

# A numerical model for light interaction with a two-level atom medium.

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The aim of this work is to study the interaction of a laser pulse with a gas described by the Bloch equations. The physical model is derived from the Maxwell-Bloch equations under the assumption that the polarization and the electric field are both oriented in a single direction, and under the slowly varying envelope approximation. The Schrödinger equation is formulated for a two-level atom medium under the rotating wave approximation and dipole interaction. A rigorous asymptotic analysis of the simplified system is performed to point out the different mechanisms associated with the physical model. A numerical approach based on a splitting technique is proposed and successfully performed.

**Key Words:** *Nonlinear Optics, Two-level Atom, Asymptotic Analysis, Splitting Scheme, Lasers pulses.*

## 1. Introduction

Many topics of interest in nonlinear optical applications are related to the propagation of light and to the interaction of the electric field with material media (see for example [23,7,18] for numerical study). The regime of the laser sources (small wavelength) displays quantum mechanical coupling via the optical properties of the medium (see for example the classical textbooks [19,8,17]). The density of the material medium is either high [23] or low [16]. Then according to the intensity of the laser beams, we can obtain different levels of linear and nonlinear interactions. Modeling and computing those behaviors are difficult numerical challenges. The full description of the light-matter interaction involves the resolution of the Maxwell equation coupled to the atomic wave function which obeys the Schrödinger equations [8,19]. The numerical approach of this model is only possible for simplified media with a small number of atoms. The nonlinear Maxwell-Bloch system is a macroscopic model taking into account the quantum mechanical coupling for a large class of media. It contains some essential numerical difficulties. In some cases, the full wave integration of this system is unavoidable and has been investigated in the finite difference time-domain (FDTD) context [22,15]. In general the computational time needed for those applications is very expensive (see [7,12,9] for general nonlinearity and [5,4,24,23,20] for Maxwell-Bloch systems). However, we are concerned with the propagation of a quasi-monochromatic optical field in a dilute atomic vapor. Atoms with two energy levels

connected by an electric-dipole transition are embedded in the medium. The laser beam frequency is nearly resonant with the atomic transition and sufficiently intense to remove a significant fraction of the population from the atomic ground state to the excited state.

We assume that the envelope of the optical field is slowly varying and that the nonlinear polarization is a perturbation term. The polarization and the electric field are supposed to be oriented with the same fixed direction so that they can be treated as scalar quantities. The Schrödinger equation is formulated for a two-level atom medium under the rotating wave approximation [8] and dipole interaction. In order to obtain an efficient numerical scheme, a nonlinear transformation is introduced to simplify the derived system. This transformation is inspired from [13] and is one of the key point of this work. Using a set of parameters associated to an industrial application, we perform a scaling of the equations and identify a small parameter. The asymptotic analysis is then performed and leads to the characterization of the important operators governing the coupling mechanism. According to this characterization, a numerical model, that respects the properties of the main operators, is proposed. This method is applied to a boundary value problem. This paper is organized as follows: in Section 2, the physical model is derived from the Maxwell-Bloch system. In Section 3, rigorous asymptotic expansions are performed. We present the numerical method in Section 4. In Section 5, we give some numerical results. We validate our numerical approach in the asymptotic regimes described in Section 3. Finally, in Section 6, we list some open questions concerning this problem.

## 2. Physical model

### 2.1. Statement of the basic equations

We are interested in the isotopic separation of uranium using an ionization by interaction with a nearly resonant laser. The uranium atomic gas is composed of  $U^{235}$  ( $\sim 0.1\%$ ) and  $U^{238}$  ( $\sim 99.9\%$ ) isotopes. In order to separate the  $U^{235}$  isotope, the  $U^{235}$  is ionized before going across a Coulomb electric field. The ionization is obtained by an intense laser that is resonant with the transition frequency of the  $U^{235}$  isotope. However, the transition frequency of both isotopes are very close so that a large part of the gas is excited. The aim here is to propose an efficient numerical approach to compute the laser interaction with the  $U^{238}$  isotope. Indeed, this interaction involves restrictive numerical constraints related to the finite-difference stability and makes the computations inefficient. For the sake of simplicity, we restrict ourselves to the 2-D case (the unknowns depend only on two variables but live in  $\mathbf{R}^3$ ). We call  $(x, z) \in \mathbf{R}^2$  the basic coordinates and  $(e_x, e_y, e_z)$  the basis of  $\mathbf{R}^3$ .

