

FDTD Analysis of Wave Propagation in Nonlinear Absorbing and Gain Media

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Abstract—An explicit finite-difference time-domain (FDTD) scheme for wave propagation in certain kinds of nonlinear media such as saturable absorbers and gain layers in lasers is proposed here. This scheme is an extension of the auxiliary differential equation FDTD approach and incorporates rate equations that govern the time-domain dynamics of the atomic populations in the medium. For small signal intensities and slowly varying pulses, this method gives the same results as frequency-domain methods using the linear susceptibility function. Population dynamics for large signal intensities and the transient response for rapidly varying pulses in two-level (absorber) and four-level (gain) atomic media are calculated to demonstrate the advantages of this approach.

Index Terms—FDTD methods, nonlinear wave propagation.

I. INTRODUCTION

THERE are two main aspects to the interaction of electromagnetic radiation with a collection of atoms: 1) the effects of the medium on the field and 2) the change in the material parameters due to the incident field. When an electromagnetic wave propagates in a medium, the field induces a time varying dipole moment in the individual atoms that comprise the medium. The oscillating atoms lose energy through radiative and nonradiative mechanisms. The total field, which is the sum of the incident field and the fields radiated by the atoms, can thus be attenuated or amplified and phase shifted by the medium. The effects of the medium on electromagnetic wave propagation can be modeled by suitably defining the polarization vector of the medium and solving the equation for the macroscopic polarization along with Maxwell's equations. In this way, the standard finite-difference time-domain (FDTD) methodology [1] can be extended to model linear dispersive media [2], [3]. This method, known as the auxiliary differential equation finite-difference time-domain (ADE-FDTD) method has also been modified to model nonlinear dispersion [4], [5] due to Kerr and Raman effects.

The ADE-FDTD approach has been modified to model gain in lasers [6], [7] by using a frequency-dependent negative conductivity term in Maxwell's equations. These formulations assume that the gain and absorption due to the medium are independent of signal intensity and only vary with frequency. For small signal intensities and for slowly varying pulses the above approximations are reasonable and give the correct results. At larger signal intensities and for rapidly varying signals

the materials response may become strongly nonlinear. The origin of this nonlinearity is the change in atomic populations with time due to signal induced transitions. The effect of gain saturation has been incorporated phenomenologically into the gain model [8] and was utilized to demonstrate saturation of oscillation intensities and to calculate output power levels in a Fabry–Perot laser cavity. A complete nonlinear model for wave propagation in a two-level system of atoms, capable of predicting saturation effects as well as self-induced transparency, has been demonstrated [9] using an iterative predictor-corrector FDTD method to solve the Maxwell–Bloch system of equations.

We present here an alternative formulation that incorporates the atomic rate equations in the ADE-FDTD model. The rate equations describe the time evolution of the atomic energy level populations under the influence of applied signals. Since this model takes into account the effect of the propagating waves on the material parameters, it is capable of describing nonlinear gain and absorption effects and is valid over a large range of signal intensities. The formulation presented here is *fully explicit* and so the electromagnetic fields and atomic energy level populations at any time step can be calculated in terms of known fields and populations, thus eliminating the need for an iterative scheme. Also, the approach used here is easily generalized to more complex situations such as media with multiple resonances and having more than two atomic energy levels. The model is applied to an absorber comprising a two-level atomic system and also to a gain medium consisting of a four-level atomic system. Small signal frequency responses of the two media are computed using FDTD and compared with theoretical models for the same. Population dynamics under the influence of varying incident signal intensities are also calculated for both media. Transient responses of the medium are studied by observing the propagation of fast pulses through the medium.

II. CLASSICAL ELECTRON OSCILLATOR MODEL

Using the classical electron oscillator (CEO) model [10] (also known as the Lorenz Model), the net macroscopic polarization $\bar{P}(t)$ for an isotropic dielectric medium can be described by the following equation:

$$\frac{d^2 \bar{P}(t)}{dt^2} + \gamma_{\text{ceo}} \frac{d \bar{P}(t)}{dt} + \omega_a^2 \bar{P}(t) = N \frac{e^2}{m} \bar{E}(t) \quad (1)$$

where e is the charge of an electron, m is the mass of an electron, and N is the number of electrons per unit volume.

