In comparison, the CRAY Y-MP I used is not as well endowed, having but a trifling 28 megaword RAM available to any one user. While the CRAY is faster, the problem size is more restricted.

2. Basic approach

The transformation of Maxwell's equations from continuous differential equations into discrete numerical approximations is straight forward. Space and time are first discretized into an ordered lattice of cells called a mesh. Each cell in the mesh contains a field quantity or medium parameter that is considered to be ap-

proximately homogeneous within the cell. The location of the field is either at the center of an edge or at the center of the cell and is referred to as a "field node". An array of field nodes then produces an image of the field occupying the problem space at a given time. Finally, central differencing is used between adjacent cells to produce the numerical equivalent to a continuous derivative:

$$\lim_{\Delta x \rightarrow 0} \frac{f(x_o + \frac{1}{2}\Delta x) - f(x_o - \frac{1}{2}\Delta x)}{\Delta x} = \left. \frac{df(x)}{dx} \right|_{x_o} \quad (3.1)$$

where Δx represents the spacing between two consecutive steps in either space or time. By this process, Maxwell's equations are solved discretely, and in the limit of infinitely fine discretization, this gives an exact representation.

The fields in a source free region must satisfy Maxwell's curl equations:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (3.2a)$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \sigma \mathbf{E} \quad (3.2b)$$

where D, E, B and H are related through the constitutive relations

$$D = \epsilon E$$

$$B = \mu H$$

and σ is the conductivity of the medium. We assume the constitutive relations are local and let $\mu = \mu_0$, $\sigma = \sigma(\mathbf{r})$, and $\epsilon = \epsilon(\mathbf{r})$. Equations (3.2 a,b) are expressed in rectangular coordinates below.

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -\mu_0 \frac{\partial H_x}{\partial t} \quad (3.3a) \quad \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} = \epsilon(\mathbf{r}) \frac{\partial E_x}{\partial t} + \sigma(\mathbf{r}) E_x \quad (3.3d)$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -\mu_0 \frac{\partial H_y}{\partial t} \quad (3.3b) \quad \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = \epsilon(\mathbf{r}) \frac{\partial E_y}{\partial t} + \sigma(\mathbf{r}) E_y \quad (3.3e)$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -\mu_0 \frac{\partial H_z}{\partial t} \quad (3.3c) \quad \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} = \epsilon(\mathbf{r}) \frac{\partial E_z}{\partial t} + \sigma(\mathbf{r}) E_z \quad (3.3f)$$

We restrict the problem space to two dimensions by forcing $\partial/\partial y = 0$. Equations (3.3a-f) then separate into two independent sets, TE_z and TM_z.

$$\begin{array}{ll} \underline{\text{TE}}_z & (3.4) \\ \frac{\partial E_y}{\partial z} = \mu_0 \frac{\partial H_x}{\partial t} \\ \frac{\partial E_y}{\partial x} = -\mu_0 \frac{\partial H_z}{\partial t} \\ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = \epsilon(\mathbf{r}) \frac{\partial E_y}{\partial t} + \sigma(\mathbf{r}) E_y \end{array} \quad \begin{array}{ll} \underline{\text{TM}}_z & (3.5) \\ -\frac{\partial H_y}{\partial z} = \epsilon(\mathbf{r}) \frac{\partial E_x}{\partial t} + \sigma(\mathbf{r}) E_x \\ \frac{\partial H_y}{\partial x} = \epsilon(\mathbf{r}) \frac{\partial E_z}{\partial t} + \sigma(\mathbf{r}) E_z \\ \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -\mu_0 \frac{\partial H_y}{\partial t} \end{array}$$

The orientation and type of problem excitation will determine which mode set is excited. We will first produce the finite difference formulation for the TM_z set. With the groundwork laid we will then procede to generate the finite difference approximation for the TE_z set.

Using central differencing, the TM_z mode set (3.5) is expressed as a finite difference approximation:

$$\begin{aligned} & - \frac{H_y(x, z + \frac{1}{2}\Delta z, t) - H_y(x, z - \frac{1}{2}\Delta z, t)}{\Delta z} \\ & = \epsilon(x, z) \frac{E_x(x, z, t + \frac{1}{2}\Delta t) - E_x(x, z, t - \frac{1}{2}\Delta t)}{\Delta t} \\ & \quad + \sigma(x, z) \frac{E_x(x, z, t + \frac{1}{2}\Delta t) + E_x(x, z, t - \frac{1}{2}\Delta t)}{2} \end{aligned} \quad (3.6a)$$

$$\begin{aligned}
& \frac{H_y(x + \frac{1}{2}\Delta x, z, t) - H_y(x - \frac{1}{2}\Delta x, z, t)}{\Delta x} \\
&= \epsilon(x, z) \frac{E_z(x, z, t + \frac{1}{2}\Delta t) - E_z(x, z, t - \frac{1}{2}\Delta t)}{\Delta t} \\
&\quad + \sigma(x, z) \frac{E_z(x, z, t + \frac{1}{2}\Delta t) + E_z(x, z, t - \frac{1}{2}\Delta t)}{2} \quad (3.6b)
\end{aligned}$$

$$\begin{aligned}
& \frac{E_z(x + \frac{1}{2}\Delta x, z, t) - E_z(x - \frac{1}{2}\Delta x, z, t)}{\Delta x} \\
&\quad - \frac{E_x(x, z + \frac{1}{2}\Delta z, t) - E_x(x, z - \frac{1}{2}\Delta z, t)}{\Delta z} \\
&= \mu_o \frac{H_y(x, z, t + \frac{1}{2}\Delta t) - H_y(x, z, t - \frac{1}{2}\Delta t)}{\Delta t} \quad (3.6c)
\end{aligned}$$

Time averaging of the electric field has been used in the conduction term. This produces a more accurate result than simply using the previously evaluated electric field.

Equations (3.6a-c) are simplified by introducing the indices j, k and n with the notation

$$\begin{aligned}
x &\stackrel{\text{def}}{=} j\Delta x \\
z &\stackrel{\text{def}}{=} k\Delta z \\
t &\stackrel{\text{def}}{=} n\Delta t
\end{aligned} \quad (3.7)$$

In Eqs. (3.6a-c) we chose to represent the fields on staggered grids. This has the advantage of placing electric field nodes between magnetic field nodes and visa versa; however, the half-indices which result from this approach complicate the notation

somewhat. We overcome this difficulty by noting that the electric and magnetic field nodes are never required to occupy the same space or time. It is therefore possible to shift the indices in order to remove half-indices from the equations and thus adopt a generic notation for both fields without losing the staggered grid. In the TM_z case we chose to use the following notation for the electric field nodes at the center of the cell edges:

$$\begin{aligned} E_z(x, z, t) &= E_z[j\Delta x, (k + \frac{1}{2})\Delta z, (n + \frac{1}{2})\Delta t] \\ &\stackrel{\text{def}}{=} E_z(j, k, n + 1) \end{aligned} \quad (3.8a)$$

$$\begin{aligned} E_x(x, z, t) &= E_x[(j + \frac{1}{2})\Delta x, k\Delta z, (n + \frac{1}{2})\Delta t] \\ &\stackrel{\text{def}}{=} E_x(j, k, n + 1) \end{aligned} \quad (3.8b)$$

The magnetic field nodes at the center of the cell areas are represented by a similar notation:

$$\begin{aligned} H_y(x, z, t) &= H_y[(j + \frac{1}{2})\Delta x, (k + \frac{1}{2})\Delta z, n\Delta t] \\ &\stackrel{\text{def}}{=} H_y(j, k, n) \end{aligned} \quad (3.8c)$$

The placement of these nodes with respect to each other is shown in Fig. (3.1). The notations indicate that the field components are labeled relative to the cell corner nearest the origin.

The FDTD approximation for the TM_z mode in Eq. (3.5) now reduces to the following equation set:

$$\epsilon(j, k) \left[\frac{E_x(j, k, n + 1) - E_x(j, k, n)}{\Delta t} \right] + \sigma(j, k) \left[\frac{E_x(j, k, n + 1) + E_x(j, k, n)}{2} \right]$$

$$= -\frac{H_y(j, k, n) - H_y(j, k - 1, n)}{\Delta z} \quad (3.9a)$$

$$\begin{aligned} \epsilon(j, k) \left[\frac{E_z(j, k, n + 1) - E_z(j, k, n)}{\Delta t} \right] + \sigma(j, k) \left[\frac{E_z(j, k, n + 1) + E_z(j, k, n)}{2} \right] \\ = \frac{H_y(j, k, n) - H_y(j - 1, k, n)}{\Delta x} \end{aligned} \quad (3.9b)$$

$$\begin{aligned} \mu_o \left[\frac{H_y(j, k, n + 1) - H_y(j, k, n)}{\Delta t} \right] = \frac{E_z(j + 1, k, n + 1) - E_z(j, k, n + 1)}{\Delta x} \\ - \frac{E_z(j, k + 1, n + 1) - E_z(j, k, n + 1)}{\Delta z} \end{aligned} \quad (3.9c)$$

These equations are then solved independently in a leap-frog manner (i.e., $\mathbf{E}$ and $\mathbf{H}$ are solved at staggered time steps) to produce the final vector FDTD solutions:

$$E_x(j, k, n + 1) = \left(E_x(j, k, n)B - \frac{H_y(j, k, n) - H_y(j, k - 1, n)}{\Delta z} \right) / A \quad (3.10a)$$

$$E_z(j, k, n + 1) = \left(E_z(j, k, n)B + \frac{H_y(j, k, n) - H_y(j - 1, k, n)}{\Delta z} \right) / A \quad (3.10b)$$

$$\begin{aligned} H_y(j, k, n + 1) = H_y(j, k, n) + \frac{\Delta t}{\mu_o} \left[\frac{E_z(j + 1, k, n + 1) - E_z(j, k, n + 1)}{\Delta x} \right. \\ \left. - \frac{E_x(j, k + 1, n + 1) - E_x(j, k, n)}{\Delta z} \right] \end{aligned} \quad (3.10c)$$

$$A = \frac{\epsilon(j, k)}{\Delta t} + \frac{\sigma(j, k)}{2}$$

$$B = \frac{\epsilon(j, k)}{\Delta t} - \frac{\sigma(j, k)}{2}$$

Once the updated fields values have been generated from the previous fields, they become the “previous values” thereby updating the fields to the current time step. By cycling through (3.10a-c) the fields are “marched” in time from the initial conditions at time $t = 0$ to the distribution at any desired time.

3. Mesh construction

Two discretization meshes are constructed from the superposition of electric and magnetic field nodes. The meshes are then displaced relative to each other by the amount $\frac{\Delta z}{2}$ in one direction and $\frac{\Delta z}{2}$ in the other as shown in Fig. (3.2). The electric and magnetic field nodes are staggered such that each node of interest lies between the two nodes corresponding to the other field components used in the differencing scheme. The indices j and k corresponding to the node locations range from 1 to j_{max} and k_{max} . The TM_z components are arranged as in Fig. (3.3) and although the field nodes are depicted as existing in a single time frame, the electric field and the magnetic field are actually staggered by a half time as shown in Fig. 3.1

4. Boundary conditions

Since any problem space must be truncated to fit within the finite limits of computer memory, boundary conditions must be chosen at the borders of the mesh. Perfect electric conductor (PEC) walls were chosen for easy software design. We now have a choice of whether to place the boundary on the electric or magnetic field nodes. For consistency between the TE_z and TM_z mode sets, all boundaries are positioned on the nodes of the $\hat{y}$ field component and, with the exception of the source wall, all boundaries are PEC's. The source boundary is also positioned on the $\hat{y}$ nodes but as we discuss in a later section, its nature depends on the type of source we are exciting.

To place the boundary on the magnetic field nodes, as is the case when modeling the TM_z mode, image theory is used. The boundary becomes an image plane and the tangential electric field has odd symmetry. The boundary in this case is constructed as follows:

$$\begin{aligned}
E_x(j, 2) &= -E_x(j, 1) & (j = 1, \dots, j_{max}) \\
E_x(j, k_{max}) &= -E_x(j, k_{max} - 1) & (j = 1, \dots, j_{max}) \\
E_z(3, k) &= -E_z(2, k) & (k = 1, \dots, k_{max}) \\
E_z(j_{max}, k) &= -E_z(j_{max} - 1, k) & (k = 1, \dots, k_{max})
\end{aligned} \tag{3.11}$$

The $k = 2$ and $k = 3$ nodes in this case straddle the boundary on the left side of the problem space. Likewise, $k = k_{max} - 1$ and $k = k_{max}$ straddle the right boundary. The nodes at $j = 2, 3$ and $j = j_{max} - 1, j_{max}$ straddle the lower and upper boundaries respectively. Similarly, when we simulate a TE_z problem we want to produce a PEC wall along the E_y nodes. In this case we simply set these field nodes to zero for all time.

$$\begin{aligned}
E_y(j, 2) &= 0 & (j = 2, \dots, j_{max}) \\
E_y(j, k_{max}) &= 0 & (j = 2, \dots, j_{max}) \\
E_y(2, k) &= 0 & (k = 2, \dots, k_{max}) \\
E_y(j_{max}, k) &= 0 & (k = 2, \dots, k_{max})
\end{aligned} \tag{3.11}$$

These boundaries are represented by the dashed lines in Fig. (3.2) and Fig. (3.3).

5. Numerical stability

The choice of discretizations Δx and Δt is not arbitrary; they must be chosen such that the wave speed does not exceed the rate at which information is passed between cells. Violation of this condition results in phase error, non-physical results, and an unstable simulation. Following the discussion in [15], the condition for the numerical speed to exceed the wave speed in two dimensions is

$$\Delta t \leq \frac{n}{c\sqrt{(\frac{1}{\Delta x})^2 + (\frac{1}{\Delta z})^2}}. \quad (3.12)$$

For safety, n is chosen as the lowest refractive index in the material. The condition (3.12) is known as the Courant stability criterion. However, when we use this in a nonlinear situation we find that it is inadequate. While the algorithm was stable, we found that when the condition was at the limit, $\Delta t = \Delta t_c = n\Delta x/(c\sqrt{2})$, some of the physics is not properly recovered. A new limit is needed for Δt for this case and it has been determined using a trial and error method. We found that a limit of $\Delta t < \Delta t_c/2$ is sufficient to recover the nonlinear physics.

6. Numerical dispersion

When Maxwell's equations are approximated by equation set (3.10a-c), some dispersion, called numerical dispersion, will result from the finite cell size in the computational mesh. In other words, the propagation velocity is slightly frequency dependent. The degree of dispersion is dependent on the relative size of a given wavelength to the cell size. Simply, smaller cells cause less dispersion. In most cases, however, since memory is usually the limiting factor in the FDTD approach, it is unreasonable to decrease the cell size arbitrarily until dispersion becomes negligible. This raises an important issue: What is the largest cell size one can have and still not significantly distort the pulse with numerical approximations?

To answer this question we look first at the origin of numerical dispersion. It is due to undersampling of the high frequency components by the grid and thus a poor approximation at these frequencies. These poorly represented components of the pulse do not move quite as far in one time step as does the rest of the pulse and the result is that a phase error is introduced. As the wavelength get smaller still, it

is suppressed altogether due to aliasing; the FDTD equations represent a low-pass filter. A discussion in greater depth on the subject of numerical dispersion is given by Taflové [16]. The numerical dispersion relation in two dimensions is rewritten in the form

$$\left(\frac{\omega}{c}\right)^2 \text{sinc}^2\left(\frac{\omega\Delta t}{2}\right) = k_x^2 \text{sinc}^2\left(\frac{k\Delta x \cos \alpha}{2}\right) + k_z^2 \text{sinc}^2\left(\frac{k\Delta z \sin \alpha}{2}\right). \quad (3.13)$$

This is in contrast to the isotropic homogeneous dispersion relation in lossless media

$$\left(\frac{\omega}{c}\right)^2 = k_x^2 + k_z^2.$$

We see that as we scale the mesh smaller the *sinc* function approaches 1.0 and we recover the ideal case. Following the discussion presented in [16], we choose a cell size of $\Delta x = \lambda_o/20$ for *fine discretization*. Here λ_o represents the shortest wavelength of interest. Then, for a Courant condition of $\Delta t = \Delta x/2c$, we find a phase error, the relative error in phase between lateral and diagonal directions of propagation with respect to the mesh.

7. The source as a scattered field

In this section we discuss the inclusion of initial conditions in the FDTD solver. The premise of our approach is that the fields in the presence of a boundary can be decomposed into incident and scattered components. In this way we can avoid the direct introduction of equivalent Huygen's sources and drive the problem in a more natural manner. We have as the basic tenet of this construction a predetermined incident field and a perfectly conducting mathematical boundary.

We begin by writing

$$\mathbf{E} = \mathbf{E}^i + \mathbf{E}^s \qquad \mathbf{H} = \mathbf{H}^i + \mathbf{H}^s \qquad (3.14)$$

We next assume that $\mathbf{E}^i$ and $\mathbf{H}^i$ have sources outside our problem space. Because these sources have not yet been specified, we are free to impose a mathematical halfspace boundary in the problem. The boundary we choose is one that will force either the tangential electric or magnetic field to be zero. Furthermore, the boundary is oriented normal to the propagation direction so as to completely suppress one of the fields in either three component mode set. Specifically, the boundary to excite the TM_z mode is a perfect magnetic conductor (PMC) plane normal to $\hat{\mathbf{z}}$; the boundary to excite the TE_z mode is a PEC plane normal to $\hat{\mathbf{z}}$. Proceeding now with the TM_z case, from (3.14) we have $\mathbf{H}^s = -\mathbf{H}^i$ on the source side of the boundary. However, when we move to the opposite side of the boundary we must change the sign of $\mathbf{H}^s$. The reason is that when we replace the boundary with freespace the field must still have a null where it did before. This requires that there be odd symmetry with respect to the plane. $\mathbf{H}^i$ is now the source which drives the fields in our problem. The TE_z case is dual.

The numerical equivalent is straight forward. We place the boundary over the nodes for the field that will be suppressed, the H_y nodes. The source will then be driven on these nodes. The boundary is a PMC imposed by forcing the E_x components to satisfy:

$$E_x(j, k_b + 1) = E_x(j, k_b) \qquad j = (1, \dots, j_{max}). \qquad (3.15)$$

where k_b is the source boundary node index, at the nodes in adjacent cells. To prevent an electric charge buildup on the boundary we must also suppress the normal component of the electric field E_z .

$$E_z(j, k_b) = 0 \quad j = (1, \dots, j_{max}). \quad (3.16)$$

We have thus numerically produced $\nabla \times \mathbf{E} \Big|_{\text{boundary}} = 0$. This is legitimate because it implies $\mu \partial \mathbf{H} / \partial t \Big|_{\text{boundary}} = 0$ where $\mathbf{H} = H_y \hat{\mathbf{y}}$ on the source boundary of our numerical scheme. The source is driven by specifying the incident field component H_y^1 on the boundary with the desired shape in time and a transverse Gaussian weighting. The resulting scattered magnetic field is then used in the calculation of the scattered electric field. This step in the propagation occurs after the source boundary is enforced (3.15 and 3.16) and before the next magnetic field is updated. Thenceforth, the fields are propagated using (3.10a-c).