The basic assumptions used for the model are :

- The elements of the dipole matrix and the electric field are singly oriented in the direction  $e_y$  :  $\mathbf{E} = \mathcal{E}e_y$ ,  $\mathbf{B} = B_x e_x + B_z e_z$  where  $\mathbf{E}$  denotes the electric field and  $\mathbf{B}$  denotes the magnetic field.
- The matter is composed of two-level atoms.
- The laser is nearly resonant with the medium.

The starting point of our model is the 2D Maxwell-Bloch equations in the transverse magnetic mode:

$$\partial_t B_z + \partial_x \mathcal{E} = 0,$$

$$\partial_t B_x - \partial_z \mathcal{E} = 0,$$

$$\partial_t \mathcal{E} - c^2(\partial_z B_x - \partial_x B_z) = -\mu_0 c^2 \partial_t P,$$

$$\partial_t C_1 + i\omega_1 C_1 = i\Omega C_2,$$

$$\partial_t C_2 + i\omega_2 C_2 = i\Omega C_1,$$

where the  $C_i$ 's are the complex representations of the populations,  $P = \mathcal{N}\mu(C_1\overline{C_2} + \overline{C_1}C_2)$  is the physical polarization,  $\mathcal{N}$  is the density of atoms per unit of volume,  $\mu$  is the dipole coupling coefficient,  $c$  is the speed of light,  $\mu_0$  the permeability of free space,  $\Omega = \frac{\mu\mathcal{E}}{\hbar}$  is the Rabi frequency and  $\hbar$  the Planck constant. The frequencies  $\omega_1$  and  $\omega_2$  are associated with each level. For a two-level atom, it is usual [17] to formulate the Bloch equations with the variables  $N = |C_1|^2 - |C_2|^2$  and  $\Lambda = C_1\overline{C_2}$ :

$$\partial_t \Lambda = i\omega_{21}\Lambda - i\Omega N, \quad \partial_t N = -2i\Omega(\Lambda - \overline{\Lambda}),$$

where  $\omega_{21} = \omega_2 - \omega_1$ . Since the laser is only nearly resonant with the medium (that is, its frequency is close to  $\omega_{21}$  but not equal to  $\omega_{21}$ ), one expects that the excitation process will be weak and that  $|C_2| \ll |C_1|$  for all time (starting with atoms that are all in the fundamental state). Moreover since  $|C_1|^2$  (resp.  $|C_2|^2$ ) is the probability for an atom to be in the energy level 1 (resp. 2), one has  $|C_1|^2 + |C_2|^2 = 1$ . Therefore we expect  $N \sim 1$  and we look for  $N$  under the form  $N = 1 - \tilde{N}$ . The Bloch equations then read:

$$\partial_t \Lambda = i\omega_{21}\Lambda - i\Omega + i\Omega\tilde{N},$$

$$\partial_t \tilde{N} = 2i\Omega(\Lambda - \overline{\Lambda}),$$

or dropping the tildes:

$$\partial_t \Lambda = i\omega_{21}\Lambda - i\Omega + i\Omega N,$$

$$\partial_t N = 2i\Omega(\Lambda - \overline{\Lambda}),$$

We now present a dimensionless form of the system formed by the Maxwell equations and the Bloch equations. Let  $T_{ref}$  be a characteristic time of the problem (taken equal to the duration of the pulse), let  $L_{ref} = cT_{ref}$  the characteristic length in the direction of propagation ( $L_{ref}$  is the length of the pulse), and let  $\rho_{ref}$  the characteristic length in the transverse direction. The characteristic value of the electric field  $\mathcal{E}_{ref}$  is given by the characteristic value of the Rabi frequency  $\omega_r = \frac{\mu\mathcal{E}_{ref}}{\hbar}$  which is given. As usual, we take  $B_{ref} = \frac{\mathcal{E}_{ref}}{c}$  as the characteristic value of  $B_x$  and  $B_y$ . We denote by  $\Lambda_{ref}$  and

$N_{ref}$  the characteristic values of  $\Lambda$  and  $N$  that are to be determined later on. Moreover we introduce the phase mismatch parameter  $\Delta = \omega - \omega_{21}$  that measures the difference between the frequency of light  $\omega$  and the characteristic frequency  $\omega_{21}$  of the medium. One obtains the following system for the dimensionless variables:

$$\partial_t B_z + \frac{cT_{ref}}{\rho_{ref}} \partial_x \mathcal{E} = 0, \quad (1)$$

$$\partial_t B_x - \partial_z \mathcal{E} = 0, \quad (2)$$

$$\partial_t \mathcal{E} - \left( \partial_z B_x - \frac{cT_{ref}}{\rho_{ref}} \partial_x B_z \right) = -\frac{\mu_0 c^2 \Lambda_{ref} \mathcal{N} \mu}{\mathcal{E}_{ref}} \partial_t (\Lambda + \bar{\Lambda}), \quad (3)$$

$$\partial_t \Lambda = i(\omega - \Delta) T_{ref} \Lambda - i \frac{\omega_r T_{ref}}{\Lambda_{ref}} \mathcal{E} + i \frac{\omega_r T_{ref} N_{ref}}{\Lambda_{ref}} \mathcal{E} N, \quad (4)$$

$$\partial_t N = 2i \frac{\omega_r T_{ref} L_{ref}}{N_{ref}} \mathcal{E} (\Lambda - \bar{\Lambda}). \quad (5)$$

We now explain how to find  $\Lambda_{ref}$  and  $N_{ref}$ . We consider the linear part of equation (4):

$$\partial_t \Lambda = i(\omega - \Delta) T_{ref} \Lambda - i \frac{\omega_r T_{ref}}{\Lambda_{ref}} \mathcal{E}. \quad (6)$$

The electric field will be of the form  $e^{i\omega T_{ref} t} \tilde{\mathcal{E}}(t)$ . Therefore, we look for a solution of (6) of the form  $\Lambda = e^{i\omega T_{ref} t} \tilde{\Lambda}$ . The equation satisfied by  $\tilde{\Lambda}$  is :

$$\partial_t \tilde{\Lambda} + i\omega T_{ref} \tilde{\Lambda} = i(\omega - \Delta) T_{ref} \tilde{\Lambda} - i \frac{\omega_r T_{ref}}{\Lambda_{ref}} \tilde{\mathcal{E}}.$$

One gets

$$\tilde{\Lambda} = \int_0^t e^{-i\Delta T_{ref}(t-s)} \left( -i \frac{\omega_r T_{ref}}{\Lambda_{ref}} \tilde{\mathcal{E}} \right) ds = -i \frac{\omega_r T_{ref}}{\Lambda_{ref}} \int_0^t e^{-i\Delta T_{ref}(t-s)} \tilde{\mathcal{E}}(s) ds$$

since  $\tilde{\Lambda}(t=0) = 0$ . We perform an integration by part in time and obtain:

$$\tilde{\Lambda} = -\frac{\omega_r}{\Delta \Lambda_{ref}} \left( \left[ e^{-i\Delta T_{ref}(t-s)} \tilde{\mathcal{E}} \right]_0^t - \int_0^t e^{-i\Delta T_{ref}(t-s)} \partial_t \tilde{\mathcal{E}} ds \right).$$