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The resonance frequency of the material ω_a is related to the atomic energy levels through

$$\omega_a = \frac{E_2 - E_1}{\hbar} \quad \text{transition frequency [rad/s]} \quad (2)$$

where \hbar is the reduced Planck's constant and E_1 and E_2 are the energy levels involved in the transition. If multiple energy levels are involved, then each transition is modeled as a separate CEO with a unique oscillation frequency and decay rate. Classically, the energy decay rate γ_{ceo} is given by

$$\gamma_{ceo} = \left(\frac{e^2}{m} \right) \frac{\omega_a^2}{6\pi\epsilon_0 c^3} \quad [1/\text{s}]. \quad (3)$$

This accounts for radiative energy loss using a simple oscillating dipole model. The radiative energy decay rate γ_r for a real atomic transition may be different from that of a classical electron oscillator. To account for the difference in these decay rates an oscillator strength F_{osc} is defined as [10]

$$F_{osc} = \frac{\gamma_r}{3\gamma_{ceo}}. \quad (4)$$

The factor of “three” assumes the atomic dipoles are fully aligned with the applied field, but can be modified to account for more complex situations [10]. These changes are incorporated in the polarization equation by replacing the term (e^2/m) in (1) by κ , which is defined as

$$\kappa = 3F_{osc} \left(\frac{e^2}{m} \right). \quad (5)$$

Another important change that needs to be made is due to the fact that real atoms undergo dephasing processes that destroy the coherence between the individual atomic dipole oscillations. Equation (1) implicitly assumes that all the atomic dipoles are oscillating in phase. The effect of the dephasing events is to increase the decay rate of the net macroscopic polarization over that of a single oscillator. The atoms in real transitions can also lose energy through other nonradiative processes. It can be shown [10] that the total energy decay rate $\Delta\omega_a$, which describes the actual linewidth of the transition, is given by

$$\Delta\omega_a = \gamma_r + \gamma_{nr} + \frac{2}{T_2} \quad \begin{array}{l} \text{total energy decay} \\ \text{rate for real transitions} \end{array} \quad (6)$$

for the homogeneously broadened case with mean time between dephasing events T_2 and nonradiative energy decay rate γ_{nr} .

The polarization vector for a collection of classical electron oscillators depends only on the number density N of oscillators per unit volume. The response of a collection of real atoms depends on the relative number of atoms in the two energy levels, hence, the total number of oscillators is replaced by the instantaneous population difference

$$N \rightarrow \Delta N(t) = N_1(t) - N_2(t) \quad \text{instantaneous population difference.}$$

An important change from the classical case is the explicit time dependence of the population difference $\Delta N(t)$ as a

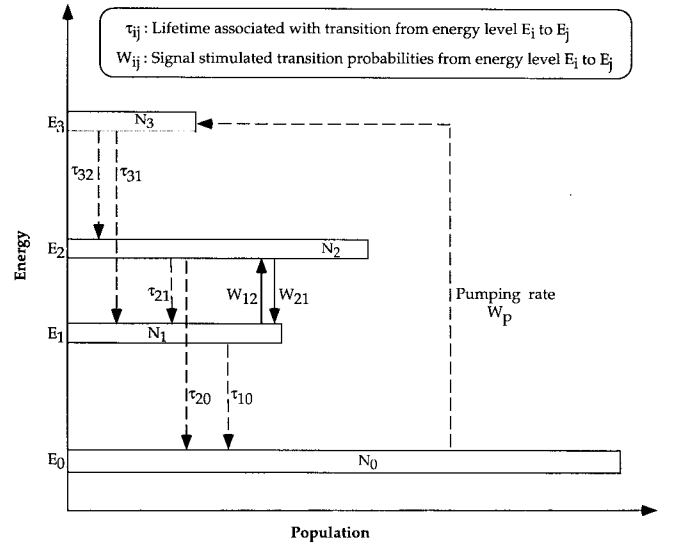


Fig. 1. Populations in the simplified four-level atomic system.

result of stimulated emission, pumping effects, and relaxation effects. If the population difference remains constant or is a slowly varying function of time (rate equation limit), then the frequency-domain susceptibility method is adequate to describe wave propagation in the medium. For large signal intensities and rapidly varying signals the time variation of $\Delta N(t)$ becomes important. Hence, the equation for the macroscopic polarization of the medium is essentially a nonlinear equation.

Consolidating all the changes discussed in this section, we see that the electric polarization in real atomic transitions can be described by the following equation:

$$\frac{d^2 \bar{P}(t)}{dt^2} + \Delta\omega_a \frac{d\bar{P}(t)}{dt} + \omega_a^2 \bar{P}(t) = \kappa \Delta N(t) \bar{E}(t). \quad (7)$$

III. RATE EQUATIONS

The rate equations are used to model the evolution of the atomic energy level populations with time. Consider here an ideal two-level system with energy levels E_1 and E_2 with populations N_1 and N_2 , respectively. For this system, the rate equations may be written [10] as

$$\frac{dN_1(t)}{dt} = -\frac{dN_2(t)}{dt} = -\frac{1}{\hbar\omega_a} \bar{E}(t) \cdot \frac{d\bar{P}(t)}{dt} - \frac{N_2(t)}{\tau_{21}} \quad (8)$$

where τ_{21} is the lifetime of the atoms in the upper energy level. This assumes the thermally stimulated transitions are negligible, which is appropriate for optical transitions. The key term here is that which relates the populations to the electric field and the macroscopic polarization associated with the transition given by $\bar{E}(t) \cdot (d\bar{P}(t)/dt)/\hbar\omega_a$. This is just the classical expression for instantaneous energy transfer divided by the energy per photon and is equivalent to the term involving stimulated transition probabilities in the rate equations more commonly used in texts. For computational purposes, these equations can be more conveniently expressed in terms of the