As an alternate point of view, the scattered field can be thought of as a field produced by Huygen's sources [15] on the boundary. Following Harrington [17], the scattered fields are treated as source free fields away from the boundary. This then allows us to make use of the induction theorem. We suppress the fields outside the problem space with the introduction of surface currents.

$$\mathbf{J}_s = \hat{\mathbf{n}} \times (\mathbf{H}^s - \mathbf{H}) \quad \mathbf{M}_s = (\mathbf{E}^s - \mathbf{E}) \times \hat{\mathbf{n}} \quad (3.17)$$

where $\hat{\mathbf{n}}$ is the normal unit vector on the boundary pointing into the problem space and $\mathbf{J}_s$ and $\mathbf{M}_s$ are electric and magnetic currents on the surface of the boundary. These currents then radiate in the presence of the boundary.

The problem is further simplified when the boundary is a perfect conductor since one of the fields (the magnetic field for the TM_z case we have focused on) is zero. For instance, for a PEC boundary, on the source side of the boundary we can therefore write

$$\hat{n} \times \mathbf{H}^s = -\hat{n} \times \mathbf{H}^i = -\mathbf{J}_s.$$

This is equivalent to removing the conductor and having an electric current radiating directly into free space.

The method outlined by Merewether [15] for driving sources in an interior problem relies on the Huygen's sources presented above. However, we have shown that this is equivalent, both analytically and numerically, to simply impressing the desired fields on their respective perfectly conducting boundaries and propagating the resulting scattered fields.

There is a difficulty encountered when driving finite aperture sources such as the incident Gaussian beam. It arises because the aperture field is not being exactly represented by the field points in the mesh. In fact, along the source boundary there is a step discontinuity in H_y at each cell boundary. Each of these discontinuities acts as if it were a small independent current source radiating a cylindrical wave. The global effect of these many transverse radiators is to produce a surface wave that propagates along the source boundary. This then causes a distortion at the tail of the pulse which appears as a dip at the beam axis and a rise at the wings. This type of distortion is also reported by Sheen [18].

Figures (3.4) and (3.5) show this tail distortion for two different beam waists. The observation that the reader should make is that with a wider beam, the field more closely resembles its source. The wider beam has a smaller difference in the field amplitudes at two transversely adjacent cells than a tighter beam and, hence, the resulting sources are smaller. The tail distortion is therefore reduced. A tight beam with finer gridding also results in smaller longitudinal currents and less distortion.

The source formulation presented thus far radiates a beam of given cross section normally to the source plane. In some problems, however, it would be advantageous to direct the beam at a specified angle. Such problems of interest to this research include oblique incidence to an interface which lies parallel to a coordinate axis. To this end we introduce a linear time delay to the source functions along the source plane. The delay per element $\Delta delay$ for a propagation angle θ_i measured from the source plane is given by

$$\Delta delay = \frac{\Delta x \cos \theta_i}{u} \quad (3.18)$$

where u is the speed of light in the medium. In order to keep the desired beam waist w_o constant, the aperture must be decreased in size by the factor $\sin \theta_i$. The source function now becomes the product of an adjusted weighting function $W_a(j\Delta x)$ and a linearly delayed time history $F(n\Delta t - t_o \pm j\Delta delay)$. We have included a delay t_o in the time argument to insure that causality will be maintained.

8. A vector FDTD simulation of the pulsed Gaussian beam in chapter 2

In this section we present some numerical results to support the method outlined in this chapter. The simulation is that of a Gaussian aperture PG beam. The mode set is TM_z and the behavior of the amplitude of the total electric field (i.e. $\sqrt{E_x^2 + E_z^2}$) is analyzed. This demonstration is intended to strengthen confidence in the paraxial beam approximation presented in chapter 2, as well as provide a confirmation of the general FDTD precepts.

For the results presented in Fig. (3.7) a mesh size of $63\mu m$ longitudinally and $63\mu m$ transversely was used. The discretization ranged from $.030\mu m$ per cell to $.0168\mu m$ per cell. The Courant condition, derived from Eq. (3.12), in this case

is .707, or $\Delta t = .707\Delta t_c$. The excitation pulse is Gaussian in time with a total $1/e$ duration of $1.45fs$. Thus the sampling ranges from approximately 15 cells to 25 cells per pulse length (pulse length in this case is defined by $(1/e)$ amplitude points). The amplitude radius of the beam is $2.5\mu m$. We have thus reproduced the model of the beam used in chapter 2.

The models are in generally good agreement with one another. However, we notice from a comparison between the analytical and numerical results that the diffraction length is shorter and the diffraction angle is greater for the numerical case. This would suggest that the effective frequency is higher for the FDTD simulation than for the analytical Gaussian beam result. We should not be overly concerned with this discrepancy since one case represents two dimensional behavior while the other represents three dimensional behavior. The other discrepancy that is apparent from this exercise is the diffraction angle decreases with increasing numerical size. It is important to note here that as the pulse transitions from the near to the far zone that it acquires a time derivative. The main contribution to the far zone behavior is therefore the higher components of the frequency spectrum. The implication is then that finer discretization is required in the far zone than the general $\lambda_o/15$ rule-of-thumb. This conclusion is supported by the three numerical results shown in Fig. (3.7).

Figure (3.1), Positioning of meshes in space and time. The electric and magnetic fields are staggered from one another by one half cell. They are also staggered in time by one half time increment.

Figure (3.2), Field approximation mesh for TM_z mode. Dotted line indicates the boundary to the problem space.

Figure (3.3), Field approximation mesh for TE_z mode. Dotted line indicates the boundary to the problem space.

Figure (3.4), Longitudinal on-axis slice of a Gaussian aperture PW beam showing tail distortion. Distortion is non-trivial because of a narrow waist size $\omega_0 = 2.5\mu m$ relative to the pulse length.

Figure (3.5), Longitudinal on-axis slice of a Gaussian aperture PW beam showing tail distortion. Distortion is reduced from Fig (3.4) due to a larger waist size $\omega_0 = 5.0\mu m$ relative to the pulse length.

Figure (3.6), Longitudinal slice of a Gaussian aperture PW beam showing onset of one time derivative behavior. Time signal at $z = 16.0\mu m$.

Figure (3.7), Profiles for the 1/e intensity of the beam spread for a Gaussian aperture PW beam. The near-far field boundary, defined as the distance at which the intensity waist doubles, is between $z = 25 \mu m$ and $z = 35 \mu m$. Three numerical cases and one analytical case are compared. The initial waist $w_o = 2.5 \mu m$ and the wavelength $\lambda_{rad} = 1.367 \mu m$.

CHAPTER 4

NONLINEAR SELF-FOCUS IN KERR MEDIA

The full vector FD-TD technique provides a model of self-focusing that is more accurate than is achieved with existing scalar models. In this chapter we model the self-focusing of an ultra-short PG beam in a nonlinear Kerr material. The Kerr medium model is introduced in section 1 and a frequency domain expression is derived for the nonlinear susceptibility. We then show that both the refractive index and the absorption coefficient are dependent on the electric field intensity in this medium. In section 2 we develop a nonlinear wave equation and produce a crude approximation to the focal length of a monochromatic beam. A wideband pulse is next considered and a qualitative analysis of expected nonlinear behavior is made in section 3. In section 4 we formulate a numerical expression for the Kerr model and develop the FD-TD mesh on which the electrical coefficients will be calculated. Numerical results are presented in section 5 for both the TE_z and TM_z cases. It will also be shown in this section that the full-wave, time dependent, vector approach recovers the physics predicted by standard scalar models. In addition, we report a number of nonlinear events not recoverable from the scalar models; back reflection and optical vortices in the wake field of the self-focus, multiple foci, and limiting of the self-focus by coupling of energy into the longitudinal field component.

1. Reorientational Kerr effect for single frequency

Self-focusing is a nonlinear effect that results from field dependent material constants. Specifically, the self-focusing effect in this discussion is due to the presence of an electric field intensity dependent susceptibility term. The model describing the nonlinear susceptibility in this case is the following differential equation.

$$\tau \frac{\partial \chi^{NL}}{\partial t} + \chi^{NL} = \epsilon_2 |\mathbf{E}|^2. \quad (4.1)$$

This is the nonlinear form of the Debye equation with τ as the relaxation time constant. It is a good approximation for the rotational molecular mode in a liquid consisting of anisotropic molecules. This is generally known as the orientational Kerr effect and while it was originally conceived to describe light/liquid interactions, some isotropic solids also exhibit a Kerr-like effect [30].

The difference in magnitudes of the induced dipole moment parallel and perpendicular to the principal (longest) molecular axis is the main contribution to the coefficient ϵ_2 . For this reason long thin molecules produce the greatest nonlinear effects. Because of molecular interaction and kinetic energy in the medium, these molecules are not allowed to rotate freely. Rather, molecular rotation is frustrated and the overall response of the medium is damped. At high electric field intensities however, the force on the dipole molecule to align with the field begins to overcome the molecules chaotic motion. The result is an intensity dependent susceptibility.

The induced susceptibility change is directly related to the nonlinear refractive index which causes a beam to self-focus or defocus (self-bloom). As we shall show in this section, the refractive index is also intensity dependent and governed by the relation

$$n = n_b + n_2 |E|^2. \quad (4.2)$$

where n_b is the background linear index. The beam initially has a Gaussian cross section with its maximum on axis thus the susceptibility is inclined to change more in the center of the beam than at the periphery. This produces a lens like structure. As in a lens, the optical path length (phase delay) is different in the center of the

beam than it is at the edge since the phase velocity, $v_p = c/n$, is different. As a result, the beam converges (self-focuses) or diverges (self-blooms) depending on the type of nonlinearity (positive or negative). As the beam begins to focus in a medium with a positive nonlinearity its center intensity grows self-inducing an even greater phase delay with respect to the edge of the beam. The spot size continues to decrease while the intensity increases until saturation and/or longitudinal field events limit the focus. The final spot size is generally many times smaller than for a linear focus.

It can be shown that the Kerr medium model (4.1) is similar to an intensity dependent refractive index (4.2) combined with nonlinear dispersion and absorption. First we will need to derive the third order frequency domain susceptibility $\chi_o^{(3)}$. Consider the case of a monochromatic beam incident on a Kerr medium. The beam is considered to be propagating in the z direction and linearly polarized transversely to the propagation direction. It is written in the form

$$\mathbf{E} = \frac{1}{2} [E(\omega)e^{-i\omega t} + c.c.] \hat{\mathbf{x}}. \quad (4.3)$$

The nonlinear polarization is expressed as the convolution of three electric fields with a fourth order response tensor:

$$\mathbf{P}^{(3)}(t) = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_3 \mathbf{R}^{(3)}(t_1, t_2, t_3) : \mathbf{E}(t-t_1) \mathbf{E}(t-t_2) \mathbf{E}(t-t_3). \quad (4.4)$$

For the sake of simplicity, the response tensor is assumed to be diagonal to remove any directional coupling. The scalar response function will hereafter be referred to as $R^{(3)}(t_1, t_2, t_3)$ and (4.4) is reduced to a scalar relation. The product of the three fields is

$$E(t-t_1)E(t-t_2)E(t-t_3) = \frac{1}{8} [E^3(\omega)\gamma_1 e^{-i3\omega t} + |E(\omega)|^2 E(\omega)\gamma_2(t_1, t_2, t_3)e^{-i\omega t} + c.c.] \quad (4.5)$$

where

$$\begin{aligned}\gamma_1(t_1, t_2, t_3) &= e^{i\omega(t_1+t_2+t_3)} \\ \gamma_2(t_1, t_2, t_3) &= [e^{i\omega(t_1+t_2-t_3)} + e^{i\omega(t_1-t_2+t_3)} + e^{i\omega(-t_1+t_2+t_3)}].\end{aligned}$$

The reason for using the coefficients $\gamma_1(t_1, t_2, t_3)$ and $\gamma_2(t_1, t_2, t_3)$ is for simplification in a later step. We choose the following representation for the polarization term to reflect that it has both ω and 3ω terms.

$$\begin{aligned}P^{(3)}(t) &= \frac{1}{2} [P^{(3)}(3\omega)e^{-i3\omega t} + P^{(3)}(\omega)e^{-i\omega t} + c.c] \\ &= \frac{1}{2} [\epsilon_o \chi^{(3)}(3\omega) E^3(\omega) + \epsilon_o \chi^{(3)}(\omega) |E(\omega)|^2 E(\omega) + c.c]\end{aligned}\quad (4.6)$$

Inserting (4.5) into (4.4) and comparing phase terms with those in (4.6), one obtains the following nonlinear susceptibilities

$$\epsilon_o \chi^{(3)}(3\omega) = \frac{1}{4} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_3 R^{(3)}(t_1, t_2, t_3) \gamma_1(t_1, t_2, t_3) \quad (4.7a)$$

$$\epsilon_o \chi^{(3)}(\omega) = \frac{1}{4} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_3 R^{(3)}(t_1, t_2, t_3) \gamma_2(t_1, t_2, t_3). \quad (4.7b)$$

To proceed we need to find a representation for the scalar response function $R^{(3)}$. The Green's function representation for our medium model (4.1) is

$$[\tau \frac{\partial}{\partial t} + 1] G(t, t_1) = \epsilon_2 \delta(t - t_1). \quad (4.8)$$

With the boundary condition $G = 0$ for $t < t_1$ (causality), we obtain

$$G(t, t_1) = \frac{\epsilon_2}{\tau} \theta(t - t_1) e^{-(t-t_1)/\tau} \quad (4.9)$$

where $\theta(t)$ is the Heaviside function

$$\theta(t) = \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases}. \quad (4.10)$$

If we now define the operator L as the differential equation describing the medium

$$L \stackrel{\text{def}}{=} \left[\tau \frac{\partial}{\partial t} + 1 \right]$$

and the inner product as

$$\langle u, v \rangle \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} uv \, dt,$$

we obtain a relation analogous to Green's second relation

$$\langle \chi^{(3)}(t), L G(t, t_1) \rangle - \langle L \chi^{(3)}(t), G(t, t_1) \rangle = \int_{-\infty}^{\infty} \left[\chi^{(3)}(t) \frac{\partial G(t, t_1)}{\partial t} - G(t, t_1) \frac{\partial \chi^{(3)}(t)}{\partial t} \right] dt.$$

By choosing as boundary conditions $G = 0$ as t goes to $\pm\infty$, the right hand side is zero. Green's function properties and Eq. (4.1) produce the following relation

$$\chi^{(3)}(t) = \int_{-\infty}^{\infty} G(t - t_1) |\mathbf{E}(t_1)|^2 dt_1 = \int_{-\infty}^{\infty} G(t_1) |\mathbf{E}(t - t_1)|^2 dt_1 \quad (4.11)$$

We notice that equation (4.4) is symmetric with interchange of t_1 , t_2 , and t_3 . Therefore, the relation (4.11) must also exhibit this symmetry. If (4.11) is rewritten in the completely symmetric form

$$\chi^{(3)}(t) = \frac{1}{3} \left[\int_{-\infty}^{\infty} G(t_1) |\mathbf{E}(t - t_1)|^2 dt_1 + \int_{-\infty}^{\infty} G(t_2) |\mathbf{E}(t - t_2)|^2 dt_2 + \int_{-\infty}^{\infty} G(t_3) |\mathbf{E}(t - t_3)|^2 dt_3 \right] \quad (4.12)$$

then the relation between Green's function and the response function is

$$R^{(3)}(t_1, t_2, t_3) = \frac{\epsilon_0}{3} \left[G(t_1) \delta(t_1 - t_2) \delta(t_3) + G(t_1) \delta(t_3 - t_1) \delta(t_2) + G(t_1) \delta(t_2 - t_3) \delta(t_1) \right]. \quad (4.13)$$

Rather than perform three equivalent integrations, we can reduce $\gamma_2(t_1, t_2, t_3)$ and $R^{(3)}$ from (4.13) to the following forms

$$\gamma_2(t_1, t_2, t_3) \Rightarrow 3e^{i\omega(t_1+t_2-t_3)}$$

$$R^{(3)}(t_1, t_2, t_3) \Rightarrow \epsilon_o G(t_1) \delta(t_1 - t_2) \delta(t_3).$$

We then obtain by substitution into (4.7a,b)

$$\begin{aligned} \epsilon_o \chi^{(3)}(3\omega) &= \frac{\epsilon_o}{4} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_3 G(t_1) \delta(t_1 - t_2) \delta(t_3) \gamma_1(t_1, t_2, t_3) \\ &= \frac{\epsilon_o}{4} \int_{-\infty}^{\infty} dt_1 G(t_1) e^{i2\omega t_1} \end{aligned} \quad (4.14a)$$

and

$$\epsilon_o \chi^{(3)}(\omega) = \frac{3\epsilon_o}{4} \int_{-\infty}^{\infty} dt_1 G(t_1) e^{i2\omega t_1}. \quad (4.14b)$$

After substitution of Eq. (4.9) for $G(t_1)$ we obtain

$$\chi^{(3)}(3\omega) = \frac{\epsilon_2}{4\tau} \int_{-\infty}^{\infty} dt_1 \theta(t_1) e^{-t_1/\tau} e^{i2\omega t_1} = \frac{\epsilon_2}{4(1-i2\omega\tau)} \stackrel{\text{def}}{=} \chi_o^{(3)} \quad (4.15a)$$

and

$$\chi^{(3)}(\omega) = \frac{3\epsilon_2}{4(1-i2\omega\tau)} = 3\chi_o^{(3)}. \quad (4.15b)$$

The nonlinear polarizations in terms of $\chi_o^{(3)}$ are then written as follows:

$$P^{(3)}(3\omega) = \epsilon_o \chi_o^{(3)} E^2(\omega) E(\omega) \quad (4.16a)$$

$$P^{(3)}(\omega) = 3\epsilon_o \chi_o^{(3)} |E(\omega)|^2 E(\omega) \quad (4.16b)$$

The refractive index for the beam at ω is now defined by the relation

$$n^2 = (1 + \chi^{(1)} + 3\chi_o^{(3)}|E(\omega)|^2) \quad (4.17)$$

where

$$(1 + \chi^{(1)}) \stackrel{\text{def}}{=} n_b^2 \quad (4.18)$$

is the linear contribution to the background refractive index. Since a plane wave solution in this medium has the form

$$\mathbf{E}(z, t) = E_o e^{-i\omega t} e^{in(\omega/c)z} e^{-\alpha z} \hat{\mathbf{x}},$$

as long as the nonlinear effects are mild (i.e., if the pump field can be assumed to be undepleted), the total refractive index n can be approximated by the real part of (4.17) and the absorption coefficient α by the imaginary part of (4.17) times ω/c . In particular, if $n_b^2 \gg 3\chi_o^{(3)}|E(\omega)|^2$, then, when $\chi_o^{(3)}$ is sorted into its real and imaginary components, we find

$$n \approx n_b + n_2|E(\omega)|^2 \quad (4.19)$$

where the nonlinear index

$$n_2 = \frac{3}{2n_b} \text{Re} [\chi_o^{(3)}] = \frac{3\epsilon_2}{8n_b[1 + (2\omega\tau)^2]} \quad (4.20)$$

and the absorption coefficient

$$\alpha = \frac{\omega}{c} \text{Im} [n] \approx \frac{3}{2n_b} \frac{\omega}{c} \text{Im} [\chi_o^{(3)}] |E(\omega)|^2 = \frac{3\omega\epsilon_2(2\omega\tau)^2 |E(\omega)|^2}{8n_b c [1 + (2\omega\tau)^2]} \quad (4.21)$$

Equation (4.19) is now congruous with the assumption (4.2) made earlier that the refractive index is dependent on field intensity. Equations (4.20) and (4.21) are

significant because they show not only that the nonlinearity is intensity dependent, but also the index and the absorption dependence on ω and τ . The nonlinear refractive index coefficient n_2 is maximum for the case where the optical oscillation period is much shorter than the relaxation time, i.e., $\omega\tau \gg 1$. The nonlinear absorption is zero for d.c. and is linearly dependent on frequency for low frequencies. As the frequency increases, the nonlinear index reaches a break point and then rolls off at the rate of 20.0 dB per decade as shown in Fig (4.1). Concurrently, the nonlinear absorption coefficient peaks and then rolls off at the rate of 10.0 dB per decade as shown in Fig (4.2). Given this dependence of the plane-wave behavior on $\omega\tau$, one would also expect the $\omega\tau$ product to have a large influence on the physics of the self-focusing phenomena. For instance, a beam of sufficient power to self-focus to a very small waist in a short relaxation time medium might focus to a larger waist in a medium where the relaxation time is on the order of the radial frequency of the beam. In this case the spot-size (waist for a nonlinear focus) is being limited by the greater absorption in high intensity regions. Furthermore, in a slowly relaxing medium the nonlinearity might be so damped that the same beam will focus at a greater distance or may not focus at all.

