

# Modeling of Electromagnetic Waves Propagation in Four-Level Two-Electron Atomic Systems Governed by Pauli Exclusion Principle Using the TLM Method

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**Abstract**— This paper presents a computational model of electrons dynamics and gain in four-level two-electron atomic systems. These systems, submitted to an electromagnetic wave, are governed by Pauli Exclusion Principle and they are modeled using the Time-Domain Transmission Line Matrix (TLM) method with the symmetrical condensed node (SCN) with novel voltage sources. The development of the proposed model is based on the incorporation, in Maxwell's equations, of the coupled rate equations with Pauli Exclusion Principle, taking into account the dynamic pumping in the TLM formulation. The scattering matrix characterizing the SCN with the new voltage sources is provided and the numerical results are compared with those of the literature or with the theoretical ones.

**Index Terms**— Atomic media, TLM method, Pauli Exclusion Principle.

## I. INTRODUCTION

During the propagation of an electromagnetic (EM) wave in a medium, it can be submitted to three processes: spontaneous emission, stimulated absorption and emission. These processes contribute, according to the rate equations, to the evolution of the population densities of electron energy states during propagation [1]. On the other hand, the space-time evolution of EM waves, during propagation, obeys Maxwell's equations, and depends on the macroscopic polarization density owing to the response of the medium to the EM wave. When the field has a low intensity, the polarization density is supposed proportional to the electric field intensity. This kind of non-linear interaction allows the exchange of energy between EM waves and the electrons of the medium. Several papers have modeled these interactions using FDTD method [2]-[5], in particular the approach based on the auxiliary differential equation (ADE), to study absorption in two-energy level atomic systems and gain of four-level systems [2]. By coupling Maxwell's equations and the rate equations describing electrons population, this method can model EM wave propagation in random gain media [3]. It was also used, by including Pauli Exclusion Principle and the dynamic pumping, to study EM wave

interaction with four-level two-electron atomic systems [4] and multi-level multi-electron atomic systems [5].

The Transmission Line Matrix (TLM) method [6]-[11] was rarely used for modeling this kind of phenomena, the first approach modeling quantum properties of two energy level atomic systems were proposed in [8]. In order to explore this field and to contribute to the development of a novel numerical model using the Time-Domain TLM method with the symmetrical condensed node (SCN), we have introduced novel voltage sources to this node [9]-[11] by including Pauli Exclusion Principle and dynamic pumping. This new model describes the space-time evolution of electrons populations' densities in each energy level and gives the frequency evolution of the gain in the atomic system of four-level two-electron. Furthermore, the scattering matrix characterizing the SCN with the new voltage sources is provided and the simulation's results are compared to those of the literature or obtained by the theoretical solutions.

## II. FORMULATION

The propagation of EM waves in atomic systems induces a time depending dipolar moment in the different atoms [1]. This shows the importance of the dipolar radiation theory which allows to give a simple interpretation of several phenomena related with EM waves interactions with material in the classical model. In addition to Maxwell's equations which govern EM wave propagation in this medium, it is necessary to take into account the equations of the oscillations due to wave and material interactions, and also the energy level population rate equations, which allow to predict the number of electrons in each energy level, coupled with Pauli Exclusion Principle.

### A. Macroscopic polarization equations

Electron transitions in atomic systems with four energy levels  $E_i$  and respective normalized densities  $N_i$  ( $i = 0, 1, 2, 3$ ) are considered as in a simplified model of two oscillating dipoles:  $P_a$  for  $E_1$  to  $E_2$  transitions with a frequency  $\omega_a$  and  $P_b$  for  $E_0$  to  $E_3$  transitions with a pumping frequency  $\omega_b$  illustrated in Fig. 1.