The near resonance hypothesis implies (see below for numerical values) :

$$\omega T_{ref} \gg \Delta T_{ref} \gg 1.$$

The dominant term in this expression is therefore:

$$\tilde{\Lambda} = -\frac{\omega_r}{\Delta\Lambda_{ref}}\tilde{\mathcal{E}} + O\left(\frac{1}{\Delta T_{ref}}\right).$$

In order to obtain order  $O(1)$  effects on  $\tilde{\Lambda}$ ,  $\Lambda_{ref}$  is set to

$$\Lambda_{ref} = \frac{\omega_r}{\Delta}. \quad (7)$$

As explained before,  $|C_1| \approx 1$  and  $|C_2| \ll 1$ , therefore since  $N = 1 - (|C_1|^2 - |C_2|^2) = 2|C_2|^2$  (we have used  $|C_1|^2 + |C_2|^2 = 1$ ) and since  $|\Lambda| = |C_1||C_2| \approx |C_2|$ , it follows that

$$N_{ref} = 2\Lambda_{ref}^2. \quad (8)$$

System (1)-(5) now reads:

$$\begin{aligned} \partial_t B_z + \frac{cT_{ref}}{\rho_{ref}}\partial_x \mathcal{E} &= 0, \\ \partial_t B_x - \partial_z \mathcal{E} &= 0, \\ \partial_t \mathcal{E} - (\partial_z B_x - \frac{cT_{ref}}{\rho_{ref}}\partial_x B_z) &= -i\frac{\mu_0 c^2 \mu^2 \omega_{21} T_{ref} \mathcal{N}}{\Delta \hbar}(\Lambda - \bar{\Lambda}), \\ \partial_t \Lambda &= i(\omega - \Delta)T_{ref}\Lambda - i\Delta T_{ref}\mathcal{E} + i\frac{2\omega_r^2 T_{ref}}{\Delta}\mathcal{E}N, \\ \partial_t N &= iT_{ref}\Delta\mathcal{E}(\Lambda - \bar{\Lambda}). \end{aligned}$$

We now introduce the following parameters:

$$\varepsilon = \frac{1}{\Delta T_{ref}}, \quad \nu = \frac{1}{\omega T_{ref}}, \quad \varepsilon_1 = \frac{\rho_{ref}}{cT_{ref}}, \quad \beta = \frac{\mu^2 \omega_{21} T_{ref} \mathcal{N}}{2\varepsilon_0 \Delta \hbar} \text{ and } \alpha = \frac{2T_{ref}\omega_r^2}{\Delta}.$$

The system reads:

$$\begin{aligned} \partial_t B_z + \frac{1}{\varepsilon_1}\partial_x \mathcal{E} &= 0, \\ \partial_t B_x - \partial_z \mathcal{E} &= 0, \\ \partial_t \mathcal{E} - (\partial_z B_x - \frac{1}{\varepsilon_1}\partial_x B_z) &= -2i\beta(\Lambda - \bar{\Lambda}), \\ \partial_t \Lambda &= \frac{i}{\nu}\Lambda - \frac{i}{\varepsilon}\Lambda - \frac{i}{\varepsilon}\mathcal{E} + i\alpha\mathcal{E}N, \\ \partial_t N &= \frac{i}{\varepsilon}\mathcal{E}(\Lambda - \bar{\Lambda}). \end{aligned}$$