Equation (4.15a) is also significant because it implies third harmonic frequency conversion. The susceptibility at 3ω produces a polarization at 3ω that is due solely to the field at ω . Since at high intensities much of the field energy is converted into higher frequencies, nonlinear self-focusing phenomena can be influenced by this frequency conversion characteristic. Because the minimum waist size for linear focus is ω dependent, this third harmonic generation will in some cases produce a more confined focus. Alternately, if the $\omega\tau$ product is large enough that n_2 is at or beyond the break point in Fig (4.1), third harmonic generation leads to a conversion of energy into a poorly focusing regime and results in an overall decrease in the energy

available in the regime that is more conducive to self-focusing. The inclusion of linear dispersion to the medium could further enhance or degrade the influence that frequency conversion has on self-focusing. Additionally, the presence of a resonance in the medium close to the third harmonic will completely suppress frequency up conversion and the result is energy loss. It is however not practical to include third harmonic effects in a self-focusing model without resorting to intensive numeric techniques due to the complexity it would involve. The following sections make use of the previously derived single frequency results to generate some predictions about self-focusing in a Kerr medium. The explicit third harmonic and attenuation characteristics are therefore excluded in the analysis below.

2. Approximation to scalar self-focus

The following is typical of the development of a scalar approximation commonly used to predict the onset of self-focus in an intensity dependent index medium. While it is of limited accuracy, its value is in its convenience because the resulting analytical expression is relatively simple. This scalar model is insufficient to meet the requirements of the research presented here but two important features arise from it which are relevant to the selection of example problems to be modeled with our vector technique. We will demonstrate that the beam power is the dominating factor in determining if self-focusing will occur and, if it does, what the focal length will be. For a nonlinear focus, the beam power must exceed a certain threshold that is exclusively a function of the medium parameters n_1 and n_2 .

Given the relation between the electric field intensity and the refractive index we can derive a scalar expression that will approximate the behavior of the beam. The approximation is based on the paraxial Gaussian beam model for a monochromatic source from chapter 2 and the assumption that there is negligible field variation in

the axial direction. Likewise, the loss in the medium is assumed to be small. The result is similar to the wave equation with a nonlinear driving term.

We start by rewriting Maxwell's curl equations (3.2a,b)

$$\nabla \times \mathbf{E} = -\mu_o \frac{\partial}{\partial t} \mathbf{H} \quad (4.23a)$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} \quad (4.23b)$$

Consider Ampere's law (4.23b) expressed with the nonlinear susceptibility χ^{NL} included through the electric flux density term,

$$\mathbf{D} = \epsilon_o \mathbf{E} + \mathbf{P},$$

where

$$\begin{aligned} \mathbf{P} &= \mathbf{P}^L + \mathbf{P}^{NL} \\ &= \epsilon_o \chi^L \mathbf{E} + \epsilon_o \chi^{NL} \mathbf{E}, \end{aligned}$$

χ^L being the linear susceptibility term:

$$\nabla \times \mathbf{H} = \epsilon_o \frac{\partial}{\partial t} [(1 + \chi^L + \chi^{NL}) \mathbf{E}] \quad (4.24)$$

Taking the curl of both sides of (4.23a) and (4.24) and neglecting terms involving $\nabla \cdot \mathbf{E}$ we obtain the wave equation:

$$\nabla^2 \mathbf{E} - \frac{n_b^2}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} (\chi^{NL} \mathbf{E}) = \mu_o \frac{\partial^2}{\partial t^2} \mathbf{P}^{NL} \quad (4.25)$$

If we now choose the following representation for the electric field,

$$\mathbf{E} = \frac{1}{2} \left[E(\mathbf{r}) e^{i(\omega t - k z)} + c.c. \right] \hat{\mathbf{x}} \quad (4.26)$$

and set

$$k_b = \frac{n_b \omega}{c},$$

then the frequency domain wave equation resulting from (4.25) is expressed as

$$\nabla^2 \mathbf{E} + k_b^2 \mathbf{E} = -\mu_o \omega^2 P^{(3)} = -\left(\frac{\omega}{c}\right)^2 \chi^{(3)}(\omega) \mathbf{E}. \quad (4.27)$$

A further simplification is achieved by using the slowly varying envelope approximation (SVEA). This is the assumption that a wavelength is small in comparison to any variations in the field envelope.

$$\left| \frac{\partial^2}{\partial z^2} E(\mathbf{r}) \right| \ll \left| k \frac{\partial}{\partial z} E(\mathbf{r}) \right| \ll \left| k^2 E(\mathbf{r}) \right|. \quad (4.28)$$

The action of the Laplacian on the field now becomes

$$\begin{aligned} \nabla^2 (E e^{-ikz}) &= (\nabla_t^2 E) e^{-ikz} + \frac{\partial^2}{\partial z^2} (E e^{-ikz}) \\ &\simeq (\nabla_t^2 E) e^{-ikz} + \left[-2(ik) \frac{\partial E}{\partial z} - k^2 E \right] e^{-ikz} \end{aligned} \quad (4.29)$$

where the $\mathbf{r}$ dependence on E is now implied and we have introduced the transverse Laplacian operator

$$\nabla_t^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

In the SVEA the nonlinear wave equation (4.27) then reduces to the form:

$$\nabla_t^2 E - 2ik_b \frac{\partial E}{\partial z} = -\omega^2 \mu_o P^{(3)} = -\left(\frac{\omega}{c}\right)^2 3\chi_o^{(3)} |E|^2 E \quad (4.30)$$

where we have introduced the nonlinear susceptibility derived in Sec 4.1. Neglecting the imaginary part of the complex susceptibility, we substitute (4.21) into the last equation to obtain the widely used scalar nonlinear Schrödinger equation model for self-focusing:

$$\nabla_{\perp}^2 E - 2ik_b \frac{\partial E}{\partial z} + \frac{n_2 k_b^2}{2n_b} |E|^2 E = 0 \quad (4.31)$$

Equation (4.31) is solved with several known numerical techniques [21] [30]. We can, however, expand this equation in a Taylor series and, given initial conditions, derive a useful analytical expression that describes the self-focusing behavior of a beam. Unfortunately, the Taylor series provides direct information only about the initial behavior of the beam; and we must extrapolate this information to conclude what conditions are required for self-focusing to occur and the distance in which it will occur. The accuracy of this approach is therefore contingent on the number of terms kept in the series approximation and the magnitude of the nonlinear term $n_2 |E|^2$. Furthermore, when the nonlinearity grows large enough (immediately prior to and during the focus), higher order terms in the Taylor's expansion begin to dominate the expression.

In the following derivation I have expounded on the method outlined by Yariv [27]. We first consider the geometry presented in Fig. (4.3). A Gaussian beam is incident normally on a block of homogeneous nonlinear material. The coordinate system is such that the origin is located at the interface. The transverse coordinate is now the radial distance r from the axis of propagation; it is the argument used in our Gaussian beam expressions. The beam waist is displaced from the interface so that we can account for the input beam's state of either convergence or divergence. The location of the nonlinear self-focus is labeled z_f .

We next consider the Gaussian beam solution in chapter 2 with its focus displaced from the interface to the plane $z = z'$.

$$\begin{aligned}
 E &= E_o \exp \left\{ \frac{-r^2}{\omega_o^2 \left[1 + \left(\lambda(z - z') / \pi \omega_o^2 \right)^2 \right]} - \frac{ikr^2}{2(z - z') \left[1 + \left(\pi \omega_o^2 / \lambda(z - z') \right)^2 \right]} \right\} \\
 &= E_o \exp \left\{ \frac{-r^2}{\omega_o^2 \left[1 + (z - z' / z_o)^2 \right]} - \frac{ikr^2}{2(z - z') \left[1 + (z_o / (z - z'))^2 \right]} \right\}. \quad (4.32)
 \end{aligned}$$

We have introduced the Rayleigh distance

$$z_o = \frac{\pi \omega_o^2}{\lambda}$$

to simplify the expression. Substituting $z = 0$ into (4.32), the expression for the input beam at the plane of the interface is now expressed as a function of z' .

$$\begin{aligned}
 E(x, y, z = 0) &= E_o \exp \left\{ \frac{-r^2}{\omega_o^2 \left[1 + (z' / z_o)^2 \right]} + \frac{ikr^2}{2z' \left[1 + (z_o / z')^2 \right]} \right\} \\
 &= E_o \exp \left[-r^2 \frac{(1 - i\theta)}{d^2} \right] \quad (4.33)
 \end{aligned}$$

where we have introduced the focusing parameter θ :

$$\begin{aligned}
 \theta &\stackrel{\text{def}}{=} \frac{k\omega_o^2 \left[1 + (z' / z_o)^2 \right]}{2z' \left[1 + (z_o / z')^2 \right]} \\
 &= \frac{k\omega_o^2 z'}{2z_o^2} = \frac{z'}{z_o} \quad (4.34)
 \end{aligned}$$

and the distance d from the beam axis to the $1/e$ amplitude at the initial plane:

$$\begin{aligned} d^2 &\stackrel{\text{def}}{=} \omega^2(0) = w_o^2 \left[1 + \left(\frac{k\omega_o^2 z'}{z_o^2} \right)^2 \right] \\ &= \frac{2z'}{k\theta} (1 + \theta^2). \end{aligned} \quad (4.35)$$

For the case where the linear beam waist occurs before the nonlinear medium, the beam is diverging when it interacts with the interface and $\theta < 0$. If the beam is still converging, then $\theta > 0$.

An approximation to the field intensity along the axis as a function of z is now obtained from a Taylor expansion of (4.29). We expand $|E(0, 0, z)|^2$ at $z = 0$ making repeated use of (4.32) to obtain derivatives of $|E|^2$ with respect to z .

$$\begin{aligned} \frac{\partial E}{\partial z} &= \frac{1}{2ik} \nabla_i^2 E + \frac{n_2 k}{in_b} |E|^2 E \\ \frac{\partial E^*}{\partial z} &= -\frac{1}{2ik} \nabla_i^2 E^* + \frac{n_2 k}{in_b} |E|^2 E^* \end{aligned} \quad (4.36)$$

$$\begin{aligned} \frac{\partial |E|^2}{\partial z} &= \left\{ E^* \frac{\partial E}{\partial z} + \text{c.c.} \right\} \\ &= \left\{ \frac{1}{2ik} E^* \nabla_i^2 E + \text{c.c.} \right\} \end{aligned} \quad (4.37)$$

$$\begin{aligned} \frac{\partial^2 |E|^2}{\partial z^2} &= \left\{ E^* \frac{\partial^2 E}{\partial z^2} + \frac{\partial E^*}{\partial z} \frac{\partial E}{\partial z} + \text{c.c.} \right\} \\ &= \frac{1}{4k^2} \{ (\nabla_i^2 E)(\nabla_i^2 E^*) - E \nabla_i^2 (\nabla_i^2 E^*) \\ &\quad + \frac{n_2 k^2}{2n_b} E [|E|^2 \nabla_i^2 E^* - \nabla_i^2 (|E|^2 E^*)] + \text{c.c.} \}. \end{aligned} \quad (4.38)$$

We now have all the requisite derivatives in z in terms of the transverse derivatives. The Gaussian beam profile at the interface (4.33) is used since for small z the beam

has not yet changed significantly. Cylindrical coordinates are more appropriate in the case of the lowest order (i.e., ϕ symmetric) Gaussian beam.

$$\nabla_t^2 = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r}.$$

From (4.33) we have the necessary terms to complete the second order expansion.

$$E^* \nabla_t^2 E \Big|_{r=0} = -4E_o^2 \frac{1-i\theta}{d^2} \quad (4.39a)$$

$$(\nabla_t^2 E^*) (\nabla_t^2 E) \Big|_{r=0} = 16E_o^2 \frac{1+\theta^2}{d^4} \quad (4.39b)$$

$$E^* \nabla_t^2 (\nabla_t^2 E) \Big|_{r=0} = 32E_o^2 \left(\frac{1-i\theta}{d^2} \right)^2 \quad (4.39c)$$

$$E^* |E_o|^2 \nabla_t^2 E \Big|_{r=0} = -4E_o^4 \frac{1-i\theta}{d^2} \quad (4.39c)$$

$$E^* \nabla_t^2 (|E|^2 E) \Big|_{r=0} = -4E_o^4 \frac{3-i\theta}{d^2} \quad (4.39d)$$

A solution of the axial beam intensity is finally obtained when, with assistance from Eqs. (4.37) and (4.38), elements of the equation set (4.39a-d) are substituted for their corresponding elements in the Taylor series expansion:

$$|E|^2 \Big|_{x,y=0} \simeq E_o^2 \left[1 + (4\theta) \frac{z}{kd^2} + \left(-4 + 12\theta^2 + \frac{n_2 k^2 d^2}{n_b} E_o^2 \right) \frac{z^2}{k^2 d^4} \right]. \quad (4.40)$$

Conservation of energy requires that the inverse of the axial intensity is roughly proportional to the area of the the beam. The self-focus, then, should occur when

the area goes to zero, i.e., the intensity goes to infinity. However, Eq. (4.40) is only accurate for the initial behavior of the beam in the nonlinear medium. Hence, its region of validity is limited. Since the degree of accuracy is unknown, it is reasonable to limit z such that the sum of the second two terms on the right hand side are between -1 and 1 . Within these limits we can then approximate the inverse of the intensity (4.40) using a series expansion found in [31]:

$$(1+x)^{-1} = 1 - x + x^2 - \dots (-1 < x < 1). \quad (4.41)$$

Using only the first three terms of this series produces a fourth order polynomial which, when truncated to second order gives the desired approximation to the inverse:

$$area \propto \frac{1}{|E|^2} \bigg|_{x,y=0} \simeq \left[1 - (4\theta) \frac{z}{kd^2} + \left(4 + 4\theta^2 - \frac{n_2 k^2 d^2}{n_b} E_o^2 \right) \frac{z^2}{k^2 d^4} \right]. \quad (4.42)$$

We can now predict if and where a self-focus will occur based on the zeros of this equation. If we define

$$P_{th} \stackrel{\text{def}}{=} \frac{\pi \epsilon_o c^3}{n_2 \omega^2}, \quad (4.43)$$

then the distance in which this area goes to zero, z_f , can be expressed as a function of beam power (P), threshold power (P_{th}), and the focusing parameter, (θ). The zeros of (4.42) are

$$\begin{aligned} z_f &= \left(\frac{kd^2}{2} \right) \frac{(4\theta) \pm \sqrt{(4\theta)^2 - 4 \left(4 + 4\theta^2 - \frac{n_2 k^2 d^2}{n_b} E_o^2 \right)}}{\left(4 + 4\theta^2 - \frac{n_2 k^2 d^2}{n_b} E_o^2 \right)} \\ &= \left(\frac{kd^2}{2} \right) \frac{1}{\sqrt{\frac{P}{P_{th}} - 1} + \theta}, \end{aligned} \quad (4.44)$$

where we have chosen the positive value of the $\pm$ pair to produce the -1 in the square root term. The initial beam power is expressed assuming that the intensity is uniform within the beam waist and zero elsewhere.

$$P = \pi d^2 \frac{1}{2} \epsilon_0 c n_b E_0^2 \quad (4.45)$$

For $\theta > 0$, the actual power for self-focusing to occur, P_{cr} , is simply $P_{cr} \equiv P_{th}$. The power required to produce a nonlinear focus in the case where the focusing parameter θ is negative (i.e. the beam is initially diverging) is increased. For $\theta < 0$, P_{cr} is then expressed as

$$P_{cr} \Big|_{\theta < 0} = P_{th} (1 + \theta^2) \quad (4.46)$$

The threshold power for self-focusing to occur for the case where the interface is located at the focal plane as given by (4.43) with n_2 given by (4.20) is plotted as a function of the relaxation time τ in Fig (4.4). Figure (4.5) shows the focal length as a function τ for a 220 kW beam focused on the interface.

Although the approximation presented here and the scalar model from which it is derived does give an introductory description of the nonlinear interaction, it has inherent flaws and is inadequate as a serious design tool for the following five reasons. First, it is based on a bidirectional beam approach which does not account for propagation transverse to the axis and is not a solution of Maxwell's equations. It assumes that the field varies as an e^{ikz} plane wave solution which does not apply when dealing with finite beams. In this model, all the fields are polarized radially thus have no longitudinal field components. This is contrary to Maxwell's equations. The Gaussian beam is an excellent model for the far field beam behavior where the transverse field components are dominant. However, a nonlinear self-focus is a near

field event in which all the field components have significant contributions. Second, the first two terms of the Taylor series expansion will at best provide only the initial focusing behavior of the beam since the higher order terms are absent. Third, the scalar model, (4.29), predicts that the beam will focus to a singular point with infinite amplitude. Such is not the case in nature. Fourth, the scalar model is unable to predict the events occurring during and immediately following self-focus. In contrast, the vector approach is able to model a number of interesting phenomena that take place at this time. For instance, back reflection from the focal region, generation of multiple foci, and optical vortices in the wakefield are phenomena that are not predicted by the scalar approach. Fifth, the approximation to (4.31) assumes a CW beam, hence, (4.44) does not necessarily hold for broad band pulses which is the exclusive regime for the problems addressed in this research. Equation (4.44) will therefore have limited application to our results other than as a rough approximation to threshold power and, with less accuracy, to focal distance.

3. Exact solution to the nonlinear Debye model for a pulse excitation

Without going into the great detail required for a formal analysis, we can analyze the medium model to obtain a qualitative feel for the behavior of high power pulses in a nonlinear medium. This section is devoted to exploring the medium behavior when subject to a pulse of energy rather than a CW beam and some possible limitations to the unbounded increase in energy density and associated diminishing beam waist at the focus predicted by the scalar model. Conclusions are made based on the physics and associated intuition and are supported by our results and the experimental and theoretical results of other authors.