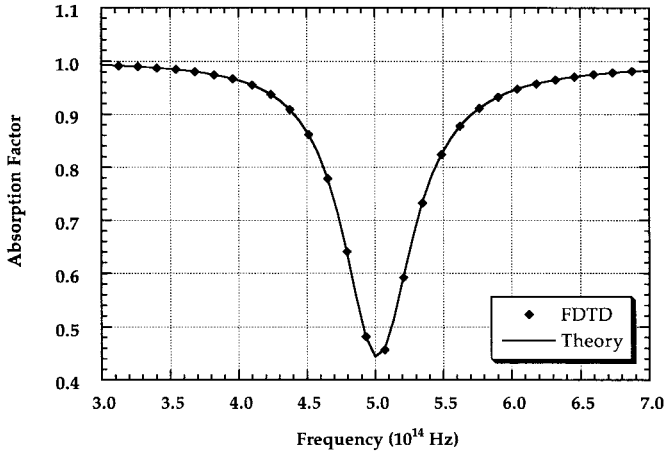


Fig. 2. Comparison of the field absorption factor as computed by FDTD and linear susceptibility theory. The FDTD results are obtained by allowing a Gaussian pulse with carrier frequency f_a to propagate a distance of $0.6 \mu\text{m}$ through an absorbing medium with a resonance frequency $f_a = 5 \times 10^{14}$ Hz and linewidth of 5×10^{13} Hz.

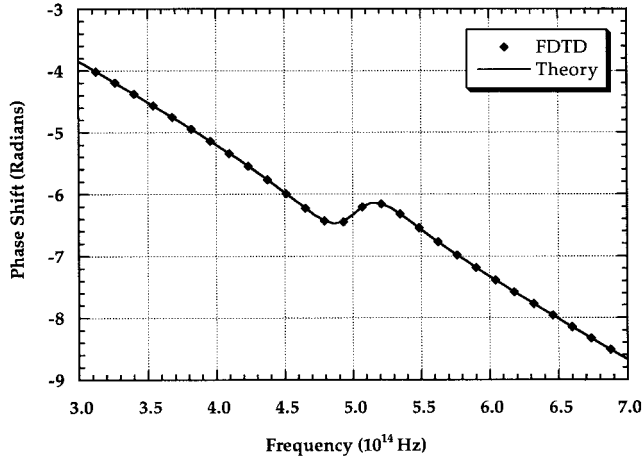


Fig. 3. Phase shift experienced by the various frequency components of a Gaussian pulse with carrier frequency f_a after propagating a distance of $0.6 \mu\text{m}$ through an absorbing medium with a resonance frequency $f_a = 5 \times 10^{14}$ Hz and linewidth of 5×10^{13} Hz.

population difference ΔN as follows:

$$\frac{d\Delta N(t)}{dt} = -\frac{2}{\hbar\omega_a} \overline{E}(t) \cdot \frac{d\overline{P}(t)}{dt} - \frac{\Delta N(t) - \Delta N_0}{\tau_{21}} \quad (9)$$

where ΔN_0 is the population difference at thermal equilibrium, which is an initial condition for the computation.

We also consider here a simplified yet realistic four-level atomic system (depicted in Fig. 1) with energy levels E_0, E_1, E_2, E_3 , and populations N_0, N_1, N_2 , and N_3 , respectively. The ground-state population N_0 is assumed to be very large compared to the populations of the higher energy levels and is basically constant with time. There is some external pumping mechanism that transfers $W_p(t)$ atoms per unit time from the ground state E_0 into the level E_3 . The energy level spacing is assumed to be sufficiently large so that the thermally stimulated transition rates are small. Thus, we consider here only spontaneous emission and signal-induced stimulated emission. Furthermore, we consider a system where the applied signal has a frequency that is close to the transition frequency

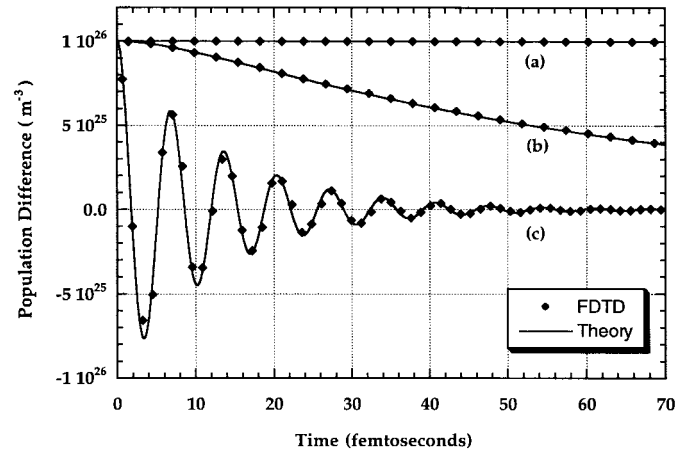


Fig. 4. Time evolution of the population difference $\Delta N(t) = N_1(t) - N_2(t)$ for applied step signals of varying amplitudes. (a) The curve is plotted for an incident electric field amplitude of 100 V/m . (b) The curve for $2.5 \times 10^8 \text{ V/m}$ and curve (c) for $5 \times 10^9 \text{ V/m}$.