**Numerical values:** For our particular physical situation, one has  $T_{ref} = 2.10^{-8}s$ ; this gives  $L_{ref} = 6m$ . We choose  $\rho_{ref} = 1cm$ . The density of polarized atoms is  $\mathcal{N} = 5.10^{18}atoms/m^3$  (this is a very dilute gas). The characteristic value of the Rabi frequency

is  $\omega_r = 10^9 \text{rad/s}$ . The dipole coupling coefficient is  $\mu = 5.10^{-31}$  in usual units, the electric dipole frequency is  $\omega_{21} \sim \pi 10^{15} \text{rad/s}$  and the phase mismatch  $\Delta \sim 10^{10} \text{rad/s}$ . The laser frequency is also of order  $\pi 10^{15} \text{rad/s}$ . We recall the value of the constant:  $\varepsilon_0 = 8.85.10^{-12} \text{F/m}$  and  $\hbar = 10^{-34} \text{Js}$ . With these values we obtain:

$$\varepsilon \sim 5.10^{-3}, \nu \sim 10^{-8}, \varepsilon_1 \sim 10^{-3}, \beta \sim 1 \text{ and } \alpha \sim 1.$$

We therefore have three small parameters. The aim of the next section is to perform an asymptotic expansion in order to obtain a simplified model. We could make the expansion  $\varepsilon, \nu$  and  $\varepsilon_1 \rightarrow 0$  and obtain a very simplified model, but doing that we would loose a lot of physical information. In fact, these three parameters have different significations. The parameters  $\nu$  and  $\varepsilon_1$  are related to the form of the pulse and are useful for the paraxial approximation. More precisely,  $\nu$  measures the efficiency of the envelope approximation. Indeed the electric field is of the form  $\mathcal{E}e^{it/\nu}$  with  $|\partial_t \mathcal{E}| \ll \frac{1}{\nu} |\mathcal{E}|$ . Since  $\nu$  is very small, we will make this approximation here. The parameter  $\varepsilon_1$  measures the diffraction effects in the transverse direction. If we keep  $\varepsilon_1$  fixed, we overlook the diffraction effects that are of great importance for the propagation. In order to recover the usual paraxial approximation we will choose:

$$\varepsilon_1 = \sqrt{\frac{\nu}{2\mathcal{L}}}.$$

The parameter  $\varepsilon$  has a completely different status: it is linked to the way that the phase mismatch modifies the propagation of the laser in the gas. We choose to keep it fixed in order to keep this phenomenon in the final model. The dimensionless system is finally:

$$\partial_t B_z + \frac{\sqrt{2\mathcal{L}}}{\sqrt{\nu}} \partial_x \mathcal{E} = 0, \tag{9}$$

$$\partial_t B_x - \partial_z \mathcal{E} = 0, \tag{10}$$

$$\partial_t \mathcal{E} - \left( \partial_z B_x - \frac{\sqrt{2\mathcal{L}}}{\sqrt{\nu}} \partial_x B_z \right) = -2i\beta(\Lambda - \bar{\Lambda}), \tag{11}$$

$$\partial_t \Lambda = \frac{i}{\nu} \Lambda - \frac{i}{\varepsilon} \Lambda - \frac{i}{\varepsilon} \mathcal{E} + i\alpha \mathcal{E} N, \tag{12}$$

$$\partial_t N = \frac{i}{\varepsilon} \mathcal{E}(\Lambda - \bar{\Lambda}). \tag{13}$$

## 2.2. Derivation of the model.

We now perform an almost standard geometric optics expansion on (9)-(13) as  $\nu \rightarrow 0$ . We make the following ansatz:

$$(B_x, B_z, \mathcal{E}) = \sum_{j=0}^2 (B_x^j, B_z^j, \mathcal{E}^j) \nu^{j/2} e^{i\frac{(t-z)}{\nu}} + c.c.,$$

where *c.c.* stands for complex conjugate and

$$\Lambda = (\Lambda^0 + \nu^{1/2} \Lambda^1 + \nu \Lambda^2) e^{i\frac{(t-z)}{\nu}},$$

because the fields  $(B_x, B_z, \mathcal{E})$  are real while  $\Lambda$  is complex.  $N$  is non-oscillatory (see [13]) and is expanded as

$$N = N^0 + \nu^{1/2} N^1 + \nu N^2.$$

We now substitute this ansatz in (9)-(13).