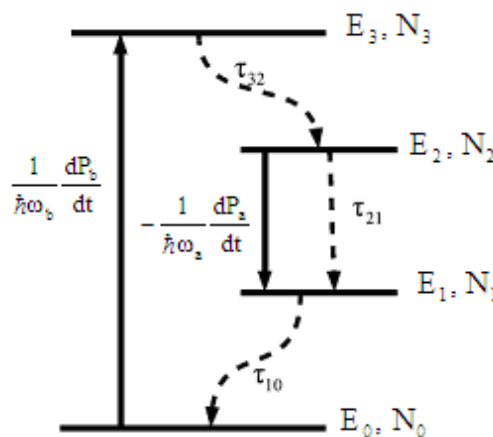


Fig. 1. Four-level two-electron model.

The equations of macroscopic polarization are [4]:

$$\begin{aligned} \frac{d^2 \overline{P}_a(t)}{dt^2} + \Delta\omega_a \frac{d\overline{P}_a(t)}{dt} + \omega_a^2 \overline{P}_a(t) &= k_a (N_1 - N_2) \overline{E}(t) \\ \frac{d^2 \overline{P}_b(t)}{dt^2} + \Delta\omega_b \frac{d\overline{P}_b(t)}{dt} + \omega_b^2 \overline{P}_b(t) &= k_b (N_0 - N_3) \overline{E}(t) \end{aligned} \quad (1)$$

Where  $k_a = \frac{6\pi\epsilon_0 c^3}{\omega_a^2} \gamma_{ra}$ ,  $k_b = \frac{6\pi\epsilon_0 c^3}{\omega_b^2} \gamma_{rb}$ .

$\epsilon_0$  is the permittivity of free space and  $\gamma_{ra} = \frac{1}{\tau_{21}}$ ,  $\gamma_{rb} = \frac{1}{\tau_{30}}$  are the radiative energy decay rates.

$\Delta\omega_a$  and  $\Delta\omega_b$  are the total energy attenuation rate which describe the spectral line width of the transition taking into account the energy loss by pumping and relaxation effects.

### B. Pauli Exclusion Principle

In an atom having many electrons, we must take into account Pauli Exclusion Principle which forbids two electrons to have the same quantum state. This principle allows to determine electron distributions in the different energy levels. In a four-level two-electron atomic system, submitted to a dynamic pumping, this principle appears through the rate equations describing electrons populations' densities in each energy level by introducing a factor  $(1-N)$ , where  $N$  is the normalized density of the population in the lower energy level. In this case, the modified rate equations are given by [4]:

$$\begin{aligned} \frac{dN_3}{dt} &= -\frac{N_3(1-N_2)}{\tau_{32}} - \frac{N_3(1-N_0)}{\tau_{30}} + \frac{1}{\hbar\omega_b} \overline{E} \frac{d\overline{P}_b}{dt} \\ \frac{dN_2}{dt} &= \frac{N_3(1-N_2)}{\tau_{32}} - \frac{N_2(1-N_1)}{\tau_{21}} + \frac{1}{\hbar\omega_a} \overline{E} \frac{d\overline{P}_a}{dt} \\ \frac{dN_1}{dt} &= \frac{N_2(1-N_1)}{\tau_{21}} - \frac{N_1(1-N_0)}{\tau_{10}} - \frac{1}{\hbar\omega_a} \overline{E} \frac{d\overline{P}_a}{dt} \\ \frac{dN_0}{dt} &= \frac{N_3(1-N_0)}{\tau_{30}} + \frac{N_1(1-N_0)}{\tau_{10}} - \frac{1}{\hbar\omega_b} \overline{E} \frac{d\overline{P}_b}{dt} \end{aligned} \quad (2)$$

Where  $N_i$  is the normalized density of electrons populations in the energy levels  $E_i$  ( $i = 0, 1, 2, 3$ ) and  $\tau_{ij}$  is the life-mean -time of electrons between energy levels  $E_i$  and  $E_j$ .