The phenomenological susceptibility equation (4.1) can be solved explicitly if the time history of the electric field is known at a specified point in space. The

solution must exhibit exponential decay with time and it must also include a time dependent coefficient to account for the nonlinear driving term $|E|^2$. The solution is therefore given in the following form.

$$\chi^{NL} = F(t) \exp [G(t)] \quad (4.47)$$

When this equation is substituted into (4.1), we obtain

$$\left(\frac{\partial F}{\partial t} + F \frac{\partial G}{\partial t} + \frac{F}{\tau} \right) \exp (G) = \frac{\epsilon_2}{\tau} |E|^2. \quad (4.48)$$

The left side of (4.48) can be separated into two subsections and rewritten as

$$F \frac{\partial G}{\partial t} \exp (G) = \frac{\epsilon_2}{\tau} |E|^2 \quad (4.49a)$$

$$\frac{\partial F}{\partial t} + \frac{F}{\tau} = 0. \quad (4.49b)$$

The solution of (4.49b) is immediate $F(t) = F(0) \exp(-t/\tau)$. Equation (4.49a) now becomes

$$\frac{\partial G}{\partial t} \exp (G) = F(0) \exp \left(\frac{t}{\tau} \right) \frac{\epsilon_2}{\tau} |E|^2 \quad (4.50)$$

The solution is obtained by integration on both sides of Eq. (4.50):

$$\begin{aligned} \exp (G) &= F(0) \frac{\epsilon_2}{\tau} \int_{-\infty}^t \exp \left(\frac{t'}{\tau} \right) |E|^2 dt' \\ \chi^{NL} &= \frac{\epsilon_2}{\tau} \int_{-\infty}^t \exp \left[\frac{(t' - t)}{\tau} \right] |E|^2 dt' \end{aligned} \quad (4.51)$$

In the nonlinear self-focus problem, the field at the source boundary is known for all time; and the susceptibility can thus be obtained near this plane. If the

assumption can be made that the field structure will not change until it has propagated a significant distance from the source boundary, then something about the initial focusing behavior can be learned from the susceptibility model (4.51). If on the other hand, the pulse begins to focus before it even leaves the source boundary, then Eq. (4.59) is of little use since it no longer describes the medium behavior close to the boundary. The following analysis is therefore based on assumption that the initial nonlinear index change is small.

We must give careful consideration to the choice of the time history of the source excitation. If a vector FD-TD scheme is to be used, then a mono- or bipolar field is suitable as a source. Either is readily discretized and is easy to model on the mesh. The function chosen for the source in the self-focusing problems is a raised cosine pulse, i.e., a cosine raised above zero and restricted to one cycle. Figure (4.6) shows this pulse shifted in time such that it begins at $t = 0$:

$$\begin{aligned} f(t) &= \frac{1}{2} \left[1 + \cos \left(2\pi \frac{t}{T} \right) \right] \theta \left(\frac{T}{2} - |t| \right) \\ &= \cos^2 \left(\pi \frac{t}{T} \right) \theta \left(\frac{T}{2} - |t| \right) \end{aligned} \quad (4.52)$$

In addition to being continuous when turned on and off, this function is adequate for our purposes because its first derivative at the on/off points is also continuous. This is desirable because sharp changes in the field relative to the cell size tend to cause noisy transitions and result in pulse distortion. The cause of this distortion would be the first derivative of the electric or magnetic field in the calculation of the corresponding dual field. A smooth first derivative allows more precision in the initial FD-TD calculation for the equation set in section 3 of chapter 3, making the field values at all subsequent times less noisy.

For the raised cosine source pulse (4.52), it is now a straightforward calculation to determine the initial medium response in the z direction (propagation axis). This is accomplished by substituting Eq. (4.52) into Eq. (4.51) and integrating. For simplification we introduce the ratio of pulse length to response time:

$$\Gamma = \frac{T}{\tau}. \quad (4.53)$$

The solution to the nonlinear susceptibility for our chosen source excitation, when shifted by $T/2$ so that calculation begins at $t = 0$, is now the following expression:

$$\chi^{NL}(t) = \begin{cases} \frac{\epsilon_2 |E_0|^2}{8} \left\{ 3 + \frac{\cos(4\pi t/T) + (4\pi/\Gamma) \sin(4\pi t/T)}{1 + (4\pi/\Gamma)^2} \right. \\ \quad \left. - \frac{4[\cos(2\pi t/T) + (2\pi/\Gamma) \sin(2\pi t/T)]}{1 + (2\pi/\Gamma)^2} \right\} \\ \quad - e^{-\Gamma t/T} \left[\frac{12(2\pi/\Gamma)^4}{1 + 5(2\pi/\Gamma)^2 + 4(2\pi/\Gamma)^4} \right] \quad \text{for } 0 < t < T \\ \frac{\epsilon_2 |E_0|^2}{8} [1 - e^{-\Gamma}] \left[\frac{12(2\pi/\Gamma)^4}{1 + 5(2\pi/\Gamma)^2 + 4(2\pi/\Gamma)^4} \right] \quad \text{for } t > T \end{cases} \quad (4.54)$$

For a medium with an instantaneous response, $\Gamma \gg 1$, we recover the source function as expected. The refractive index as a function of time can then be calculated from relations (4.19) and (4.20). The effective conductivity is related to the time derivative of χ^{NL} as

$$\sigma_{eff} = \epsilon_0 \frac{\partial \chi^{NL}}{\partial t}. \quad (4.55)$$

Figure (4.7) shows the nonlinear refractive index (4.54) and Figure (4.8) shows the effective nonlinear conductivity, both as functions of time. Plots are given for four different relaxation times ranging from slow in comparison to the pulse (retarded) to fast in comparison to the pulse (instantaneous regime).

We see in Fig. (4.7) that the peak nonlinear index is closer to the tail of the pulse than the front of the pulse (latest in time in the figure) and that the delay increases with increasing τ . One would therefore expect the sharpest focus to occur on the trailing edge of the pulse and only linear diffraction to occur at the front. This intuition is further strengthened by analyzing the conductive behavior in Fig (4.8). Positive conductivity at the leading edge of the pulse results in the removal of energy. However, immediately following the peak intensity, there is a region of negative conductivity. This produces a gain effect on the tailing portion of the pulse and also in the background noise that is generated behind the pulse. The noise results from either the numerical approximations in the mesh or spontaneous scattering from quantum mechanics. Eventually, these effects cause the tail of the pulse to undergo an intense steepening also known as a “shock”. These trailing events can lead to some other interesting local effects. These are presented in the last section of this chapter.

This tail phenomenon has been predicted in a number of other works [24] [26]. For instance, Shen reports the presence of a horn shaped pattern in the pulse due to linear diffraction at the front and nonlinear self-focusing at the tail. Shimizu, studying the effect of dispersion, pulse distortion, and optical filaments that are caused by self-focusing in Kerr liquids, also reports an intense steepening and an asymmetric focus. However, instead of the compression occurring at the tail of the pulse, the first half of the pulse is compressed while the tail gradually spreads. An optical shock is eventually formed at the pulse front. This difference can be attributed to the fact that the second author has included normal (linear) dispersion in his scalar model. On the other hand, as anticipated by Shimizu, in nondispersive media the pulse center lags relative to its wings as a result of the positive nonlinear index. Therefore, the pulse gradually forms a shock at its tail. Similarly, Reintjes,

Carman, and Shimizu [23] note that if dispersion is absent, the leading edge of the pulse does not experience a significant nonlinear index because of the finite response time of the nonlinear medium. Consequently, the early part of the pulse diffracts as if the medium were linear and, because of the integral nature of the transient response, the tendency for focusing increases further into the pulse, causing the diameter to decrease towards the back of the pulse.

The nonlinear Debye model has an advantage over dispersionless nonlinear models (i.e., models that behave like Eq. (4.19) such as the one presented by either Feit and Fleck [20] or Malloney and Newell [22]) because it has a built-in mechanism for limiting the intensity of the focus. If left alone, a scalar model like (4.31) will continue to increase the lensing of the medium, increase the intensity, and focus the beam in a runaway fashion so that the field approaches a singularity. However, Marburger [21] asserts that before this can happen, higher order nonlinear effects and nonlinear saturation will limit the focus. The nonlinear Debye model, on the other hand, is a physical model that removes energy from the beam as it focuses and will tend to dampen the shock and reduce the beam power until the self-focusing stops.

While the finite response time of the Kerr medium model does influence the sharpness of focus, this may not be sufficient to preventing an eventual collapse to a singularity. Other physical limitations on the size of the focus include but are not limited to parametric interaction (scattering) [27] and filamentation [25]. In some cases scattering is a limiting factor because when the threshold for Raman scattering is reached, energy is backscattered at the expense of the input beam. Additionally, Shen has shown that for nanosecond pulse self-focusing in some Kerr liquids, when the input power exceeds $10P_{th}$, multiple filaments of highly dense energy form and remain stable for distances of up to one meter. However, these phenomena occur

to varying degrees and are thus not necessary for limiting the self-focus process. Consequently, we do not include these aspects of nonlinear beam self-focusing in our analysis.

Two physical processes that limit self-focusing and are not included in conventional scalar models, are the generation of longitudinal field components and propagation of energy into the transverse to z direction (diffraction). Unlike scattering, filamentation, and higher order nonlinearities, linear diffraction is always present for a beam in any homogeneous media. While the nonparaxial approaches of Feit and Fleck generate field components off axis and also predict an eventual saturation of the focus, propagation and power flow is still restricted to only one direction so these models must rely on nonphysical loss mechanisms to account for the energy that is propagating off-axis. To model the physics of combined nonlinear lensing and linear diffraction requires a full set of vector fields. The following section therefore details the implementation of the nonlinear Debye model into the FDTD framework developed in chapter 3.

4. FDTD implementation for the nonlinear Debye model

In this section we discuss the implementation of the Kerr medium Debye model (4.1) into the appropriate vector FDTD equation set ((3.4) or (3.5)) for two space dimensions and time. The medium is modeled in such a way that it occupies its own mesh and must be updated simultaneously with the fields. The method which follows is analogous to the method which produced the FDTD equation sets in chapter 3.

To begin, we develop a discretization mesh and calculate the medium parameters on the mesh as we did for the field components. We next use central differencing to represent our medium model. The electrical coefficients, ϵ_{eff} and σ_{eff} , are treated

as homogeneous volume quantities over the entire cell and the medium cells are updated with each cycle. Because there is an electric field intensity dependence on those coefficients, an averaging scheme is used to determine the intensity within each cell. In the TM_z case we treat the electric field components as edge quantities bordering all four edges of the the medium cell. The averaging provides coupling between the transverse and longitudinal electric field components since the medium “feels” both components in each cell. In contrast, in the TE_z case we place the electric field node at the center of the cell and treat this node as the sole contribution to the electric field intensity in the medium cell. Therefore, there is no direct nonlinear coupling between field components for the TE_z case.

When a medium is nonlinear, it can be treated by incorporating the field dependence into the susceptibility, hence, the polarization density. The Debye model for the nonlinear susceptibility of the medium in each polarization case is expressed as follows:

$$\text{TM Case:} \quad \partial_t \chi^{NL} + \frac{1}{\tau} \chi^{NL} = \frac{1}{\tau} \epsilon_2 (|E_x|^2 + |E_z|^2) \quad (4.56a)$$

$$\text{TE Case:} \quad \partial_t \chi^{NL} + \frac{1}{\tau} \chi^{NL} = \frac{1}{\tau} \epsilon_2 |E_y|^2. \quad (4.56b)$$

Consider again Ampere's law expressed in the form of (4.24).

$$\nabla \times \mathbf{H} = \epsilon_o \frac{\partial}{\partial t} [(1 + \chi^L + \chi^{NL}) \mathbf{E}]. \quad (4.57)$$

Unless the medium response is instantaneous, the time derivative of χ^{NL} influences the propagation of the beam. Equation (4.57) is now re-expressed to show this contribution as an effective conductivity term.

$$\nabla \times \mathbf{H} = \epsilon_o (1 + \chi^L + \chi^{NL}) \frac{\partial \mathbf{E}}{\partial t} + \sigma_{eff} \mathbf{E}. \quad (4.58)$$

The effective nonlinear conductivity σ_{eff} is given by (4.55) and can have either a positive or negative sign representing, respectively, either loss or gain. We treat the linear susceptibility, which is responsible for any linear dispersion effects, as a constant.

Since ϵ_{eff} and σ_{eff} represent volume quantities in each cell, the notation used to describe them is borrowed from the H -field representation. In particular,

$$\chi^{(3)}(x, z, t) \simeq$$

$$\chi^{(3)} \left[\left(j + \frac{1}{2} \right) \Delta x, \left(k + \frac{1}{2} \right) \Delta z, \left(n + \frac{1}{2} \right) \Delta t \right] \stackrel{\text{def}}{=} \chi^{(3)}(j, k, n) \quad (4.59a)$$

$$\chi^{(3)} \left[\left(j + \frac{1}{2} \right) \Delta x, \left(k + \frac{1}{2} \right) \Delta z, \left(n - \frac{1}{2} \right) \Delta t \right] \stackrel{\text{def}}{=} \chi^{(3)}(j, k, n-1) \quad (4.59b)$$

The nonlinear debye equations (4.56a,b) are now represented by the following numerical approximation.

TM Case:

$$\begin{aligned} & \left[\frac{\chi^{(3)}(j, k, n) - \chi^{(3)}(j, k, n-1)}{\Delta t} \right] + \frac{1}{\tau} \left[\frac{\chi^{(3)}(j, k, n) + \chi^{(3)}(j, k, n-1)}{2} \right] \\ &= \frac{\epsilon_2}{\tau} \left\{ \frac{[E_x(j, k+1, n) + E_x(j, k, n)]^2 + [E_x(j+1, k, n) + E_x(j, k, n)]^2}{4} \right\} \end{aligned} \quad (4.60a)$$

TE Case:

$$\left[\frac{\chi^{(3)}(j, k, n) - \chi^{(3)}(j, k, n-1)}{\Delta t} \right] + \frac{1}{\tau} \left[\frac{\chi^{(3)}(j, k, n) + \chi^{(3)}(j, k, n-1)}{2} \right]$$

$$= \frac{\epsilon_2}{\tau} [E_y(j, k, n)]^2 \quad (4.60b)$$

As in the case of the field equations, these results are simplified using the coefficients A , B , and I defined below. The nonlinear Debye equations become

$$\chi^{NL}(j, k, n) = [B\chi^{NL}(j, k, n) + \epsilon_2 I(j, k)] / A \quad (4.61)$$

where

$$A = \frac{\tau}{\Delta t} + \frac{1}{2}$$

$$B = \frac{\tau}{\Delta t} - \frac{1}{2}$$

$$I(j, k, n) = \begin{cases} \left\{ [E_x(j, k+1, n) + E_x(j, k, n)]^2 \right. \\ \quad \left. + [E_z(j+1, k, n) + E_z(j, k, n)]^2 \right\} / 4 & \text{TM Case} \\ E_y^2(j, k, n) & \text{TE Case} \end{cases}$$

The expression for ϵ_{eff} is now

$$\epsilon_{eff} = \epsilon_o (1 + \chi^L + \chi^{NL}) \quad (4.62)$$

The expression for the effective conductivity

$$\sigma_{eff} = \epsilon_o \frac{\partial \chi^{NL}}{\partial t}$$

is found by approximating the time derivative of χ^{NL} obtained from its central differencing form (4.61):

$$\begin{aligned} \sigma_{eff}(j, k, n) &= \epsilon_o \left[\frac{\chi^{NL}(j, k, n+1) - \chi^{NL}(j, k, n)}{\Delta t} \right] \\ &= \frac{\epsilon_o}{A \Delta t} [B\chi^{NL}(j, k, n+1) + \epsilon_2 I(j, k, n+1) - A\chi^{NL}(j, k, n)] \end{aligned} \quad (4.63)$$

where A , B and I are defined in (4.61).

Arbitrary structures and inhomogeneities are now easily modeled, within the limits of the finite grid size, by simply specifying the appropriate values for $\chi^{(L)}$ and ϵ_2 in each cell. Some simple structures including a slab waveguide and a linear/nonlinear interface are presented in chapter 5.

Since dispersion in this case is independent of the magnetic field, the magnetic field and the medium parameters can be updated simultaneously. The coefficients ϵ_{eff} and σ_{eff} are therefore computed from Eqs. (4.61) and (4.63) at the same time step as the $\mathbf{H}$ field. The coefficients are then substituted into either Eqs. (3.10a-c) in the case for the TM_z mode set or Eqs. (3.10d-f) in the case for the TE_z mode set for the subsequent $\mathbf{E}$ field update. The result is a complete model of Maxwell's equations in a medium exhibiting the kind of nonlinear dispersion described by relation (4.1). Unlike a nonlinear two dimensional scalar approach, no approximations have been made by this technique aside from the fact that space and time are discretized.

5. Initial parameters for the vector FD-TD self-focus simulation

The numerical problem deals with two space dimensions and time. The direction of propagation is along z ; the transverse direction is along x . The computational grid is excited by driving the initial transverse boundary with a Gaussian weighted (in space), raised cosine (in time) pulse:

$$H_y(x, z = 0, t) = H_0 \exp[-(x/w_0)^2] F(t), \quad (4.64)$$

where $F(t)$ is given by Eq. (4.52). The initial waist was taken to be $w_0 = 10.0 \mu\text{m}$. The Fourier transform of $F(t)$ is

$$\tilde{F}(\omega) = e^{i\omega T/2} \frac{\sin[(\omega/\omega_0)\pi]}{\omega} \frac{1}{1 - (\omega/\omega_0)^2}. \quad (4.65)$$

The pulse length was taken to be $T = 20.0 fs$. Thus, the 6-dB amplitude roll-off point of this spectrum is located at $\omega = \omega_0$ or $f_0 = 1/T = 5.0 \times 10^{13} Hz$ ($\lambda_0 = c/f_0 = 6.0 \mu m$). The frequency $1/e$ roll-off point is at $f \approx 1.18 f_0 = 5.9 \times 10^{13} Hz$. The first null in this spectrum occurs at $\omega = 2\omega_0$ or $f = 1.0 \times 10^{14} Hz$. The initial pulse actually contains wavelengths of relevance which range (in free space) from more than $10.0 \mu m$ to less than $1.0 \mu m$. We note that the choice of the initial pulse is arbitrary; any continuous, finite time pulse can be used with the FDTD approach as long as the spatial and temporal resolution is chosen sufficiently to capture the relevant physics. If the medium were simply a nonlossy dielectric, the numerical Maxwell's equations solver would then generate and numerically simulate the propagation of a pulsed Gaussian beam whose initial waist is defined by the Gaussian weighting function.

Because this input pulse is very narrow and, hence, has a broad frequency bandwidth, the estimate of the location of the nonlinear focus and the associated focused beam waist cannot be obtained with the standard formulae discussed in Sec 4.2 since a unique choice of wavelength or frequency can not be made. Moreover, the nonlinear medium will drastically change the propagation speeds of these various frequency components, hence, the actual wavelengths in the medium. In addition, as discussed in Chap 2, recent results [29] for the propagation of ultra-wide bandwidth pulsed Gaussian beams have shown that the intensity and energy profiles of the beam are not the same. Thus some care must be exercised to determine the critical focal distance and electric field strength in the short pulse case.

For the simulation runs we set the nonlinear medium parameter to the value $n_2 = \epsilon_2/(2n_0) = 1.0 \times 10^{-18} (m^2/V^2)$, where $n_0 = 1.0$, and set the input electric field am-

plitude to $E_0 = 18.25 \times 10^8 (V/m)$. We note that the index of refraction choices do not correspond to a particular material, but they are chosen simply as a representative case. It would be a straightforward matter to tailor the problem to specific materials. The calculation is simply limited by the amount of available computer memory. With the resources available to us, these values simplified the analysis of the results and insured that the focusing would occur near the center of the computational grid.

The effective frequency of the excitation pulse, which has been shown²³ to be a good measure of the frequencies involved in the diffraction process for a broad bandwidth pulse, is $f_{rad} = f_0/\sqrt{3} = 2.89 \times 10^{13} Hz$; the corresponding free space wavelength $\lambda_{rad} = 10.39 \mu m$. The associated Rayleigh distance for an aperture driven raised cosine pulsed beam is then

$$L_R = \frac{\pi w_0^2}{\lambda_{rad}} = 30.24 \mu m, \quad (4.66)$$

which has been confirmed by numerical simulation [29].