associated with energy level E_1 and E_2 and differs from the transition frequencies associated with the other transitions by several linewidths. Thus, signal stimulated transition terms appear only in the rate equations for populations N_1 and N_2 . Under the above mentioned approximations, the populations can be modeled by the following rate equations:

$$\begin{aligned} \frac{dN_3(t)}{dt} &= W_p(t) - \frac{N_3(t)}{\tau_3} \\ \frac{dN_2(t)}{dt} &= \frac{N_3(t)}{\tau_{32}} + \frac{1}{\hbar\omega_a} \overline{E}(t) \cdot \frac{d\overline{P}(t)}{dt} - \frac{N_2(t)}{\tau_2} \\ \frac{dN_1(t)}{dt} &= \frac{N_3(t)}{\tau_{31}} - \frac{1}{\hbar\omega_a} \overline{E}(t) \cdot \frac{d\overline{P}(t)}{dt} + \frac{N_2(t)}{\tau_{21}} - \frac{N_1(t)}{\tau_1} \end{aligned} \quad (10)$$

where $\gamma_{ij} = 1/\tau_{ij}$ is the transition probability per unit time from level E_i to E_j and $\gamma_i = 1/\tau_i$ is the total transition probability per unit time from level E_i to all lower levels. This system has been studied extensively [10] and the steady-state solutions in the absence of an applied signal are known. From these it is readily seen that $W_p > 0$ and $\tau_2 > \tau_1$ are the necessary conditions for population inversion to take place between the energy levels E_1 and E_2 . Thus, if these conditions are satisfied then the four-level atomic system will behave like a gain medium for signals with frequencies within a linewidth of the transition frequency $\omega_{12} = (E_2 - E_1)/\hbar$.

IV. FDTD FORMULATION

The effects of the nonlinear medium on the propagation of electromagnetic waves is incorporated into the analysis through the polarization response of the medium. Maxwell's equations for such a medium may be written in the form

$$\begin{aligned} \nabla \times \overline{E}(t) &= -\frac{\partial \overline{B}(t)}{\partial t} \\ \nabla \times \overline{H}(t) &= \overline{J}(t) + \epsilon \frac{\partial \overline{E}(t)}{\partial t} + \frac{\partial \overline{P}(t)}{\partial t} \end{aligned} \quad (11)$$

where the macroscopic polarization $\overline{P}(t)$ is given by (7) in Section II. Equations (7) and (11) and the rate equation