### C. TLM Model for a Four-Energy-Level Two-Electron Atomic Systems

In order to implement a numerical model for the simulation of the interaction of EM wave with four-energy level two-electron atomic systems using the TLM method with the SCN and novel voltage sources, we combine the equations (1) and (2) with those of Maxwell:

$$\begin{aligned} \nabla \Lambda \overline{H} &= \epsilon_0 \frac{\partial \overline{E}(t)}{\partial t} + \frac{\partial (\overline{P}_a(t) + \overline{P}_b(t))}{\partial t} \\ \nabla \Lambda \overline{E} &= -\mu_0 \frac{\partial \overline{H}(t)}{\partial t} \end{aligned} \quad (3)$$

Let's consider an EM wave propagating in a 3D regular mesh ( $\Delta x = \Delta y = \Delta z$ ), Maxwell's equations time-discretization with a time step  $\Delta t$  gives at a time  $t^n = n\Delta t$ , the following expressions:

$$\begin{aligned}
 E^{n+1}(i, j, k) &= E^n(i, j, k) - \frac{1}{\epsilon_0}(P_t^{n+1}(i, j, k) - P_t^n(i, j, k)) + \frac{\Delta t}{\epsilon_0} \nabla \Lambda H^{n+\frac{1}{2}}(i, j, k) \\
 H^{n+1}(i, j, k) &= H^n(i, j, k) - \frac{\Delta t}{\mu_0} \nabla \Lambda E^{n+\frac{1}{2}}(i, j, k)
 \end{aligned}
 \tag{4}$$

Where  $P_t(i, j, k) = P_t(i, j, k) + P_t(i, j, k)$ .

The TLM approach modeling EM wave interactions with atomic systems governed by Pauli Exclusion Principle is formulated from the equations given below. In these equations, we have replaced the EM parameters (E, H) by their equivalent voltages and currents (V, I):

$$V = E \cdot \Delta L, I = H \cdot \Delta L \text{ and } V = Z_0 \cdot I \tag{5}$$

Where  $\Delta l$  is the space step and  $Z_0$  is the intrinsic impedance of vacuum. Thus, the equations (4) become:

$$\begin{aligned}
 V^{n+1}(i, j, k) &= V^n(i, j, k) - \frac{\Delta l}{\epsilon_0}(P_t^{n+1}(i, j, k) - P_t^n(i, j, k)) + \frac{\Delta t}{\epsilon_0} \Delta l \cdot \nabla \Lambda H^{n+\frac{1}{2}}(i, j, k) \\
 I^{n+1}(i, j, k) &= I^n(i, j, k) - \frac{\Delta t}{\mu_0} \Delta l \cdot \nabla \Lambda E^{n+\frac{1}{2}}(i, j, k)
 \end{aligned}
 \tag{6}$$

The fields (E, H) in the curls of equations (6) are converted into local incident and scattered voltage pulses  $V^i$  and  $V^r$  on the faces of the SCN of the TLM Method [6]-[7]. Thus making use of charge and energy conservation principle through the transmission lines forming the SCN, and imposing the continuity conditions on the electric and magnetic fields [6], we obtain at time  $n\Delta t$  the following scattering matrix of the SCN with voltage sources:

$$\begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \\ V_7 \\ V_8 \\ V_9 \\ V_{10} \\ V_{11} \\ V_{12} \end{pmatrix}^r = \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & -1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \\ V_7 \\ V_8 \\ V_9 \\ V_{10} \\ V_{11} \\ V_{12} \end{pmatrix}^i + \frac{1}{4} \begin{pmatrix} V_{sx} & 0 & 0 \\ V_{sx} & 0 & 0 \\ 0 & V_{sy} & 0 \\ 0 & V_{sy} & 0 \\ 0 & 0 & V_{sz} \\ 0 & 0 & V_{sz} \\ 0 & 0 & V_{sz} \\ 0 & V_{sy} & 0 \\ V_{sx} & 0 & 0 \\ 0 & 0 & V_{sz} \\ 0 & V_{sy} & 0 \\ V_{sx} & 0 & 0 \end{pmatrix} \tag{7}$$