The numerical study of the self-focusing problem consists of a two dimensional Gaussian beam incident on a Kerr medium with a non-instantaneous relaxation time. The variable parameters are beam power (proportional to the waist size intensity-on-axis product), pulse width to response time ratio, and the choice of mode set, TE_z or TM_z . A respectable number of permutations on the self-focus theme have been explored here but by no means has a thorough study of all the available parameter variations been made.

6. Theoretical model of PG beam self-focus

If a narrow bandwidth signal with amplitude E_0 , initial waist w_0 , and center

frequency f_{rad} propagates in a nonlinear medium, its self-focusing distance is then $\sim (E_{cr}/E_0) L_R$, where in the instantaneous response regime

$$E_{cr} = (n_2/n_0)^{-1/2} \lambda_{rad}/[\pi w_0] = 3.307 \times 10^8 \left(\frac{V}{m}\right) \quad (4.67)$$

is the critical field amplitude. Thus, with the indicated parameters, the self-focusing distance would be $5.48 \mu m$. This result was found in Sec. 7 to be a large underestimate of the critical nonlinear self-focusing distance. We found that the following reasoning provided a better estimate in the pulse case.

Self-focusing occurs because of changes to the index of refraction of the medium, hence, the speed of propagation and wavenumbers in that medium. The distance over which the focusing process occurs changes by varying the field strengths, but the time for it to occur does not. Thus, the focusing should occur at the time

$$\tau_R = \frac{L_R}{c} = \frac{\pi w_0^2}{c \lambda_{rad}} = 100.8 \text{ fs} , \quad (4.68)$$

Moreover, the intensity pattern of the raised cosine beam does not expand at the CW rate: $\theta_{int}^{CW} = \lambda_{rad}/[\pi w_0]$, but rather at the rate:

$$\theta_{int} = 8.317^\circ \approx 0.439 \frac{\lambda_{rad}}{\pi w_0} , \quad (4.69)$$

the specific value having been obtained here numerically as in chapter 2. The critical focal distance is then more appropriately defined by

$$z_{cr} \approx \frac{w_0}{\theta_{int}} = 68.89 \mu m , \quad (4.70)$$

which takes into account the actual beam spread rate. Therefore, we expected the critical focus in the instantaneous response cases to occur at

$$z_f = \left(\frac{E_0^{cr}}{E_0} \right) z_{cr} = 12.48 \mu m. \quad (4.71)$$

Since a portion of the pulse would not experience the nonlinearity in a finite response time case, we expected the critical focus distance to be bound by the value z_f and the value $cT_R = L_R$.

7. TM_z simulation

Several TM cases were considered by varying the medium response time τ with respect to the input pulse width T . In particular, we ran cases with $T = 0.2 \tau$, $T = 2.0 \tau$, $T = 5.0 \tau$, and $T = 20.0 \tau$, i.e., $\tau = 100.0 fs$, $\tau = 10.0 fs$, $\tau = 4.0 fs$, and $\tau = 1.0 fs$, respectively. These choices provided access to the nonlinear phenomena associated with mediums exhibiting slow to almost instantaneous response times.

Several grid sizes have been used to test the numerical stability and accuracy of the approach. Direct comparisons were made between simulations with a 600×800 grid, where $\Delta x = \Delta z = 0.05 \mu m$ or $30.0 \mu m \times 40.0 \mu m$, and a 1500×2000 grid, where $\Delta x = \Delta z = 0.020 \mu m$ or $30.0 \mu m \times 40.0 \mu m$. These discretizations provided a spatial resolution of $\Delta z = \lambda_0/120$ and $\Delta z = \lambda_0/300$, respectively. The coarser resolution was adequate to minimize the numerical dispersion effects in the cases treated; the finer grid simply reduced them further. A Courant stability condition (the time step must be chosen for a two-dimensional problem with $\Delta x = \Delta z$ so that $\Delta t \leq \Delta z/\sqrt{2}c$) of $\Delta z/c\Delta t = 0.38$ was maintained in both cases; this means we chose $\Delta t = 0.045 fs$ and $\Delta t = 0.018 fs$, respectively. The enhanced spatial resolution provided a better resolution of the very sharp field patterns that are formed in the focal regions and

reduced the numerical noise. The algorithm did not model the physics well when it was run at the linear equation Courant limit, but did for values $\Delta z/c\Delta t \leq 0.50$. The nonlinear version of the Courant limit is not known at this time. With four unknowns and additional overhead, the corresponding total memory requirement was approximately 3.0 *MWords* and 10.0 *MWords*, respectively. The time requirement is proportional to the number of unknowns and the number of time steps. The 10.0 *MWords* problem took approximately 510 CONVEX/240 cpu minutes to compute 7550 time steps, approximately 0.5 μs per unknown. In terms of the problem parameters, this corresponds to the pulse propagating $40 \mu m \sim 7 cT$ with a resolution of 240 cells over the spatial pulse width $cT = 6.0 \mu m$.

We found that the self-focusing distance Z_{sf} , i.e., the axial distance to the point where the maximum intensity occurred, was between z_f and L_R . However, in each case the time at which the focusing occurred for the cases considered was approximately $\sim T_R \approx 100.0 fs$. The actual self-focus distance was very dependent upon the ratio T/τ . For $T = 0.2\tau$, the distance $Z_{sf} \sim 24.0 \mu m$; for $T = 2.0\tau$, $Z_{sf} \sim 19.8 \mu m$; for $T = 5.0\tau$, $Z_{sf} \sim 17.1 \mu m$; and for $T = 20.0\tau$, $Z_{sf} \sim 14.2 \mu m$. As noted above, the focus locations are drastically different between each of the cases because the wave speeds in their nonlinear regimes are very different. Their distances are only accurate to within $\pm 0.45 \mu m$ corresponding to the output frame time spacing of 1.5 fs that we chose.

We note that, as anticipated from the full-wave, vector analysis, we found that the self-focusing is restrained by the generation of the longitudinal field component and the associated transverse power flow and by reflections from the waveguiding region. The augmented Helmholtz scalar models also predict that the beam does not experience any catastrophic focusing, i.e., does not focus to a point [25]. This is achieved by the removal of higher wavenumber components and these models do not

take into account the important energy transfer mechanisms between the transverse and longitudinal field components which occurs during self-focusing. The FDTD approach however, does not depend upon nonphysical loss mechanisms to limit the self-focusing and it incorporates all beam angles and models the physical flow of power in all directions.

The $T = 0.2 \tau$ case is a representative ultra-slow medium relaxation problem. It illustrates the behavior that sub-femtosecond pulsed laser beams, when they become available, will exhibit when they interact with the electronic properties of a material. Because the pulse width is shorter than the relaxation time of the medium, the medium does not have adequate time to respond to the presense of the pulse. Consequently, the front part of the pulse propagates in the medium as a linear beam. Because of this, one finds nonlinear decay, not growth on the front edge of the pulse. The build-up of the nonlinearity occurs in the rising portion of the pulse causing nonlinear tail effects on the back side of the pulse. The pulse then experiences a mild shock formation with a corresponding creation of a set of up-shifted (anti-Stokes) frequency components as it passes into the negative resistivity region. Focusing occurs to a waist (defined by the minimum width for the contour representing $1/e$ of the value on axis) of $3.05 \mu\text{m}$ for the intensity, $5.05 \mu\text{m}$ for the total field energy. The pulse breaks-up into two packets: the front lobe being broader, hence, consisting of the lower frequencies; the back lobe being compressed and including the higher, nonlinearly generated frequencies. The front lobe components travel at rates of speed different from the rear lobe because they see a linear rather than a nonlinear medium. The distance between the intensity peaks of these lobes at the time of maximum focus is $\sim 4.0 \mu\text{m}$; the front lobe intensity half-width is $\sim 6.0 \mu\text{m}$ and the back lobe is $\sim 1.1 \mu\text{m}$. The intensity peaks have approximately the same value, the trailing peak being ~ 1.4 times as large as the leading peak. There

is a correspondingly large growth in the longitudinal E_z field component where the null between the lobes in the transverse field components E_x and H_y occurs. It has its peak value off-axis at $x = 5.2 \mu\text{m}$. There is no noticeable reflection out of the focusing region since the medium responds so slowly that the nonlinear channel formation occurs very gradually. Rather, the back lobe forms and follows behind the front lobe which is diffracting linearly.

The remaining TM cases include response times on the order of or shorter than the pulse. These cases represent fast to almost instantaneous problems. Thus, they are more amenable to comparison with most of the scalar model results and are more accessible to experimental verification. When $T = 2.0 \tau$, we find that the medium responded to the pulse in a fashion similar to the $T = 0.2 \tau$ case, but more quickly. Focusing occurs to a waist of $1.25 \mu\text{m}$ for the intensity, $5.0 \mu\text{m}$ for the energy. Again, the front edge of the pulse acts in linear manner, i.e., responds to the presence of a linear medium; the build-up of the nonlinearity occurs on the rising portion of the pulse. The pulse then exhibits a strong shock formation as it passes through the negative resistivity region with a corresponding creation of a set of up-shifted (anti-Stokes) frequency components. The distance between the intensity peaks of the front and back lobes is now $\sim 1.1 \mu\text{m}$; the front lobe intensity half-width is $\sim 6.2 \mu\text{m}$ and the back lobe is $\sim 0.8 \mu\text{m}$. The back lobe exhibits a slightly higher intensity value than the front lobe, approximately 5.9 times as large. The back lobe develops within a shorter distance since the medium is responding more quickly to the large field enhancements. The lower frequency components remain with the front lobe; the higher frequency components get channeled to the rear lobe. We see a strong growth of the longitudinal component at the cost of the transverse components; and we begin to see some reflection of some longer wavelength components out of the focus region. In the focal region, the longitudinal component has a maximum at

$x = 0.72 \mu m$. The peak value of $|E_x|$, 1.09×10^9 (V/m), is 3.30 times the critical value and 3.52 times larger than the peak value of $|E_z|$. There is a corresponding growth in the transverse power flow S_x in the focus region.

Typical results for the $T = 2.0 \tau$ case are shown in Figs. (4.9-16) Plots of the $1/e$ -profiles of the electric field intensity $I = |E_x|^2 + |E_z|^2$ and the total field energy density integrated along the z -axis: $\int dz \{ \frac{1}{2} \epsilon_{eff} [|E_x|^2 + |E_z|^2] + \frac{1}{2} \mu_0 |H_y|^2 \}$ versus time are given in Fig. (4.9). Note that the initial $1/e$ -intensity waist is $7.07 \mu m$, corresponding to the initial amplitude waist $w = 10.0 \mu m$. As indicated, the intensity profile is much narrower than the energy profile. This results from the spreading of the energy throughout space-time from the focusing process. The intensity is merely a point quantity in any transverse plane; the energy is an average value of the intensity in time. The energy profile is smoother than the intensity curve because it is an average in space of the signal intensity. The initial growth in the profiles occurs because the search for the values occurs over the numerical simulation volume, not including the initial boundary values.

Consider Fig. (4.10) where the intensity of the transverse electric field component $|E_x|^2$ along the propagation axis is given at the time $t = 103.0 fs$ corresponding to when the maximum intensity focus occurs. As shown in this figure, the pulse gradually forms a horn pattern with the shock at the tail as predicted by Reintjes, Carman, and Shimizu for a pulse in the presence of a nonlinear medium in the absence of linear dispersion. The early part of the pulse diffracts as if the medium were linear. This behavior is characterized by the gradually increasing front lobe (in distance this is the largest z -value portion of the plot) shown in Fig. (4.10); the intensity increases in the linear area towards the back of the pulse and the nonlinear region. There is significant distortion of the pulse, resulting in a pulse which is significantly shorter in the high-intensity region than the input pulse dura-

tion. The high intensity region which is in the rear of the pulse is formed primarily by the nonlinear index change set up by the early portion of the pulse. Because there is no dispersion, an associated spectral asymmetry occurs and only up-shifted, anti-Stokes frequency components occur from the latter part of the focused pulse. Fig. (4.11) compares the power spectrum of the intensity $|E_x|^2$ shown in Fig. (4.10) to the power spectrum of the input signal. This illustrates the spectral asymmetry caused by the generation of only up-shifted, anti-Stokes frequency components which occurs in the latter part of the focused pulse.

A contour plot of the total electric field intensity $I = |E_x|^2 + |E_z|^2$ in the focal region shown in Fig. (4.10) is given in Fig. (4.12). One can see that the high intensity regions continuously radiate a significant amount of light away from them at large angles as they propagate. The front (large z) portion corresponds to the linear diffraction region; the rear (smaller z) portion incorporates the nonlinear effects. This is the horn pattern referred to in Sec. 3 of Chap. 4. Fig. (4.12), however, shows that the actual field structure is more complicated than the simple scalar equation picture and two field lobes are formed in the focal region.

The behavior of the longitudinal electric field component E_z is addressed specifically in Figs. (4.13) and (4.14). The maximum intensity of the longitudinal electric field component $|E_z|^2$ occurs off-axis along the axial slice $x = 0.72 \mu m$ and at a time that is slightly larger than the time $t \sim 103.0 fs$ when the transverse electric field component $|E_x|^2$ shown in Fig. (4.10) achieves its maximum. A plot of $|E_z|^2$ along the axial slice $x = 0.72 \mu m$ when it achieves its maximum is given in Fig. (4.13). A contour plot of the $|E_z|^2$ intensity field at the same time is shown in Fig. (4.14). With the corresponding plots of the electric field intensity given in Figs. (4.10) and (4.11), one sees that E_z has grown out of the noise in the transition layer to the negative resistivity region. Moreover, one can see a second peak in the longitudinal

field component appearing. The energy that gets transferred out of the focus to the longitudinal field component provides the energy for the next focus. This longitudinal field component behavior is unavailable from the scalar models. Its presence is necessary to produce waveguiding conditions in the nonlinear focal region that satisfy Maxwell's equations.

The corresponding axial power density $S_z = E_z H_y$ values along the propagation axis are shown in Fig. (4.15). A slight negative component occurs in the region of the back lobe. Its shape indicates that it consists essentially of low frequency, longer wavelength components that have been reflected back from the waveguiding region. As the leading portion of the pulse transitions through the focal region, there is an associated π phase change in the transverse electric field component which provides this sign change. These negative values of the z -directed power of the power flow increase (see Fig. (4.22) below) as the response becomes more instantaneous; the channel forms faster causing the reflection coefficients from the channel to increase. In general, scalar models such as (4.27) do not model this back reflection because in the SVEA, propagation occurs in only one direction.

Similar to Feit and Fleck's [2] nonparaxial algorithm for the Helmholtz equation the FDTD approach is valid for wide-angled beams. In contrast, it accounts for the large wavenumber components which are lost by their algorithm when self-focusing is developing. No unnecessary evanescent waves are introduced; hence, there is no nonphysical loss of power associated with those nonpropagating waves. However, the full-wave, vector algorithm does show the anticipated [2] reduced power transmission in the forward direction which is accompanied by radiation scattered from the nonlinear focal region and the conversion of energy between the transverse and the longitudinal field components. This produces the reduced power results from the change in the field patterns as the process of the pulse

focusing, separating, and defocusing repeats itself. It produces the splitting of the field pattern into the linear and nonlinear lobes, causing less energy to be available in any of the lobes in the next focus region. This effective splitting of the pulse is illustrated in Fig. (4.10). The loss of energy during the focusing process to the nonlinear conductivity term is shown in Fig. (4.16). The total field energy density $\frac{1}{2}\epsilon_{eff}[|E_x|^2 + |E_z|^2] + \frac{1}{2}\mu_0|H_y|^2$ integrated over the spatial band (a) $(x, z) \in [0.0, 1.2 \mu\text{m}] \times [0.0, 40.0 \mu\text{m}]$, and over the larger spatial band (b) $(x, z) \in [0.0, 2.4 \mu\text{m}] \times [0.0, 40.0 \mu\text{m}]$, and then normalized by the area of those bands, is given versus time. After the initial rise of the average field energy in those bands as the pulse enters the simulation volume, there is a gradual decrease in the field energy as the pulse transitions into the negative conductivity region. There is an increase of the average energy in the band closer to the axis in the focal region with a corresponding decrease in the larger band. In contrast to the corresponding figures in Ref. [2], there is not an abrupt loss of energy after the pulse passes through the focus; rather, there is a steady redistribution of energy back to the larger transverse distances as the pulse unfocuses and a loss of energy to the increased conductivity of the medium.

Fig. (4.17) is a time sequence of plots that illustrates the importance of the growth of the longitudinal field component in the self-focusing process. Contour plots of $|E_x|^2$ and $|E_z|^2$ and the on-axis distributions of the intensity $|E_x|^2$ and the power flux $S_z = E_z H_y$ are given at the times $t = 83.3 \text{ fs}$, $t = 96.6 \text{ fs}$, and $t = 109.9 \text{ fs}$ for the $T = 5.0\tau$ case. The first time set occurs long before the first main focus is reached; the second time set is just before the focus time $t \sim 100.0 \text{ fs}$; and the third time set is an equal interval after the focus. The longitudinal component E_z has reached a maximum off-axis value already in the first time set and, as the pulse propagates, acts as a catalyst for re-focusing some of the scattered field energy. The off-axis

field energy is also focused as the nonlinear channel grows. As the pulse approaches the true focal region where its waist reaches a minimum, the peak field pattern now exhibits the passage of the pulse through two transition regions. The latter one reflects the presence of the intensity focus, the former the initial transition into the negative conductivity region. Following the pulse evolution, the front portion of the pulse corresponds to the original nonlinear transition; the back portion to the focused field intensity. The benign region in between both sets simply corresponds to energy carried along with the pulse. The appearance of a second E_z peak is seen in the first time set. The growth of this second peak and the resulting changes in the transverse component are seen from the second set, particularly in the intensity of the transverse field component on-axis. Note that the power flux acquires negative values as the focal region is reached. In the third set one can see that a third lobe in the intensity has appeared because of the power which has reflected back out of the focal region. The large off-axis value of E_z is now causing the power to flow away from the focal region which will eventually feed the next focusing process when it experiences the next channel formation from the front part of the pulse.