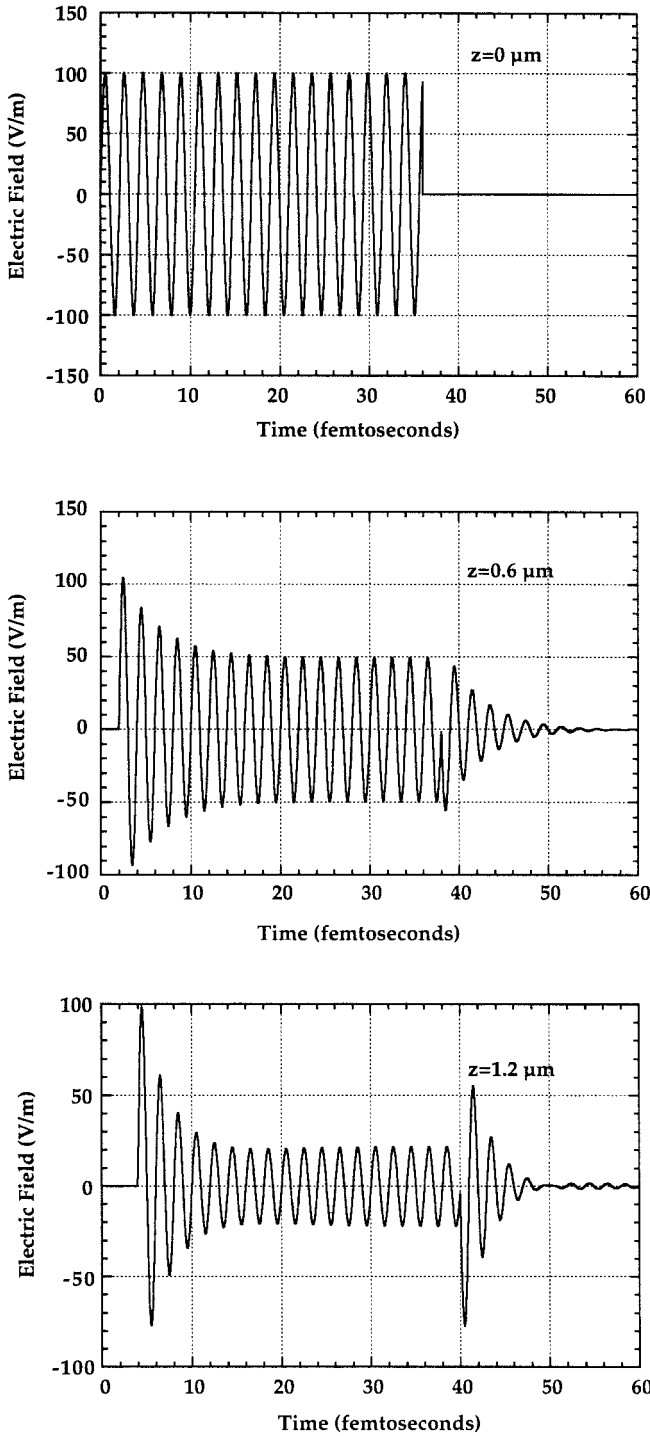


Fig. 5. Transient response of the medium (in the linear regime) to a square pulse with extremely small rise and fall times. The incident pulse shape and the pulse shapes recorded at progressively larger distances into the absorbing medium are depicted here.

(9) for $\Delta N(t)$ form a self-consistent set of equations that accurately models the two-level atomic system. For the four-level atomic system, (9) is replaced by (10). Another minor variation required is the use of $\Delta N_{12}(t) = N_1(t) - N_2(t)$ instead of $\Delta N(t)$ in (7).

Let us consider a one-dimensional problem of a TEM wave propagating in the $+z$ direction so that E_x and H_y are the only

field components present. Correspondingly, the macroscopic polarization has a nonzero component in the x direction alone. Using the central differencing scheme and spatial and temporal interleaving of the fields [1], we can write the discretized equations for the electric and magnetic fields as

$$\begin{aligned} H_y^{n+1/2}[i+1/2] &= \frac{-\Delta t}{\mu_0 \Delta z} (E_x^n[i+1] - E_x^n[i]) \\ &\quad + H_y^{n-1/2}[i+1/2] \\ E_x^{n+1}[i] &= E_x^n[i] - \frac{1}{\epsilon_0} (P_x^{n+1}[i] - P_x^n[i]) \\ &\quad + \frac{\Delta t}{\epsilon_0 \Delta z} (H_y^{n+1/2}[i-1/2] \\ &\quad - H_y^{n+1/2}[i+1/2]). \end{aligned} \quad (12)$$

For the macroscopic polarization, we use

$$\begin{aligned} P_x^{n+1}[i] &= \frac{2\Delta t^2}{2 + \Delta\omega_a \Delta t} \left(\kappa \Delta N^n[i] E_x^n[i] \right. \\ &\quad + \left(\frac{2}{\Delta t^2} - \omega_a^2 \right) P_x^n[i] \\ &\quad + \left(\frac{\Delta\omega}{2\Delta t} - \frac{1}{\Delta t^2} \right) P_x^{n-1}[i] \Big) \end{aligned} \quad (13)$$

and, similarly, the discretized rate equation for the two-level atomic system is

$$\begin{aligned} \Delta N^{n+1}[i] &= \left(\frac{2\tau_{21}\Delta t}{2\tau_{21} + \Delta t} \right) \left(\Delta N^n[i] \left(\frac{1}{\Delta t} - \frac{1}{2\tau_{21}} \right) \right. \\ &\quad + \frac{\Delta N_0}{\tau_{21}} - \frac{(E_i^{n+1} + E_i^n) \cdot (P_x^{n+1}[i] - P_x^n[i])}{\Delta t \hbar \omega_a} \Big). \end{aligned} \quad (14)$$

Equation (10), which describes the population levels for the four-level atomic system, can be discretized similarly. An important point is that the polarization $\bar{P}(t)$ and the atomic level populations are colocated in space and time with the electric fields.

In order to keep the formulation explicit, the time derivatives of $P_x(t)$ in (13) are centered at time step n , while in all other equations they are centered about time step $n + \frac{1}{2}$. It has been demonstrated previously [11] that inconsistent time centering of the discretized derivatives results in a more restrictive stability condition than the original FDTD formulation for nondispersive media. There it was determined that choosing the time step Δt such that it finely resolves the smallest time scale in the problem ensures the stability of the algorithm. The guidelines provided by [11] suggest that the time step be chosen such that

$$\Delta t < \frac{T_a}{100}. \quad (15)$$

Here, $T_a = 1/f_a$ is the time period associated with the material resonance and is the shortest time-scale characteristic of the medium. Note that the above condition is also ordinarily required for a high level of accuracy [11], thus, it is not an overly restrictive requirement.