The obtained matrix models EM wave propagation in an atomic system taking into account the physical effects related with the medium polarization with the voltage sources  $(V_{sx}, V_{sy}, V_{sz})$  which are expressed as follows:

$$V_{su}^{n+1} + V_{su}^n = - \frac{\Delta l}{\epsilon_0} (P_{tu}^{n+1}(i, j, k) - P_{tu}^n(i, j, k)) \tag{8}$$

Where  $u=x, y, z$ .  $P^{n+1}$  is the medium's polarization at time  $t^{n+1} = (n+1)\Delta t$ . Its expressions are deduced from the time discretization of equations (1):

$$\begin{aligned} P_{au}^{n+1}(i, j, k) &= \frac{2\Delta t^2}{2+\Delta\omega_a\Delta t} \left[ \left( \frac{2}{\Delta t^2} - \omega_a^2 \right) P_{au}^n(i, j, k) + \left( \frac{\Delta\omega_a}{2\Delta t} - \frac{1}{\Delta t^2} \right) P_{au}^{n-1}(i, j, k) + k_a(N_{1u}^n - N_{2u}^n) \frac{V_u^n(i, j, k)}{\Delta l} \right] \\ P_{bu}^{n+1}(i, j, k) &= \frac{2\Delta t^2}{2+\Delta\omega_b\Delta t} \left[ \left( \frac{2}{\Delta t^2} - \omega_b^2 \right) P_{bu}^n(i, j, k) + \left( \frac{\Delta\omega_b}{2\Delta t} - \frac{1}{\Delta t^2} \right) P_{bu}^{n-1}(i, j, k) + k_b(N_{0u}^n - N_{3u}^n) \frac{V_u^n(i, j, k)}{\Delta l} \right] \end{aligned} \tag{9}$$

The TLM method with voltage sources algorithm implementation is based on a recursive computation of  $P_{au}^{n+1}(i, j, k)$  and  $P_{bu}^{n+1}(i, j, k)$  given by the equation (9). This allows to update voltage sources given by (8),  $V^{n+1}(i, j, k)$  from (6) and to determine the population densities  $N_i^{n+1}$  with  $i=0, 1, 2, 3$  given by (2). Local scattered voltage pulses  $V^r$  at the SCN are obtained from the scattering matrix expressed in (7). Finally, we establish connections between nodes along the spatial TLM lattice.

### III. NUMERICAL RESULTS

The proposed model was used to simulate the effect of an incident EM wave on a four-level two-electron atomic system. This allows to predict the electrons dynamic between energy levels by the modified rate equations, by introducing Pauli Exclusion Principle and pumping dynamic as well as the incident signal amplification by this system. The physical parameters characterizing this atomic system of four energy levels  $E_0 < E_1 < E_2 < E_3$  with two electrons are [2]:  $\omega_a = 2\pi \cdot 10^{14}$  rad/s,  $\omega_b = 2\pi \cdot 10^{16}$  rad/s,  $\Delta\omega_a = \Delta\omega_b = 4\pi \cdot 10^{12}$  rad/s, with the electron life-time between energy levels  $\tau_{32} = 0,99 \cdot 10^{-10}$  s,  $\tau_{21} = 1,35 \cdot 10^{-7}$  s,  $\tau_{10} = 1 \cdot 10^{-9}$  s,  $\tau_{30} = 1 \cdot 10^{-10}$  s, and initial normalized electrons population densities in the energy level  $N_0 = N_1 = 1$  and  $N_2 = 0$ . The spatial TLM lattice considered is  $(1,1,1000)\Delta l$ , with  $\Delta l$  is the mesh width taken to be  $3 \cdot 10^{-2}$   $\mu\text{m}$ . The atomic system spans the cells located between  $8\Delta l$  and  $208\Delta l$  in the  $z$  direction. The air-system interface is excited first with a sine wave of amplitude  $2 \cdot 10^8$  V/m and frequency  $1 \cdot 10^{14}$  Hz. In order to prove the efficiency of the proposed model, we present in Fig. 2 the time evolution of the population difference  $\Delta N_{12} = N_1 - N_2$  at  $z=108\Delta l$ . The results obtained from TLM method show good agreement with FDTD method [2].