When $T = 20.0\tau$ the medium is nearly into the instantaneous response regime. The $1/e$ -profiles of the electric field intensity and the total field energy along the z -axis are given in Fig. (4.18). Focusing occurs to a waist of $0.50\mu m$ for the intensity, $1.80\mu m$ for the energy. The field values have become slightly more noisy than the $T = 2.0\tau$ and $T = 5.0\tau$ cases since the spatial and temporal resolution has remained the same even though the rate at which changes occur has increased. The energy profile is smoother than the intensity's since it is obtained by averaging the intensities over time. The axial slice of the intensity of the transverse electric field $|E_x|^2$ at the focal region time $t = 97.0 fs$ is shown in Fig. (4.19); its power spectrum is compared with the input power spectrum in Fig. (4.20). The front part of the pulse still diffracts

linearly; however, the nonlinearity turns-on extremely fast (instantaneous regime) as soon as the pulse amplitude surpasses the critical value early in the computational grid. A corresponding increase in the generation of higher frequencies is observed by comparing Fig. (4.20) with Fig. (4.11). A very steep shock forms at approximately $6.2 \mu\text{m}$, the first transition into the negative conductivity region. Some reflections of the lower frequency components are observed from this initial transition region. The resulting pulse exhibits very strong tail erosion as the nonlinear conductivity increases quickly in strength. The peak value of $|E_x|$, $1.22 \times 10^9 \text{ (V/m)}$, is 3.70 times the critical value and 2.40 times larger than the peak value of $|E_z|$. The peak intensity value of the lagging peak is noticeably higher than the forward peak, approximately 2.6 times larger; it is approximately 5.4 times larger than the peak intensity in the linear region. The shape of the back portion of the central region is also very steep corresponding to the sharp turn-off of the nonlinearity. It occurs when enough energy has left the focal region due to the resulting transverse power flow and additional reflections from the nonlinear channel. There is a corresponding peak of E_z in the region near this rear transition. A plot of the intensity of the longitudinal electric field component $|E_z|^2$ in the focal region along the axial slice $x = 0.24 \mu\text{m}$ for the focal region time $t = 97.0 \text{ fs}$ is given in Fig. (4.21). The locations of the peaks of this component occur precisely where the derivative behavior in the transverse components are found. Again, the lack of beam focusing to a point can be readily connected to the appearances of these peaks; they correspond to energy taken away from the focal region and the axis of propagation. The power flux S_z when the focal time $t = 97.0 \text{ fs}$ is reached is shown in Fig. (4.22). The negative power flow is readily apparent now. As in the $T = 5.0\tau$ case shown in Fig. (4.17), the appearance of the small lagging lobe in Fig. (4.19) is caused by the negative power flow from the focal region. The total field energy density $\frac{1}{2}\epsilon_{eff}[|E_x|^2 + |E_z|^2] + \frac{1}{2}\mu_0|H_y|^2$ integrated over

the spatial band (a) $(x, z) \in [0.0, 1.2 \mu\text{m}] \times [0.0, 40.0 \mu\text{m}]$, and over the larger spatial band (b) $(x, z) \in [0.0, 2.4 \mu\text{m}] \times [0.0, 40.0 \mu\text{m}]$, and then normalized by the areas of those bands, is plotted versus time in Fig. (4.23). The significantly higher energy density near the axis in the focal region is illustrated with this figure. The loss of field energy to defocusing and to the lossy nonlinear medium occurs after the focal time $\sim \tau_R$ has been reached. In contrast to the results given in Ref. 2, the losses in Fig. (4.23) do not occur in steps. They are more gradual, particularly in the focal regions, because there are physical loss mechanisms present which provide the energy transfer to the medium.

We note that in the $T = 20\tau$ case, a phenomenon similar to the multiple self-focusing regions reported in Ref. 2 are observed. However, the physical picture now has a more complex interpretation than simply that the beam alternately contracts and expands between those focal regions. Each transition region causes sign changes in the field components and a power flow towards and away from the propagation axis which is facilitated by the presence of the longitudinal field component. At the tail of the pulse the flow is toward the axis such that an additional intensity peak is being formed. Then, as energy gets cycled to the region behind the pulse to become the next focal region, each successive intensity peak is lower because of this redistribution of the wave energy from the transverse to the longitudinal field components. Moreover, each successive peak travels at a slower rate of speed due to the ever increasing nonlinear dispersion which causes the various components to travel at slower rates of speed. We expect that the process must eventually self-limit itself as the peak intensity decreases below the nonlinear threshold.

8. TE_z simulation

The TE equation set does not exhibit the nonlinear energy transfer phenomena

associated with the longitudinal electric field component found in the TM system. Thus, we expected and found a quantitatively different behavior for the TE cases. Consider, for instance the TE case in which the input pulse width $T = 5.0 \tau$, where $\tau = 4.0 fs$. The on-axis values and a contour plot of the intensity $|E_x|^2$ of the transverse electric field component in the TM case are given in Figs. (4.24) and (4.25), respectively, for the focal time $t = 100.0 fs$. The corresponding $|E_y|^2$ plots for the TE case are shown respectively in Figs. (4.26) and (4.27). Although there is not a major difference in the peak intensity value, the pulse shapes and their locations and distributions are quite different between the two polarizations. The intensity shown in Fig. (4.24) exhibits the loss of energy to the longitudinal component on the rear portion of the pulse (z values between ~ 16 and $17 \mu m$). In contrast, the intensity shown in Fig. (4.26) is essentially uniform over the length of the original pulse which surpasses the critical field strength $\sim 3.5 \mu m$. This also explains the difference in the widths of the intensities in the focal regions. Notice that the focus in both the TE and TM cases occurs at the same time $t = 100.0 fs$ but not at the same axial distance. The TE case focuses at $\sim 15 \mu m$ while the TM case focuses at $\sim 17 \mu m$. Moreover, comparing the contour plots in Figs. (4.25) and (4.27), one finds that the field pattern is more diffuse in the TE case than it is in the TM case. This is simply due to the fact that there are no competing nonlinear mechanisms for the field energy in the TE case. Similar results were found for the other response times.

9. Back reflection and vortices in the wakefield of a self-focus

The vector FDTD approach has produced a physical picture of the nonlinear self-focus that includes some unexpected phenomena, 1) back reflection from the focal region and 2) the generation of optical wakefield vortices in the negative conductivity region following the focus. To the best of my knowledge, this is the first

time that these nonlinear characteristics of beam focusing have been modeled by any technique. Scalar models, which do not couple the transverse and longitudinal fields, are unable to show these effects because it is the transverse power flow which produces them.

Back reflection and vortex formation occur mainly in the nearly instantaneous regime where there can be a sharp shock in the medium and a region of high negative conductivity production at the tail of the pulse. Unlike the large longitudinal field produced at the front of the pulse which causes the beam to diffract, along the transition region from positive to negative conductivity there is a large longitudinal field generated with the opposite sign. Behind the focus, power flows backwards and in towards the axis to produce circulation. Vortices thus occur at the tail where the back reflected longitudinal power flow intermixes with the transverse power flow. This circulation is enhanced by the high negative conductivity present behind the focus in an instantaneous regime. The vortices grow at the expense of the pulse and when enough energy is circulated behind the pulse a second focus will occur. This sequence continues as long as enough energy is available in the focal region to produce the next focus. Eventually, unless linear dispersion causes it to do otherwise, the procreation of foci will tend to stretch the pulse spatially and temporally.

In all the simulations that were run in this research, additional foci production has always occurred with a great deal of overlap time with the proceeding focus. This can be described as being similar to a longer continuous focus. The focus however is actually moving in relation to the pulse front as the pulse propagates forward. The multiple focal regions are too close together to be measured as separate individual foci. If a alternate experiment was conducted such as one where the initial waist is made wider, the focusing and diffracting effects would be slowed and one

might see the nonlinear self-focus as series of discrete events rather than as one continuous focus.

Figures (4.28), (4.29), and (4.30) show the focal region of a pulse in an instantaneous regime ($T = .2\tau$). The initial transverse waist was taken to be $w_o = 10.0\mu\text{m}$. The total pulse width was 20.0fs and the input electric field was set at $E_o = 18.25 \times 10^8 (\text{V/m}) = 5.5 E_{\text{crit}}$. The initial pulse is the Gaussian tapered, raised cosine pulse given by Eq. (4.64). The longitudinal power flow $S_z = E_x H_y$ in this region is shown in Fig (4.28). Negative power flow occurs at the tail of the pulse where there is a region of high negative conductivity. This is the region where the electric field has dropped abruptly and, due to a finite lag in the medium, the nonlinear susceptibility has not yet responded; i.e., where $\chi^{NL}/[\epsilon_2|\mathbf{E}|^2] < 1$. Thus, power flows backward out of an intense electric field region and is nonlinearly enhanced by the gain of the medium. Part of the energy from this process goes into the next focal region and the rest feeds the vortices. The transverse power flow $S_x = -E_z H_y$ shown in Fig. (4.29) occurs at the back end of the pulse and is directed toward the axis. This flow is necessary to direct energy into a second focal region and produce growth. Meanwhile, in the horn region power is flowing away from the axis producing linear diffraction. The longitudinal and transverse power flows near the focus and in its wakefield are combined in Fig. (4.30). The resulting plot of the Poynting's vector $\mathbf{S} = E_x H_y \hat{z} - E_z H_y \hat{x}$ reveals both power reflection from the focus and vortex formation in the wakefield of the focus caused by the transverse power flow. Both processes remove power from the focal region. The power flow in the focus itself (not depicted) is an order of magnitude larger than the surrounding flows and is directed along the propagation axis and away from it. Since the vorticity is zero originally, the large negative (clockwise) vortex formed in the wakefield of the focus is compensated by the formation of many smaller positive vortices in the transition

layer between the positive power flow associated with the propagation of the pulse and the negative power flow in the wakefield of the focus.

Figure (4.1). The nonlinear index n_2 for single frequency as a function of τ . The other parameters are those used in the numerical simulations: $E_0 = 18.25 \times 10^8$ (V/m), $f_{rad} = 2.89 \times 10^{13}$ Hz, $\epsilon_2 = 2.0 \times 10^{-18}$, $n_b = 1.0$

Figure (4.2). The absorption coefficient α for a single frequency as a function of the $\omega\tau$ product. The frequency ω is normalized to the value $\omega = 1.0 \text{ rad/sec}$; the intensity $\epsilon_2|E_o|^2$ is also normalized (unitless).

Figure (4.3). Configuration for the self-focus problem.

Figure (4.4). Power threshold approximation for single frequency to self-focus a beam in the scalar field model. P_{th} is plotted as a function of τ . The other parameters are: $f_{rad} = 2.89 \times 10^{13} \text{ Hz}$, $\epsilon_2 = 2.0 \times 10^{-18} (\text{m}^2/\text{V}^2)$. The beam is initially focused onto the medium interface.

Figure (4.5). Focal distance approximation for single frequency to self-focus a beam. z_f is plotted as a function of τ . The other parameters are: $E_o = 18.25 \times 10^8 (V/m)$, $f_{rad} = 2.89 \times 10^{13} Hz$, $\epsilon_2 = 2.0 \times 10^{-18} (m^2/V^2)$, $n_b = 1.0$. The beam is initially focused onto the medium interface. The dot-dash line represents the maximum value of τ for which the approximation will focus.

Figure (4.6). Input pulse (4.60) used in the numerical simulations.

Figure (4.7). Exact nonlinear refractive index as a function of time for the input pulse used in the numerical simulations. $E_0 = 18.25 \times 10^8 \text{ (V/m)}$, $\epsilon_2 = 2.0 \times 10^{-18} \text{ (m}^2/\text{V}^2\text{)}$.

Figure (4.8). Exact nonlinear conductivity as a function of time for the input pulse for the numerical simulations. $E_0 = 18.25 \times 10^8 (V^2/m^2)$, $\epsilon_2 = 2.0 \times 10^{-18}$.

Figure (4.9). The $1/e$ -profiles of the electric field intensity $I = |E_x|^2 + |E_z|^2$ and the total field energy density integrated along the z -axis: $\int dz \frac{1}{2} \epsilon_0 f f [|E_x|^2 + |E_z|^2] + \frac{1}{2} \mu_0 |H_y|^2$ versus time are plotted for the $T = 2\tau$ case. The original intensity waist of the input pulse was $7.07 \mu m$.

Figure (4.10). The intensity of the transverse electric field component $|E_x|^2$ along the propagation axis is given for the $T = 2\tau$ case at the time $t = 103.0 fs$ when the maximum intensity focus occurs.

Figure (4.11). The power spectrum of the signal $|E_x|^2$ (shown in Fig. 2) along the propagation axis is given for the $T = 2\tau$ case at the time $t = 103.0 fs$ when the maximum intensity focus occurs. The power spectrum of the input pulse is given for comparison purposes.

Figure (4.12). A contour plot of $|E_x|^2 + |E_z|^2$ for the $T = 2\tau$ case at the time $t = 103.0 f_s$ when the maximum intensity focus occurs, shows the breakup of the pulse into two lobes, the null appearing in the transition to the negative resistivity region.

Figure (4.13). The intensity of the transverse electric field component $|E_z|^2$ along the axial slice $x = 0.72 \mu m$ is given for the $T = 2\tau$ case at the time $t \sim 103.0 fs$ when its maximum value occurs.

Figure (4.14). A contour plot of $|E_z|^2$ for the $T = 2\tau$ case at the time $t \sim 103.0 fs$ when its maximum value occurs, shows the appearance of its peak off the propagation axis in the region where the transverse field components exhibit a null.

Figure (4.15). The longitudinal power flow S_z along the propagation axis is given for the $T = 2\tau$ case at the time $t = 103.0 \text{ fs}$ corresponding to when the maximum intensity of the transverse field component E_x occurs.

Figure (4.16). The total field energy density $\frac{1}{2}\epsilon_{eff}[|E_x|^2 + |E_z|^2] + \frac{1}{2}\mu_0|H_y|^2$ integrated over the spatial band (a) $(x, z) \in [0.0, 1.2\mu m] \times [0.0, 40.0\mu m]$, and over the spatial band (b) $(x, z) \in [0.0, 2.4\mu m] \times [0.0, 40.0\mu m]$, and then normalized to the areas of those bands are plotted versus time for the $T = 2\tau$ case.

Figure (4.17a)

Figure (4.17a-c). Contour plots of the intensities $|E_x|^2$ and $|E_x|^2$ and plots of the on-axis intensity $|E_x|^2$ and the power flow density $S_z = E_x H_y$ are given for the $T = 5\tau$ case at the times (a) $t = 83.3 fs$, (b) $t = 96.6 fs$, and (c) $t = 109.9 fs$.

Figure (4.17b)

Figure (4.17c)

Figure (4.18). The $1/e$ -profiles of the electric field intensity $I = |E_x|^2 + |E_z|^2$ and the total field energy density integrated along the z -axis:

$\int dz \frac{1}{2} \epsilon_{eff} [|E_x|^2 + |E_z|^2] + \frac{1}{2} \mu_0 |H_y|^2$ versus time are plotted for the $T = 20\tau$ case. The original intensity waist of the input pulse was $7.07 \mu m$.

Figure (4.19). The intensity of the transverse electric field component $|E_x|^2$ along the propagation axis is given for the $T = 20\tau$ case at the time $t = 97.0 fs$ when the maximum intensity focus occurs.

Figure (4.20). The power spectrum of the signal $|E_x|^2$ (shown in Fig. 11) along the propagation axis is given for the $T = 20\tau$ case at the time $t = 97.0 fs$ when the maximum intensity focus occurs. The power spectrum of the input pulse is given for comparison purposes.

Figure (4.21). The intensity of the transverse electric field component $|E_x|^2$ along the axial slice $x = 0.24 \mu m$ is given for the $T = 20 \tau$ case at the time $t \sim 97.0 fs$ when its maximum value occurs.

Figure (4.22). The longitudinal power flow S_z along the propagation axis is given for the $T = 20\tau$ case at the time $t = 97.0 fs$ corresponding to when the maximum intensity of the transverse field component E_x occurs. The negative power flow from energy reflected from the focal region is apparent.

Figure (4.23). The total field energy density $\frac{1}{2}\epsilon_{eff}[|E_x|^2 + |E_z|^2] + \frac{1}{2}\mu_0|H_y|^2$ integrated over the spatial band (a) $(x, z) \in [0.0, 1.2\mu m] \times [0.0, 40.0\mu m]$, and over the spatial band (b) $(x, z) \in [0.0, 2.4\mu m] \times [0.0, 40.0\mu m]$, and then normalized by the areas of those bands is plotted versus time for the $T = 20\tau$ case.

Figure (4.24). The intensity of the transverse electric field component $|E_x|^2$ is given for the $T = 5\tau$, TM case at the time $t = 100.0 fs$ when the maximum intensity focus occurs.

Figure (4.25). A contour plot of $|E_z|^2$ for the $T = 5\tau$, TM case is given at the time $t = 100.0 \text{ fs}$ when its maximum value occurs.

Figure (4.26). The intensity of the transverse electric field component $|E_y|^2$ is given for the $T = 5\tau$, TE case at the time $t = 100.0 f_s$ when the maximum intensity focus occurs.

Figure (4.27). A contour plot of $|E_y|^2$ for the $T = 5\tau$, TE case is given at the time $t = 100.0 f_s$ when its maximum value occurs.

Figure (4.28). Negative longitudinal power flow occurs in regions where the conductivity of the medium is increasing rapidly. Positive longitudinal power flow occurs in the negative conductivity regions where field growth occurs. This is illustrated with a contour plot of the longitudinal component of Poynting's vector S_z in the focal region for the $T = 20r$ case.

Figure (4.29). Transverse power flow occurs in regions where the longitudinal field component is not small. The flow of power away from the propagation axis is intense near the horn region where linear diffraction dominates and in the focus itself. The flow of power is towards the propagation axis in the focal region where self-focusing occurs. The transverse power flow is illustrated with a contour plot of the transverse component of Poynting's vector S_x in the focal region for the $T = 20\tau$ case.

Figure (4.30). A plot of Poynting's flux vector field $\vec{S}$ in the self-focusing region for the $T = 20\tau$ case reveals both power reflection from the focus and vortex formation in the wakefield of the focus caused by the transverse power flow. Both processes remove power from the focal region. The power flow in the focus itself (not depicted) is an order of magnitude larger than the surrounding flows and is directed along the propagation axis and away from it.

CHAPTER 5

SHORT PULSE BEHAVIOR AT A LINEAR/NONLINEAR
INTERFACE AND NONLINEAR SWITCHES

In this chapter we discuss the characteristics of the response to a PG Gaussian beam incident on a nonlinear medium. In section 1 we present the plane wave theory for reflection and transmission of light at a linear/nonlinear interface. Numerical results are also presented for a PG beam incident normally on a nonlinear medium and comparisons are made with theoretical and numerical reflection and transmission coefficients. In section 2 we attempt to produce an optical switch by exciting a well-focused beam at an incidence angle near the critical angle. However, it will be shown that this does not produce an effective switch. An improvement on the optical switch theme is made in section 3 by using a slab waveguide excited with a pulsed waveguide mode. This configuration is analyzed with numerical simulations and typical results are presented.

1. Nonlinear reflection for normally incident beams

Up to this point our attention has been focused primarily on the development of the vector FD-TD technique applied to nonlinear media. By modeling the self-focus phenomena we have shown in great detail a variety of physics that could not easily have been demonstrated otherwise. However, we have overlooked another advantage that the vector FD-TD approach has over most scalar methods: its ability to model complex structures. The next step is therefore to demonstrate that this technique is useful in modeling simple or complex geometries of linear and nonlinear media for which the scalar models are inadequate. In particular, standard scalar methods such as the beam propagation approach are designed to model propagation in only one direction. Any interface problem then poses a severe limitation of these techniques.

In contrast, to incorporate inhomogeneous media into the vector FD-TD solver is a trivial step that requires no extra memory or run-time. We will therefore exploit this advantage by modeling pulsed waves in some simple devices that include both linear and nonlinear regions.

The FD-TD mesh facilitates the construction of arbitrary structures in the problem space. Because space is divided into many independent cells, the cells can contain any desired property. Moreover, the electrical properties in each cell can be specified independently of any other cell. We consider four devices which consist of simple geometries; either a planar boundary or slab waveguide in which the nonlinearity changes the reflecting or guiding properties.