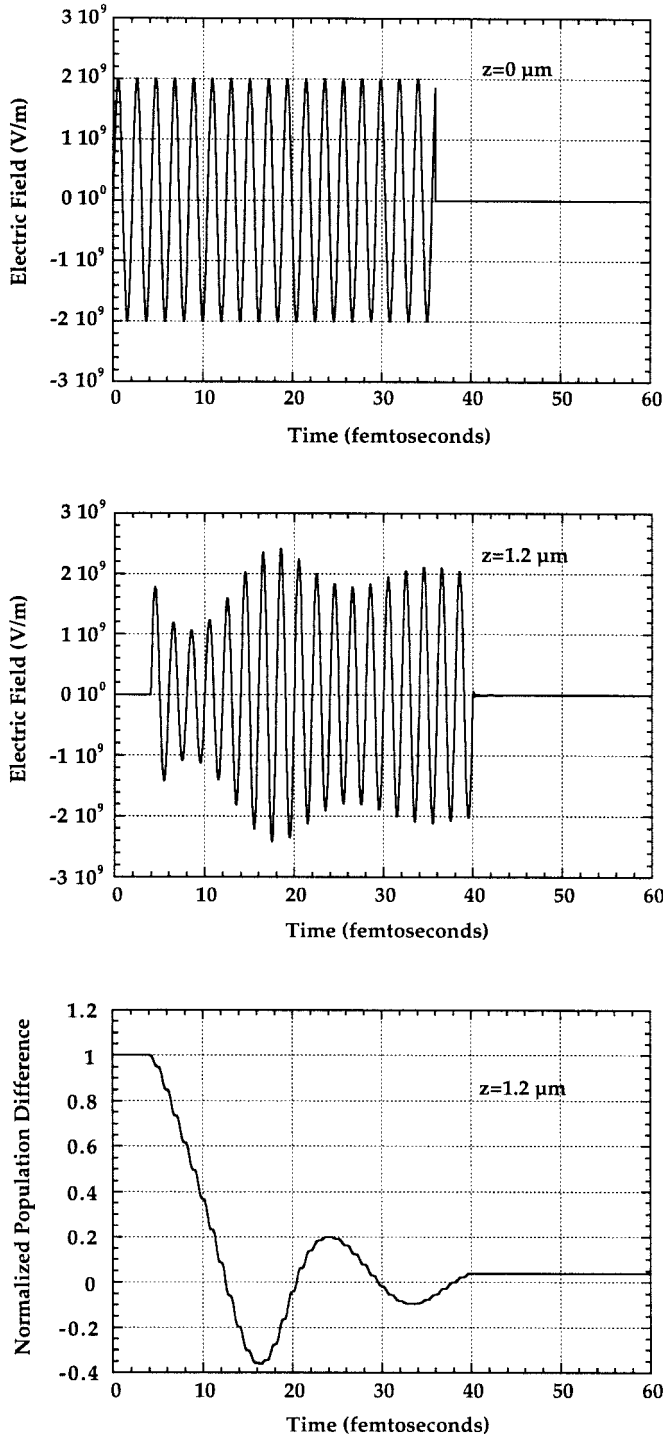


Fig. 6. Transient response of the medium to a strong pulse with small rise and fall times. The shape of the pulse after it has traveled a distance of $1.2 \mu\text{m}$ into the absorber is shown. The time evolution of the population difference at the same point is also depicted.

V. VALIDATION OF THE FDTD PROGRAM

Wave propagation in a two-level system of atoms was studied and the results compared with existing theory. The resonance frequency f_a was taken to be 5×10^{14} Hz with a homogeneously broadened linewidth Δf_a of 5×10^{13} Hz. The radiative decay rate γ_r was chosen to be $5 \times 10^7/\text{s}$. The contribution to the linewidth due to radiative

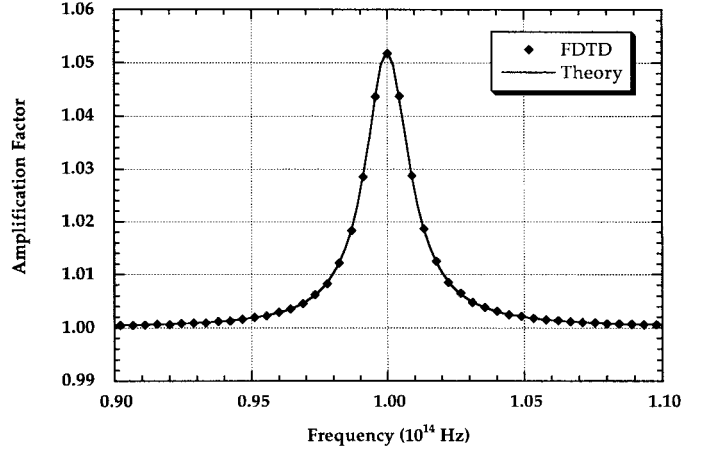


Fig. 7. Comparison of small signal gain versus frequency response for a four-level atomic system as predicted by theory and computed using FDTD.