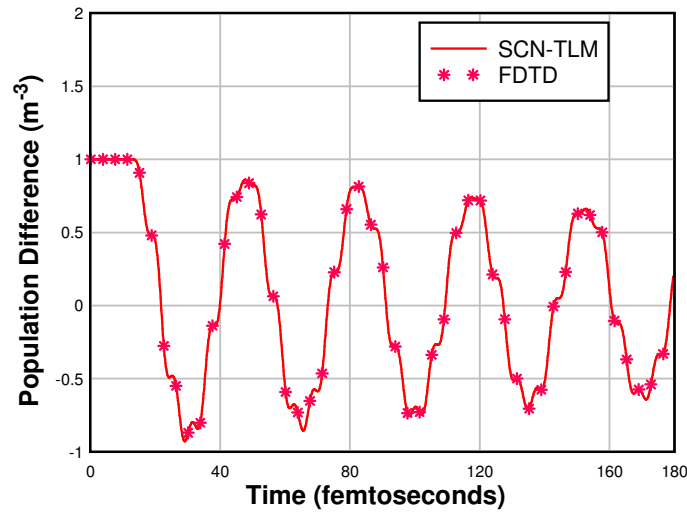


Fig. 2. Comparison of population difference as computed by SCN-TLM and FDTD methods.

In the beginning of the dynamic pumping, the electrons move from  $E_1$  to  $E_0$ , then to  $E_3$  and finally to  $E_2$ . The population in level  $E_1$  starts to decrease and the population in level  $E_2$  starts to increase. The time evolution, of the electrons population densities in the different energy levels, is shown in Fig. 3.

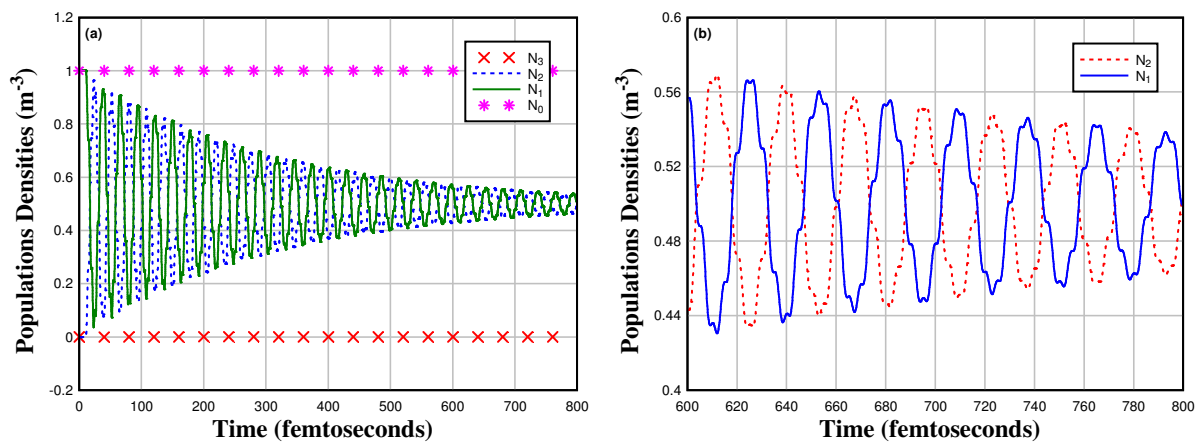


Fig. 3. (a) Time variation of the population densities  $N_0$ ,  $N_1$ ,  $N_2$  and  $N_3$ .  
(b) The inversion between energy levels  $E_1$  and  $E_2$ .