The first geometry is the simple case of an interface between a linear and a nonlinear region arranged such that the beam is incident from the linear region and arrives at an angle normal to the plane dividing the two regions. Figure (5.1) gives the problem space structure. The beam is a PG beam that is similar to the one used for the self-focusing simulation; however, the pulse in this case is modified from the original raised cosine function to a seventh order polynomial bipolar pulse. This is done in order to enhance the accuracy of the tail of the pulse when generating the source field on the simulation boundary. The time history of the source is now given by the function

$$F(t) = x(1 - x^2)^3 \theta(1 - |x|) \quad ; \quad x = \frac{2t}{T} - 1 \quad (5.1)$$

which is continuous (zero) and has continuous (zero) first and second derivatives at $x = \pm 1$. The effective wavelength λ_{eff} has been determined numerically for this pulse. It is .537 times the pulse length or, for this case, $3.22\mu m$. This function, shown in Fig. (5.2), is superior to the raised cosine in that it has continuous first

and second derivatives at the turn on and turn off points. Consequently, it is a smoother function than the raised cosine and generates little noise on the tail of the pulse as it is launched into the simulation volume. The dimensions for this problem are also similar to the self-focus problem: the discretization $\Delta x \equiv \Delta z \equiv .02 \mu m$ and the Courant condition remains 0.38 giving $\Delta t = 0.018 fs$. The dimensions of the box are $30.0 \mu m \times 40.0 \mu m$ corresponding to a total number of 1500×2000 cells. The period of the pulse is again $20.0 fs$ although the equivalent wavelength is now shorter than for the raised cosine with the same period. The initial beam waist is still $10.0 \mu m$. Placement of the interface at $15.0 \mu m$ from the source plane allows the beam to diffract prior to interacting with the boundary. This also provides adequate separation distance between the reflected and transmitted pulses.

The single frequency plane wave version of the normal incidence problem has an exact solution. The reflection coefficient for power is given by

$$|\Gamma|^2 = \left| \frac{n_{l2} - n_{l1}}{n_{l2} + n_{l1}} \right|^2 \quad (5.2)$$

where n_{l1} and n_{l2} represent the linear refractive indexes in regions 1 and 2 respectively. Since the index in the linear medium is given and the index in the nonlinear medium is a function of electric field intensity, $|E_o|$, and relaxation time, τ , as given by the relation (4.19), we can predict the exact reflection coefficient as a function of intensity for a CW plane wave at this interface. It is common practice to substitute the real approximation (4.21) for the complex relation to simplify equations involving the nonlinear coefficients. Replacing n_{l1} with 1.0 and n_{l2} by $1.0 + n_2|E_o|^2$ we obtain

$$|\Gamma|^2 \simeq \frac{n_2 |E_o|^2}{2 + n_2 |E_o|^2}. \quad (5.3)$$

This approximation to the reflection coefficient is shown in Figs. (5.3) and (5.4). The parameters used for the generation of Fig. (5.3), a plot of Eq. (5.3) as a function of E_o , are $\omega = \omega_{eff} = 5.85 \times 10^{14} \text{ rad/sec}$, $\tau = 4.0 \text{ fs}$, and $\epsilon_2 = 2.0 \times 10^{-18} (\text{m}^2/\text{V}^2)$. To produce Fig. (5.4), a plot of Eq. (5.3) versus τ , we used the same values of ω and ϵ_2 in Fig. (5.3) with $E_o = 46.9 \times 10^8 (\text{V/m})$.

The simulations were made with two variations in the relaxation time τ and one variation in the field intensity E_o . The first case was made with the maximum field amplitude of $E_o = 46.9 \times 10^8 (\text{V/m})$ and $\tau = 4.0 \text{ fs}$. The second case was characterized by reducing the maximum field amplitude to $E_o = 9.37 \times 10^8 (\text{V/m})$ and slowing slightly the medium relaxation time to $\tau = 5.0 \text{ fs}$. The third case is a beam of the same amplitude as the first case but with the medium being characterized by a much slower response time of $\tau = 40.0 \text{ fs}$. From the results of these three simulations, we obtained the corresponding reflection coefficients and focal aspects. Table (5.1) presents the results for these three cases.

Figures (5.5)-(5.8) pertain to case 1. Figure (5.5) is a contour plot showing transmitted and reflected pulses following the interaction with the nonlinear boundary. The nonlinear reflection coefficient was found by integrating $\epsilon_{eff}/2 [|E_x|^2 + |E_z|^2]$ in both regions giving $\Gamma = .239$, shy of the plane wave result $\Gamma = .54$. The beam power in this case is substantially above the critical power and, consequently, we see a very steep shock forming at the tail almost immediately. The waist of the beam where it interacts with the boundary is $7.7 \mu\text{m}$, and it has a peak intensity of $2.2 \times 10^{20} (\text{V}^2/\text{m}^2)$. The transmitted beam then propagates into the medium and subsequently undergoes a nonlinear collapse, eventually self-focusing to a waist

size of $3.8\mu m$ and a peak intensity of $2.4 \times 10^{18} (V^2/m^2)$ at about $28.7\mu m$ from the source plane. This is followed by beam diffraction, as illustrated by Fig. (5.6). Figure (5.7) shows the energy of the beam near the axis as the beam propagates forward in time. The sharp spikes on this curve are a result of the electric field in the pulse interfering with its reflection off the boundary. The second set of spikes corresponds to the reflected wave re-reflecting off the source boundary. The third set corresponds to the reflected pulse interacting with the nonlinear interface for the second time. The third set of spikes is smaller than the previous two because there is now less power to cause any reflections and because the beam has now spread slightly as a result of linear diffraction. There is significant attenuation of the beam energy near the axis in the direction of propagation. This is despite the fact that the beam is focusing and hence is adding energy to the region near the axis. This is due to energy saturation in the medium and to the loss of a majority of the energy due to diffraction out of the nonlinear channel; i.e., pulse widening in the front of the horn region. A contour of the intensity of the E_x field near the focal region, given in Fig (5.8), shows the front of the pulse diffracting while the tail reduces to a very small, intense spot.

The forward horn pattern postulated by Shen is again clearly reproduced by the fields in the focal region. However, as we saw previously, there is much more detail in the vector model. Many high intensity regions are found along the axis in the focal region, all in different stages of focusing or de-focusing. The initial portion of the pulse is only moderately affected by the nonlinearity, but it is this part of the pulse which is responsible for creating the initial nonlinear channel. The longitudinal component of the electric field E_z is generated and amplified in the rear of the front part of the bipolar pulse since it is coupled to the strong transverse component due to the negative resistivity region. This process feeds more energy to the second half

of the bipolar pulse. Once the first half of the bipolar pulse has focused and has begun to diffract, the second half begins to form its own channel and self-focuses. The focusing of the first half of the pulse goes unnoticed because the collapse of the second half is much more intense and dramatic. The shock associated with the second region is more intense due to increased energy distributed in the stronger channel. As the tail of the pulse continues to focus, energy is cycled behind the pulse into the channel to create an even sharper focus. The process repeats as long as there is enough energy left in the beam to feed more focal regions. The waist size decreases at a more or less constant rate through each subsequent foci. However, each of these foci dilute the available energy, and eventually the waist reduction cycle must stop. The beam then spreads at approximately the rate at which it focused as linear diffraction effects begin to dominate.

Case 2 represents a medium that is slightly more retarded than case 1. The Parameters for this trial are: $\tau = 5.0fs$, an increase by a factor of 1.25 from case 1, and $E_o = 9.37 \times 10^8 (V/m)$, a reduction from case 1 by a factor of 5.0. The reflection coefficient for this case is only .00853 as opposed to the previous .239, a factor of 28.0 times less. The $1/e$ energy waist is shown as a function of time in figure (5.9). As expected the focal waist size is only slightly larger than for the previous case. The rate of focus however is about $1/2$ the previous rate because the focus occurs further out at a distance of $37.0 \mu m$ as opposed to the previous distance of $28.7 \mu m$. The energy in the focal region is contained in three lobes, the third having been generated by the nonlinear coupling of energy into the longitudinal field components. Because the intensity in case 2 is lower, the longitudinal component is not coupled to the transverse field as strongly as it was in case 1. Thus, the energy did not cycle as quickly into the next lobe. The contour of the electrical intensity at maximum focus in case 2 is shown in figure (5.10). The diffraction rate following

self-focusing in case 2 is more subtle than in case 1 because the focal region is now wider than it was in the previous case. Figure (5.11) shows the beam energy in a $1.2\ \mu m$ slab along the axis. The peak corresponding to the focusing of the beam is more prominent than in case 1 because the nonlinear loss is not as high.

Case 3 shows the effect that reducing the relaxation time of the medium has on the reflection coefficient. The pulse from case 1 (fast response time) is reproduced in a medium with $\tau = 40.0\ fs$. The beam for this case propagates into the nonlinear medium with almost no initial interaction with the medium, self-focuses to relatively large spot size focus containing three lobes, and then diffracts at about the same rate at which it focused. The reflection coefficient for this case turns out to be $\Gamma = .0862$ which is a dramatic reduction from the reflection coefficient found in case 1 as well as being well above the plane wave result. The slower response time causes the nonlinear increase in refractive index to occur more slowly. Hence, the reduced reflection coefficient demonstrates that reflection from a shallowly graded or slowly increased refractive index is less than it is from a steeply graded or quickly increased refractive index. The maximum focus waist occurs at about $15.6\ \mu m$ from the interface and is $4.55\ \mu m$ wide. The reason that the focused pulse contains three lobes instead of four and is wider than the minimum waist in case 1 is because the ratio T/τ has been reduced by a factor of 10. Recall from Chap. 4 that this ratio determines the severity of the shock front and the magnitude of the negative conductivity (gain) region. This was illustrated in Figs. (4.7) and (4.8). Because there is less gain in the region of longitudinal field production, we expect there to be less cycling of energy to the additional focus (foci) trailing the pulse. Thus, there will be fewer foci, a wider nonlinear channel, and a larger waist size for the maximum focus. The $1/e$ beam waist for case 3 is shown as a function of time in Fig (5.12).

2. Optical threshold for obliquely incident finite PG beams

The modeling of a Gaussian beam normally incident on a linear/nonlinear interface is just one simple example of the device application modeling capabilities of the vector FD-TD approach. A more complicated problem is created when we introduce an incident beam angle other than normal (zero degrees). The goal in this oblique incidence case becomes to invent a system which allows a finite PG beam to either only reflect or transmit contingent exclusively on the electric field intensity of the beam. This type of threshold device is analogous to an electrical diode and could be useful as a high speed optical on/off switch. One can then make a strong case for modeling such a device. In particular, the many wave vector components of a tightly focused beam and the multi-dimensionality of such a problem require a more complete analysis than most scalar models can provide. Because the vector FD-TD technique is a complete vector model, it seems that it would be a good method for modeling the wide range of wave vectors contained in a tightly focused, strongly diffracting beam and for describing the consequence of placing a sharp index step at an oblique angle to the propagation direction.

The basic geometry of this device is a refractive index discontinuity at the interface of two transparent substrates with the incident substrate having the slightly higher index. A beam is then designed to be incident on the interface plane in a condition of total reflection, i.e. at an angle slightly greater than the critical angle as given by Snell's law. Then, by adding a positive Kerr law nonlinearity to the medium on the transmitted side of the interface, the total refractive index can be increased by the intensity of the beam and thus increasing the critical angle or even making it nonexistent (i.e., by creating a continuous index or a negative index step). The purpose for creating this condition is so that as soon as the beam intensity rises

above a threshold, transmission into the neighboring medium will begin. Ideally, when more of the beam has been transmitted into the second region, the intensity in this region will increase and, as a consequence, the index step and the interface will completely vanish. Total reflection at low power will suddenly become transparency at or above the threshold power. Figure (5.13) gives the geometry for the oblique incidence optical pulse diode.

It has been shown previously that at high intensities, a two dimensional finite Gaussian beam will break this condition of total reflectivity and will lead to a series of step changes in reflection [33]. Furthermore, a small change in the intensity produces a very strong change in the transmitted beam angle. At the threshold intensity the beam emits a self-trapped spatial solitary-like wave and forms a non-linear channel into the the transmitting medium. To the best of our knowledge, only these step-like changes in reflectivity have been measured and the spatial solitary-like waves generated by them have never been observed experimentally. This study was based on a model for a beam that was focused to a waist size of 10λ and had only a 1.22° diffraction angle and a 87° incident angle. For the phenomena being studied here we prefer to model a beam that is more tightly focused and has a smaller incident angle (by at least a few degrees). This configuration will allow for the device to be modeled on a smaller grid because the initial beam size is smaller and the interaction length is shorter, but it has the disadvantage of being further from the ideal plane wave case.

When the source is a plane wave, this device can be modeled exactly. The index in substrate 2, n_{b2} , is written in terms of n_{b1} , the index in substrate 1, as:

$$n_{b2} = n_{b1} - \Delta n + n_2 |E_o|^2 \quad (5.4)$$

where Δn is the size of the step in the linear index. Here we assume the instantaneous nonlinear model given by Eq. (4.2) and neglect linear absorption. The critical angle is now given by the following expression:

$$\theta_c = \sin^{-1} \left(\frac{n_{b1} - \Delta n + n_2 |E_o|^2}{n_{b1}} \right) \quad (5.5)$$

This expression is used as the basis for the design of the nonlinear interface optical switch. For plane waves, this model shows that such a device is realizable. However, when we model the real world of finite beams, the results are at best inconclusive. This is illustrated by the following ten examples which are summarized in table 5.2.

The first five cases that we modeled are examples of a TM_z finite beam incident upon the interface at glancing or near glancing angles. In the first 3 cases, the source (5.1), which was driven by the $z = 0$ boundary in region 1 by the method in Chap. 3, has an initial aperture waist of $\omega_o = 10.0 \mu m$, a period of $30 \mu m$, and a diffraction angle, found by the technique presented in Chap. 2, of $\theta_{int} = 8.76^\circ$. The remaining cases represent an aperture size of $\omega_o = 14.14 \mu m$ and a diffraction angle of $\theta_{int} = 6.22^\circ$. The source is excited far enough from the intersection point on the interface that the beam is in its far field and clearly diffracting. The dimensions for the mesh are $105 \mu m \times 305 \mu m$ with a discretization size per cell of $0.3 \mu m$ in the linear case and $0.125 \mu m$ in the nonlinear case. The medium used here is similar to the previous section but with a linear refractive index of $n_{b1} = 1.56$, $\Delta n = .06$, the relaxation time is $4.0 fs$, and $\epsilon_2 = 2.0 \times 10^{-18} (m^2/V^2)$. The critical angle for a plane wave is $\theta_c = 74.1^\circ$ and $\theta_i = 75.65^\circ$ to 80.0° so that $\theta_i > \theta_c$ in the first five cases.

Cases 1 and 2 represent the linear behavior of associated with an incident TM_z finite beam. The first example showed that the chosen incidence angle of 75.65°

did not produce the desired total reflection. Unfortunately, the subsequent choice of 80.0° didn't either. This is due to the fact that the tightly focused incident beam has wave vector components at angles below *and* above the critical value. In spite of this initial discouragement, we proceeded to model the nonlinear reflection cases. From Eqs. (4.21) and (5.2) and $\lambda_{rad} = 4.84 \mu m$, the nonlinear index change needed for a plane wave to overcome the condition of total reflection is $n_2|E_b|^2 = .036$ where E_b is the electric field amplitude on the boundary. The plane wave electric field which will achieve this has a threshold intensity $|E_o|^2 = 1.17 \times 10^{18} (V^2/m^2)$. In the previous chapter, we found that a much lower intensity is required for a given nonlinear index change when a PG beam is used.

Case 3 showed very little change from the linear case other than the transmitted pulse was significantly attenuated by nonlinear loss. In case 4 the beam was widened in order to reduce diffraction effects but the result did not change. Finally, case 4 was repeated as case 5 but with the intensity increased by 1.25. Nonetheless, the transmission coefficient decreased because of the nonlinear nature of the loss mechanism in region 2.

The second five cases are examples of TE_z beams incident on the interface. The electric field in this case is polarized parallel to the interface. The source function and medium are the same as in the TM_z cases as is the mesh size and discretization. The first TE_z case (case 6) is a repeat of the second TM_z case and the results are similar. For the second TE_z case (case 7) the size of the step is reduced while the incident angle is increased. The critical angle for a plane wave calculated for this index step is 82.0° and the incident angle is slightly more, $\theta_i = 84.4^\circ$. The transmission, however, increases dramatically, this being in direct contradiction to plane wave theory. Three cases of increasing beam intensity were examined next and little change in the transmission coefficient was noted. The final case began

to show a slight decrease in reflection but it was balanced by a slight increase in nonlinear attenuation in the transmission. The investigation of the obliquely incident focused beam threshold (optical diode) devices was discontinued after this series of disappointing results and the following simple conclusion was drawn: It doesn't work for a highly focused PG beam.

The difficulty resides in the ability of a finite Gaussian beam to totally reflect off the interface boundary. This is due to the fact that there are a wide range of wave vector components in a tightly focused beam, i.e., for any given angle between the propagation direction and the boundary plane there is a wide range of incidence angles for the beam components. Thus, unless the beam waist is very wide or the the index step is extreme, some transmission will always be present for a beam that is incident at an angle greater than the "critical" angle.

Another undesirable effect that we observed from a tightly focused beam was that diffraction of the wings of the pulse was completely swamping out the nonlinearity. The effect that the decreased index step had on channeling the pulse back into region 1, also known as the Goos-Hänchen effect, is also much smaller than the linear dispersion for this beam and it gave a smaller contribution than we needed. Consequently, the intensity has little effect on the direction of the beam and we don't see the big diode-like threshold that was apparent from the plane wave analysis. A more aggressive nonlinear interaction should produce a result closer to the desired effect, but the other high intensity nonlinear phenomena such as focusing and back reflection will also be present. Since our intention was to single out just the diode behavior, we had to restrict ourselves to relatively low intensity nonlinear devices. Although improvements would be gained by using a greater interaction length, smaller index step, shallower angle, and wider beam; at present, the required computer memory for such a problem is unavailable. With the questionable

success of such devices, we dropped this design in favor of the better one presented in Sec. 3.

3. Optical threshold in a waveguide

Faced with the numerous shortfalls inherent in the previous nonlinear interface model, we are forced to develop a better strategy for switching a pulsed wave. We now realize that beam diffraction is spoiling the plane wave threshold properties. Thus, our effort is now directed to containing the beam in a dielectric slab waveguide and using nonlinear properties to leak the energy out of the waveguide mode and possibly retrap it in a second waveguide. Ideally, all the energy should remain in one packet. The geometry of this device is divided into three regions; The center region makes the guiding portion of the waveguide and contains the slightly higher refractive index. Of the remaining two regions, one is made to have a positive nonlinear refractive index. This device has the advantage that a mode, if it is low intensity and if it is in a steady-state guided condition, will propagate in one dimension indefinitely. On the other hand, if the mode is of high intensity, the beam will exhibit dramatically different characteristics by coupling to the nonlinear substrate [34]. The energy emitted into the nonlinear substrate will form a channel in which it is self trapped and will propagate at an angle away from the guide. It can then be made to rendezvous with a second wave guide and be captured. This is exactly the type of high-speed switching response that we wish to emulate numerically.

In this section we have increased the complexity of our previous geometry by including an interface and creating a third region. Figure (5.3) shows the placement and contents of these three regions and the location of the pulse within this structure. The multiple wave vector problem with the obliquely incident PG beam diode

is solved by going to the slab waveguide structure shown in the figure. We have attempted to excite a source of the lowest order TE_z mode, i.e. TE_{01} , in the linear guide. This allows the beam to achieve a stable linear condition and thereby reduce the transients that might let energy escape prematurely from the waveguide. The index linear step is made small ($\Delta n_{linear} \simeq .015 - .02$) to create a weakly guiding condition that can be easily broken with a mild nonlinear increase in the refractive index outside the guide. This makes the device useful at lower power and reduces the scattering which occurs in the vicinity of strong nonlinear effects on the medium. For the moment, the second capturing guide is omitted since its function is secondary to the switching behavior of the primary waveguide.