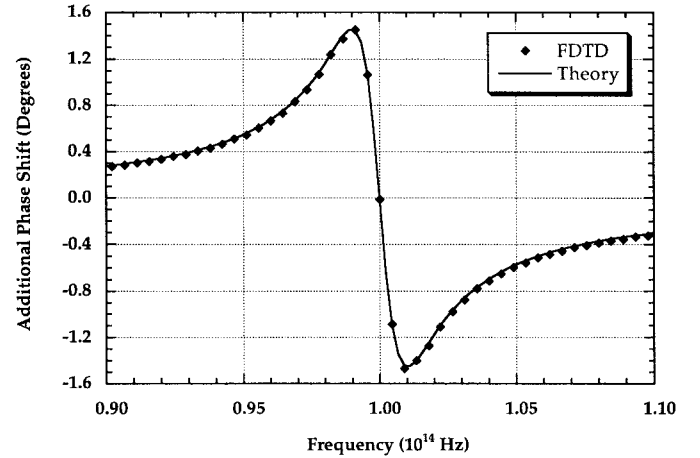


Fig. 8. Contribution of the atomic media to the phase shift versus frequency response. This phase shift is in addition to the normal phase shift that the different frequency components would have experienced if they had propagated the same distance in free space.

and nonradiative decay rates was assumed to be negligible compared to the effect of the population dephasing time T_2 (which can be estimated from the linewidth to be 6.3 fs). For the simulation, the nonradiative decay rate was assumed to be much smaller than the radiative decay resulting in a population recovery time $\tau_{21} = 1/\gamma_r = 20$ ns. The thermal equilibrium population difference ΔN_0 was set to be $1 \times 10^{26}/\text{m}^3$. The relative dielectric constant ϵ_r was chosen to be one and the conductivity of the medium was assumed to be zero. The FDTD parameters were chosen as per the guidelines in [11] to ensure stability and accuracy of the algorithm. The values $\Delta z = \lambda_a/100 = 6$ nm and $\Delta t = 1.8 \times 10^{-17}$ s were used in the simulations. Note that the time step is chosen to be slightly smaller than the value dictated by the Courant condition as the phase velocity exceeds the free-space propagation velocity in the vicinity of the resonance.

To obtain the steady-state small-signal frequency response of the medium, a Gaussian pulse of peak amplitude 100 V/m and RMS width 9 fs, modulated at the resonance frequency of the medium, was allowed to propagate through the medium and the fields were recorded at two different locations that

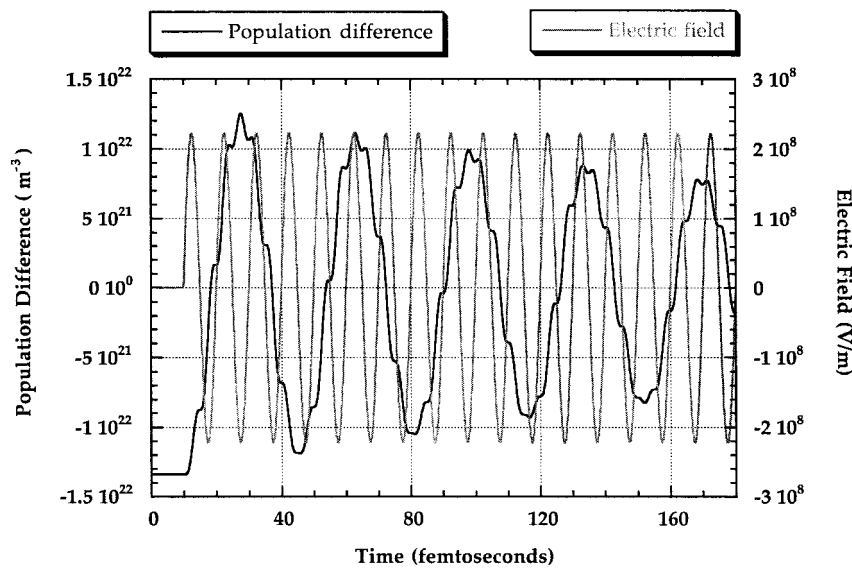


Fig. 9. Population dynamics of the four-level atomic system under the influence of strong applied electric fields. Shown here is time evolution of the population difference $\Delta N(t) = N_1(t) - N_2(t)$ along with the input signal.

were a distance $l = \lambda_a$ apart. The recorded fields were Fourier transformed to calculate the frequency response of the medium. As shown by Figs. 2 and 3, the FDTD data shows extremely good correlation with linear susceptibility theory. The maximum error in the field absorption factor was found to be 0.02% while the maximum error in the phase shift was 0.1%. Good agreement with linear susceptibility theory was to be expected here since the signal intensity was too small to appreciably perturb the populations.