Figure 4 illustrates the space evolution of the population densities after 8000 time step.  $N_1$  decreases and  $N_2$  increases quickly at  $z = 24.10^{-2} \mu\text{m}$  which corresponds to the air-system interface. Through the TLM mesh,  $N_1$  and  $N_2$  vary slightly about the same limit value 0.5 in the opposite direction, which indicates the saturation of the EM transition.

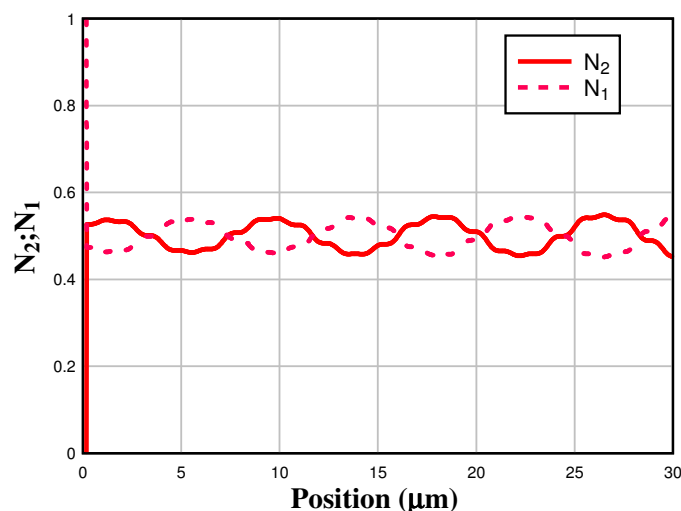


Fig. 4. Evolution of the population densities along the TLM mesh after 8000 time step.

In the second part, we have excited the air-system interface using a Gaussian wave of amplitude 1V/m and frequency  $1.10^{14}$  Hz [2]. The values of the electric field magnitudes in the two edges, air-system and system-air, allow to evaluate the amplification factor as shown in Fig. 5. Here again, the TLM method generates results in very good agreement with those of [2] and with the theoretical ones [1].

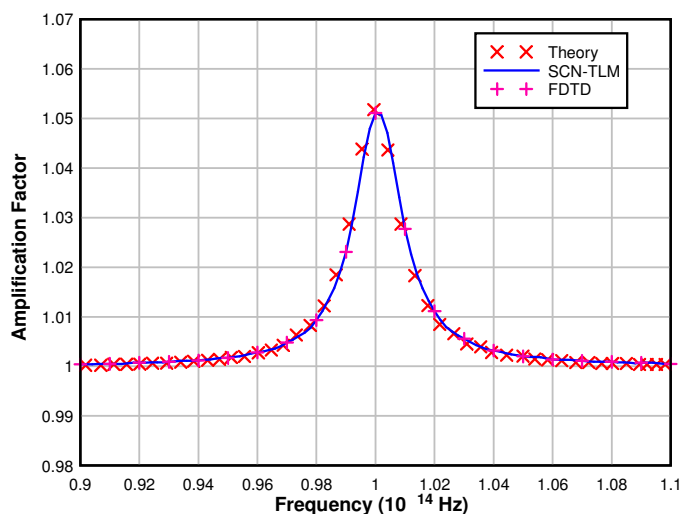


Fig. 5. Comparison of amplification factor versus frequency as computed by theory, FDTD and SCN-TLM methods.

#### IV. CONCLUSION

We have developed a novel modeling approach for EM wave propagation in four-level two-electron atomic systems, using the SCN-TLM method, with new voltage sources including Pauli Exclusion Principle and dynamic pumping coupled with the population rate equations. In order to illustrate the validity of this novel model combining both classical electrodynamics with quantum mechanics, we have simulated the electrons dynamic between two energy levels through the variation of populations' densities by the modified rate equations with Pauli Exclusion Principle, pumping equation and computing the incident field amplification. The good agreement between the novel TLM approach

results and those available in the literature proves its validity and efficiency. Hence, this study contributes to the widening of the field of the problems treated by the TLM method.

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