We initially modeled the slab waveguide threshold device in the $T = 7.5\tau$ regime using the TM_z mode set and represented three different intensity levels; $|E_o|^2 = .25 \times 10^{18} (V^2/m^2)$, $|E_o|^2 = 1.0 \times 10^{18} (V^2/m^2)$, and $|E_o|^2 = 100.0 \times 10^{18} (V^2/m^2)$. The nonlinear region is given a nonlinear permittivity coefficient $\epsilon_2 = 2.0 \times (m^2/V^2)$ as usual. The pulse time history used for the source was again the polynomial bipolar pulse given by (5.1). However, in an attempt to initiate the simulation with a steady state mode, the TE_{01} dielectric waveguide mode, the following equation was used for the aperture cross section for the source $W_a(x)$:

$$W_a(x) = \begin{cases} Au \cos u(x - x_o) e^{-jk_z z} & |x - x_o| < \frac{a}{2} \\ Bv e^{-u|x-x_o|} e^{-jk_z z} & |x - x_o| > \frac{a}{2} \end{cases} \quad (5.6)$$

where x_o is the location of the center of region two a is the width of the guide. The constants u and v are determined by solving the following transcendental equation,

$$\frac{ua}{2} \tan \frac{ua}{2} = \frac{\epsilon_d}{\epsilon_o} \frac{va}{2} \quad (5.7),$$

simultaneously with the following relation:

$$u^2 + v^2 = k_d^2 - k_o^2 = \omega_{rad}^2 \mu_o (n_e^2 - n_o^2). \quad (5.8)$$

For the case being considered here, $n_e = 1.57$, $n_o = 1.55$ and $a = 10.0 \mu m$. The device is confined to an area $100.0 \mu m$ wide and $200.0 \mu m$ long. The mesh is discretized into 1000×2000 cells. The time step $\Delta t = .18 fs$ making the Courant criterion 0.50. The pulse period T is $30 fs$ (i.e. the discretization is 60 cells per pulse length). The results are depicted in Figs. (5.13-15) as shaded images of the electric field intensity in space at different points in time.

It is apparent that some *but not all* of the energy in the waveguide channels into the nonlinear substrate. In the first (low intensity) case, the pulse is only shifted off of center within the guide. Increasing the intensity results in a pulse separating from the guide and beginning to propagate away at a slight angle. In the third case we have clearly gone too far with intensity. Energy couples into the nonlinear region quickly and propagates away at a steep angle in a solitary-like wave. However, the process quickly limits itself through the nonlinear conductivity term, producing a poorly conducting boundary at the interface between regions two and three. Although more definitive results can only come from a longer interaction distance, we nonetheless favor this geometry over the oblique incidence geometry for producing a threshold switching behavior.

This is the extent of the nonlinear switching research conducted for this thesis. The quantitative analysis and further modeling are withheld at this time pending further understanding and investigation by the author. The results presented here relative to this subject (especially the slab waveguide threshold device) are meant only as a demonstration of the modeling capabilities of the vector FDTD approach.

Figure (5.1), The normal incidence problem space is divided into two regions: the incident region which is linear and the transmission region which is nonlinear. The linear index is continuous across the interface so that a low intensity beam will propagate unchanged. As the intensity increases however, the pulse will experience some reflection and the transmitted pulse will self-focus if its intensity is high enough.

Figure (5.2), The polynomial bipolar pulse versus time. The bipolar nature of this pulse improves the distortion problem generated by the source being excited on the boundary. The effective radial frequency for this pulse is $5.85 \times 10^{14} \text{ rad/sec}$.

Figure (5.3), We show the reflection coefficient as a function of intensity for a plane wave incident on a nonlinear medium. The “exact” curve (solid line) is derived from the complex susceptibility equation (4.19) and the “approximate” curve (dashed line) represents the nonlinear index equation (4.21). An effective frequency of $\omega_{eff} = 5.86 \times 10^{14} (rad/sec)$ is assumed. The relaxation time $\tau = 4.0 fs$; the nonlinear permittivity coefficient $\epsilon_2 = 2.0 \times 10^{-18} (m^2/V^2)$.

Figure (5.4), We show the reflection coefficient as a function of relaxation time for a plane wave incident on a nonlinear medium. The “exact” curve (solid line) is derived from the complex susceptibility equation (4.19) and the “approximate” curve (dashed line) represents the nonlinear index equation (4.21). An effective frequency of $\omega_{eff} = 5.86 \times 10^{14} \text{ (rad/sec)}$ is assumed. The intensity $|E_o|^2 = 22.0 \times 10^{18} \text{ (V}^2/\text{m}^2\text{)}$; the nonlinear permittivity coefficient $\epsilon_2 = 2.0 \times 10^{-18} \text{ (m}^2/\text{V}^2\text{)}$.

Figure (5.5), The contour of the intensity of a PG beam for a frame in time following its reflection from and transmission through a nonlinear interface which is located at $z = 15 \mu m$ from the source plane (case 1). The leading edge of the forward traveling pulse diffracts linearly while the tail is already beginning to form a shock. The majority of the intensity is in the reflected pulse which is diffracting linearly. The initial beam is launched from a $10.0 \mu m$ amplitude waist Gaussian weighted aperture. The total period of the pulse is $20.0 fs$ and its time history is given by Eq. (5.1). The peak amplitude is initially $E_0 = 46.9 \times 10^8 (V/m)$. The medium parameters are the same as the ones used to generate Fig. (5.3). These parameters are not meant to be representative of any specific material; they are meant to give a general view of the behavior of this class of materials.

Figure (5.6), The $1/e$ energy waist in microns versus time for the PG beam focus after it enters the nonlinear medium (case 1). The energy was determined for a given distance from the axis by integrating $\epsilon_{eff}/2 [|E_x|^2 + |E_z|^2]$ along a line parallel to the axis. The two jagged structures at $t \simeq 60 fs$ and $t \simeq 110 fs$ resulted when the PG beam reflected off the interface and the source plane boundary respectively. The noisy region on the waist from $135 fs$ to $160 fs$ was generated by the return of the reflected pulse to the nonlinear medium.

Figure (5.7), The energy in Joules contained in a $1.2\mu m$ half band near the propagation axis (lower portion of the simulation region) for case 1. The jagged spikes in this plot correspond to the spikes in Fig. (5.6). As the beam focuses, the energy in this band rises. It then declines after the focus as the beam begins to diffract.

Figure (5.8), The contour for the intensity of the transmitted PG beam in the focal region corresponding to the case shown in Fig. (5.5). The peak intensity in the focal region is $2.4 \times 10^{18} \text{ (V}^2/\text{m}^2\text{)}$ and the $1/e$ energy waist is $3.8 \mu\text{m}$. Transverse energy cycling has produced two additional lobes on the tail of the pulse with the highest peak occurring on the final lobe. The time at which this focus occurs is 172 fs .

Figure (5.9), The $1/e$ energy waist in microns versus time for the PG beam focus after it enters the nonlinear medium (case 2). The energy was determined for a given distance from the axis by integrating $\epsilon_{eff}/2 [|E_x|^2 + |E_z|^2]$ along a line parallel to the axis. The lower intensity results in less reflection and a decrease in magnitude of the jagged structure as the pulse enters region 2.

Figure (5.10), The contour of the intensity of a PG beam for a frame in time following its reflection from and transmission through a nonlinear interface which is located at $z = 15 \mu m$ from the source plane (case 2). The leading edge of the forward traveling pulse diffracts linearly while the tail is already beginning to form a shock. The majority of the intensity is in the reflected pulse which is diffracting linearly. The initial beam is launched from a $10.0 \mu m$ amplitude waist Gaussian weighted aperture. The total period of the pulse is $20.0 fs$ and its time history is given by Eq. (5.1). The peak amplitude is initially $E_0 = 9.37 \times 10^8 (V/m)$. The medium parameters are meant to represent a typical Kerr medium. The relaxation time $\tau = 5.0 fs$; the nonlinear permittivity coefficient $\epsilon_2 = 2.0 \times 10^{-18} (m^2/V^2)$.

Figure (5.11), The energy in Joules contained in a $1.2\mu m$ half band near the propagation axis (lower portion of the simulation region) for case 2. The jagged spikes in this plot correspond to pulse interaction with the interface. They are reduced in magnitude from the spikes in Fig. (5.7). As the beam focuses, the energy in this band rises. It then declines after the focus as the beam begins to diffract.

Figure (5.12), The $1/e$ energy waist in microns versus time for the PG beam focus after it enters the nonlinear medium (case 3). The energy was determined for a given distance from the axis by integrating $\epsilon_{eff}/2 [|E_x|^2 + |E_z|^2]$ along a line parallel to the axis. The two jagged structures at $t \simeq 60 fs$ and $t \simeq 110 fs$ resulted when the PG beam reflected off the interface and the source plane boundary respectively.

Figure (5.13), The oblique incidence problem is also divided into two regions but the incident beam must be directed at a glancing angle to the interface. There is a small linear index step in the mediums with the incident medium (region 1) having the higher index. The step size is chosen such that the critical angle θ_c is smaller than the incident angle θ_i to create a condition approaching total reflection. Region 2 represents the nonlinear medium.

Figure (5.14), The general configuration for a slab waveguide threshold device. Of the three regions, region 3 is the only one with nonlinear aspects. Region two forms the dielectric waveguide. A packet of energy in the lowest order mode will either stay in the guide or leave the guide and form a channel in the nonlinear medium depending on its initial intensity.

Figure (5.15), A pulse in the slab waveguide threshold device. The linear case is depicted in the top template and the nonlinear case is depicted in the bottom template. The pulses are shown as they exist in space frozen in time at evenly spaced intervals. For the nonlinear case $|E_0|^2 = .25 \times 10^{18} (V^2/m^2)$. The parameters for the waveguide are: $n_e = 1.57$, $n_o = 1.55$, the width $a = 10.0 \mu m$, and the nonlinear permittivity coefficient in region three $\epsilon_2 = 2.0 \times 10^{-18} (m^2/V^2)$. The dimensions of the problem are $100.0 \mu m$ wide $\times 200.0 \mu m$ long. The pulse length $T = 7.5\tau$ is in the instantaneous regime.

Figure (5.16). A pulse in the slab waveguide threshold device. The linear case is depicted in the top template and the nonlinear case is depicted in the bottom template. The pulses are shown as they exist in space frozen in time at evenly spaced intervals. For the nonlinear case $|E_0|^2 = 1.0 \times 10^{18} \text{ (V}^2/\text{m}^2\text{)}$. The waveguide is the same as in Fig (5.13).

Figure (5.17), A pulse in the slab waveguide threshold device. The linear case is depicted in the top template and the nonlinear case is depicted in the bottom template. The pulses are shown as they exist in space frozen in time at evenly spaced intervals. For the nonlinear case $|E_o|^2 = 100.0 \times 10^{18} (V^2/m^2)$. The waveguide is the same as in Fig (5.13).

	case 1 :	case 2 :	case 3 :
τ	4.0 <i>fsec</i>	5.0 <i>fsec</i>	40.0 <i>fsec</i>
E_o	$46.9 \times 10^8 \left(\frac{V}{m}\right)$	$9.37 \times 10^8 \left(\frac{V}{m}\right)$	$46.9 \times 10^8 \left(\frac{V}{m}\right)$
Γ	.239	.00853	.0862
time to focus	173 <i>fsec</i>	160 <i>fsec</i>	159 <i>fsec</i>
distance to focus	28.7 μm	37.0 μm	30.6 μm
waist at focus	3.5 μm	3.9 μm	4.6 μm

Table (5.1)

Case	Mode	n_{b1}	n_{b2}	θ_i	E_o	T_{ener}
1	TM _z	1.56	1.50	75.65°	linear	.603
2				80.00°		.607
3					$8.0 \times 10^8 (V/m)$	.603
4						.599
5				$10.0 \times 10^8 (V/m)$	.587	
6	TE _z	1.56	1.50	80.00°	linear	.595
7			1.545	84.40°		.813
8					$0.584 \times 10^8 (V/m)$	.799
9					$0.825 \times 10^8 (V/m)$	.799
10					$4.0 \times 10^8 (V/m)$	.799

Table (5.1)

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

The research presented in this thesis has focused on the behavior of pulsed finite beam propagation in nonlinear media. The analysis began with the investigation of a two dimensional PW beam in free space using a paraxial approximation and linear system theory to determine its propagation characteristics. Relations were then found between the diffraction lengths and divergence angles and the beam waist and pulse shape. We then developed the vector finite difference-time domain algorithm for determining the fields of a two dimensional PW Gaussian beam in either the TE_z or TM_z modes. Meshes were introduced for the discretization of space in 2-D and time, and Maxwell's equations were solved numerically on them. Next, a model was introduced to represent a medium exhibiting the reorientational Kerr effect. We produced a numerical solver to determine the electrical properties of the medium. Then, given the nonlinear relationship between the fields and the medium, both solvers had to operate simultaneously to model the pulsed beam propagation. This technique was implemented for a number of nonlinear problems to explore such nonlinear phenomena as self-focus and self-reflection. These new vector results were compared with existing scalar models. This finally led to the design and modeling of several nonlinear optical switches.

As a precursor to the subject of optical pulse propagation in nonlinear media, a PW Gaussian beam in free space was examined. A good approximation for the propagation of a zeroth order, single frequency, radially symmetric Gaussian beam was available, and we merely had to use linear system theory to apply this relation to a broad spectrum pulse. It was shown by using both numerics and analysis that as well as diffracting away from the aperture, the pulse was also changing shape, both

longitudinally and transversely. Longitudinally, the beam clearly began developing into a first derivative of its initial form at about one diffraction length from the source. Transversely, the beam energy waist grew at a slower rate than the intensity waist did. A single frequency, ω_{rad} , can be used to describe these characteristics of a PW beam through the relations derived in Chap. 2

The vector FDTD technique introduced in Chap. 3 proved to be a useful tool in the modeling of the propagation of two dimensional beams in nonlinear media in Chap. 4. We found that for a pulse, the self-focus distance does not imitate the scalar model self-focus distance and that the longitudinal field components have a strong influence on the beam. This distance is more accurately described by a simple relation involving the beam power and the free space diffraction length, L_{rad} . The time required for the pulse to collapse remains almost constant but the distance and severity of this focus is strongly dependent on beam power and relaxation time τ . Nonlinear reflection from a normal interface is likewise a function of both of these parameters.

Several attempts were then made to produce a linear-nonlinear interface design that would give a clear on/off behavior when it was illuminated above a given threshold power. On the whole, this venture was unsuccessful as far as producing the desired result. Nonetheless, it served as a tutorial on how not to design this device. It was clearly shown that a tightly focused pulse at an interface will not behave the same way as a plane wave will, and the device will malfunction. To obtain a threshold characteristic like that of a plane wave at oblique incidence, a much wider beam than I am currently able to model is required. A guiding structure provides better results than the oblique interface because it prevents spatial dispersion and allows nonlinear effects to accumulate over greater distances. This device actually did couple an amount of energy into the nonlinear substrate region contingent on the

intensity of the input. The transfer was incomplete because energy was coupled at a cost to the pump (guided pulse). Thus, before the beam was completely redirected, the intensity at the interface decreased below threshold, and the nonlinearity turned-off leaving energy remaining in the guide. Another benefit of the guided structure is that at low intensity, no energy gets coupled into the nonlinear region. This device shows promise but extensive modeling would be required to produce a true threshold device with this configuration.

One main discrepancy between the linear and the nonlinear modeling in this research is that all the nonlinear phenomena which I treated with the FDTD methods were modeled in two dimensions. In contrast, the linear model of a PW beam in Chap. 2 was in three dimensions. A three dimensional FDTD mesh with the current resolution of our 2-D mesh would be much too large for the memory constraints of the Cray-YMP 432 and slightly large and much too time consuming for the Convex 240. Modeling the pulse in two dimensions keeps the size reasonable, however some physics may be lost when this is done. Both the TE_z or TM_z modes were modeled to compensate for the two dimensionality by showing the behaviors of modes with and without the presence of the nonlinear coupling between the longitudinal and transverse electric field components.

Instability is always an issue when modeling electromagnetics by numerical techniques, and this issue was not thoroughly discussed in the body of this thesis. In fact, Equation set (3.10a-c) shows the term A in the denominator of the electric field calculation and, given a large enough negative nonlinear conductivity term, it could tend toward zero thus causing a near infinite spike in the field at that cell. Because of floating point considerations, a spike like this would be undesirable, it would cause the calculated field value at that cell to be grossly inaccurate, and all

later time calculations would be unreliable. This has not yet presented a problem but it is anticipated that it could for a much higher power PW beam.

There are a number of extensions to this work which could be considered for future research. This includes computational refinements, three dimensional models, and alternative dispersion models. Currently, in the problems that this thesis has modeled so far, the majority of the electromagnetic fields have occupied only a small portion of the mesh at any one time. This is inefficient (and expensive) since it requires additional memory and computation time for the cells that provide little or no information. A couple of solutions for future consideration follow. First, one should consider truncating the geometry closer to the field structures in one or more directions with a boundary that radiates rather than reflects. A further refinement in this direction that would benefit a straight waveguide or collimated beam problem is to march the nodes in space as well as time so that, relative to the boundary, the wave front does not move. Alternately, Maxwell's equations could be written in stationary form meaning either one space argument, z , is replaced with $z - ut$ or the time argument is replaced by $t - z/u$, where u is the wave speed in the medium. Second, one should consider the use of nonuniform cell sizes (and shapes) to distribute the computer resources over the problem space in a way that will maintain or gain detail in specific regions, and provide less detail to the rest of the problem space where accuracy is not important.

Three dimensional modeling of vector fields is only feasible once measures have been taken to make the FDTD technique more efficient. Radial symmetry arguments can be used to extend the existing 2-D method (after adapting it to a cylindrical coordinate system) into three dimensions. However, any real beam mode that has peak power flow at the axis is radially asymmetric. To completely model the three dimensional self-focus phenomenon would therefore require that a 3-D

mesh be used. Moreover, since TE_z and TM_z mode sets become coupled, all six field components must be included for an accurate description of the self-focusing process.

Alternative models for linearly and nonlinearly dispersive media are another possible extension to this research. Pulse compression, a phenomenon resulting from the presence of both nonlinear and normal dispersion, is an example of a nonlinear effect incorporating a more complex model of the medium. Other types of third order nonlinear dispersion which could just as easily be implemented in the FDTD approach include models for optical (Raman scattering) and acoustic (Brillouin scattering) phonons. Due to the second derivative nature of these types of nonlinearities, more computation and memory are required.

The vector FDTD technique is a versatile tool which is simple to implement and allows almost any aspect of wave propagation to be included in the problem model. Without a high performance computer, however, modeling nonlinear media by this technique would be unrealistically difficult. In fact the main drawbacks to the FDTD technique are all related to the size and speed of the computer being used. The problem size and speed could be greatly extended by using one of the new massively parallel machines. Because the field calculations are isolated, this technique lends itself readily to massive parallelization. Ideally, one processor should be devoted to each node and perform simultaneously with all of the others. The fields would then be stepped in time as quickly as a single processor could perform a central differencing task for one cell. Several machines are available, such as the Intel Touchstone and the Thinking Machine's CM5, that are approaching the ability to perform this multi-processor task. It seems that the usefulness of the FDTD technique will only increase with future supercomputer advancements.

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