The next step was to model the population dynamics due to signal stimulated transitions and the results are shown in Fig. 4. A step function with carrier frequency at the resonance frequency of the medium was turned on at time $t = 0$ and the population at some point in the medium was recorded as a function of time. Curve (a) corresponds to an electric field amplitude of 100 V/m and it can be seen that the population difference remains constant. In this regime, the two-level system of atoms behaves like a linear absorber. Curve (b) shows the population response to a step function with a peak amplitude of 2.5×10^8 V/m and shows saturation of the population difference. This is the mechanism responsible for absorption saturation in nonlinear absorbers. Curve (c) which is drawn for a peak field amplitude of 5×10^9 V/m shows an interesting feature of the population response under strong signals—Rabi flopping. The exact theoretical response of the population has been calculated before [10] and the results from the FDTD solution show good agreement.

The main utility of the FDTD approach, however, is its ability to model the transient response of the medium as well as large signal effects. A pulse with rise time and fall times that are small compared to the time constant T_2 , but overall duration (36 fs) that is several times T_2 is allowed to propagate through the medium. The fields are recorded at different distances into the medium. Fig. 5 shows the evolution of the pulse shape as it propagates into the medium. The pulse shape can be explained qualitatively based on the argument that the total field is the sum of the incident pulse and the fields

reradiated by the medium. Since the material is an absorber, the reradiated fields are 180° out of phase with the incident pulse and tend to reduce the amplitude of the total fields. However, the atomic media has a finite response time and, hence, the leading edge of the pulse undergoes only a small attenuation as it propagates through the medium. Similarly, at the trailing edge the incident pulse dies out very quickly but the medium continues to radiate a canceling signal till the coherent polarization dies out with the time constant T_2 . This explains the 180° out-of-phase signal that trails the falling edge of the incident pulse. This is commonly referred to as free induction decay. It is important to note that this behavior results entirely from the linear or small signal transient behavior of the absorbing medium.

Fig. 6 shows interesting nonlinear effects of the medium when an intense pulse with short rise and fall times is allowed to propagate through the medium. The leading edge shows behavior similar to the pulse in Fig. 5. However, due to signal stimulated transitions the population difference goes to zero and even becomes negative implying that population inversion has taken place. Thus, the later portions of the pulse undergo smaller absorption and, finally, even some gain. These kinds of amplitude modulation effects have been known to exist in saturable absorbers [12]. Note that the amplitude modulation of the pulse follows the oscillation in the population difference and has the same period. Another interesting feature that is not predicted theoretically is the flattening of the population response curve at times where the electric field goes to zero. Similar behavior has been observed in other FDTD simulations [9] and is shown there to be due to time derivative effects of the field.

A four-level system of atoms with population inversion between levels E_2 and E_1 was also simulated. The transition frequency associated with the energy levels E_2 and E_1 was chosen as $f_{21} = 1 \times 10^{14}$ Hz and the linewidth was taken to be 2.0×10^{12} Hz corresponding to a dephasing time T_2 of 1.59×10^{-13} s. The radiative decay rate for this transition

from E_2 to E_1 was taken to be $7.4 \times 10^6/\text{s}$. The time constants for the population rate equations were chosen as $\tau_3 = 1 \times 10^{-10}$ s, $\tau_{32} = 0.99 \times 10^{-10}$ s, $\tau_{31} = 1 \times 10^{-6}$ s, $\tau_2 = \tau_{21} = 1.35 \times 10^{-7}$ s, and $\tau_1 = 1 \times 10^{-9}$ s. The pumping rate into level E_3 was set to be $1 \times 10^{29} \text{ m}^{-3}$ and was assumed to be uniform over the entire spatial domain. This may be easily modified to account for nonuniform spatial pumping effects. The FDTD parameters used for the simulations were $\Delta z = 30$ nanometers and $\Delta t = 9 \times 10^{-17}$ s. Here again, the time step was chosen slightly smaller than the Courant limit due to anomalous dispersion close to the resonance frequency.

A Gaussian pulse of amplitude 1 V/m and rms width 9 fs with carrier frequency 1×10^{14} Hz was allowed to propagate through the medium and the fields were recorded at two points separated by a distance of $3 \mu\text{m}$. The small signal field gain is shown in Fig. 7 and the additional phase shift contribution of the atomic media is plotted in Fig. 8. The results obtained from FDTD show good agreement with theory and the maximum error in field gain was 0.02% and the maximum error in phase was 0.12%. The time evolution of the population difference $\Delta N_{12}(t)$ under the influence of signal stimulated transitions was studied by using a step signal with carrier frequency same as f_{12} and peak amplitude 2×10^8 V/m. The electric field and the population difference at $z = 3 \mu\text{m}$ is shown in Fig. 9. The time-derivative effects [9] of the field on the population are seen as flattening of the population difference at points where the electric field goes to zero.

VI. CONCLUSIONS

The ADE-FDTD approach for modeling dispersive media was extended to accurately model nonlinear effects in absorbing and gain media by including the effects of the signal on the atomic populations through the rate equations. The results show extremely good correlation with existing theoretical models for the small-signal frequency response. Population dynamics under the influence of strong incident fields were also successfully modeled using this technique. The utility of FDTD modeling to calculate exactly transient effects in nonlinear media was demonstrated by studying pulse propagation.

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