- Terms of order  $\frac{1}{\nu}$ :

One obtains

$$iB_z^0 = 0, \quad iB_x^0 + i\mathcal{E}^0 = 0, \quad i\mathcal{E}^0 + iB_x^0 = 0, \quad i\Lambda^0 = i\Lambda^0, \quad 0 = 0,$$

which gives

$$B_z^0 = 0 \text{ and } B_x^0 = -\mathcal{E}^0. \tag{14}$$

$\mathcal{E}^0$ ,  $\Lambda^0$  and  $N^0$  are unknown at this level.

- Terms of order  $\frac{1}{\nu^{1/2}}$ :

$$iB_z^1 + \sqrt{2\mathcal{L}}\partial_x \mathcal{E}^0 = 0,$$

$$iB_x^1 + i\mathcal{E}^1 = 0,$$

$$i\mathcal{E}^1 + iB_x^1 - \sqrt{2\mathcal{L}}\partial_x B_z^0 = 0,$$

$$i\Lambda^1 = i\Lambda^1$$

$$0 = 0$$

According to (14),  $B_z^0 = 0$  and this last system gives:

$$B_z^1 = i\sqrt{2\mathcal{L}}\partial_x \mathcal{E}^0, \tag{15}$$

$$B_x^1 = -\mathcal{E}^1, \tag{16}$$

where  $\mathcal{E}^1$ ,  $\Lambda^1$  and  $N^1$  are unknown.

• Terms of order  $O(1)$ :

One gets

$$iB_z^2 + \partial_t B_z^0 + \sqrt{2\mathcal{L}}\partial_x \mathcal{E}^1 = 0, \quad (17)$$

$$iB_x^2 + \partial_t B_x^0 + i\mathcal{E}^2 - \partial_z \mathcal{E}^0 = 0, \quad (18)$$

$$i\mathcal{E}^2 + \partial_t \mathcal{E}^0 - (\partial_z B_x^0 - iBB_x^2 - \sqrt{2\mathcal{L}}\partial_x B_z^1) = -2i\beta\Lambda^0, \quad (19)$$

$$i\Lambda^2 + \partial_t \Lambda^0 = i\Lambda^2 - \frac{i}{\varepsilon}\Lambda^0 - \frac{i}{\varepsilon}\mathcal{E}^0 + i\alpha\mathcal{E}^0 N^0, \quad (20)$$

$$\partial_t N^0 = -\frac{i}{\varepsilon}\mathcal{E}^0 \bar{\Lambda}^0 + \frac{i}{\varepsilon}\bar{\mathcal{E}}^0 \Lambda^0. \quad (21)$$

We have kept only the resonant terms in these equations and have dropped all others harmonics.

We now subtract (18) from (19) and using (14) we get:

$$\partial_t \mathcal{E}^0 + \partial_z \mathcal{E}^0 + \sqrt{2\mathcal{L}}\partial_x B_z^1 + \partial_t \mathcal{E}^0 + \partial_z \mathcal{E}^0 = -2i\beta\Lambda^0$$

and (15) gives

$$\partial_t \mathcal{E}^0 + \partial_z \mathcal{E}^0 + i\mathcal{L}\partial_x^2 \mathcal{E}^0 = -i\beta\Lambda^0. \quad (22)$$

Now (20) implies

$$\partial_t \Lambda^0 = -\frac{i}{\varepsilon}(\Lambda^0 + \mathcal{E}^0) + i\alpha\mathcal{E}^0 N^0 \quad (23)$$

and (21) gives

$$\partial_t N^0 = \frac{2}{\varepsilon}Im(\mathcal{E}^0 \bar{\Lambda}^0). \quad (24)$$

The 3-D extension of the system (22)-(24) reads ( $\Delta_\perp = \partial_x^2 + \partial_y^2$ ):

$$\begin{cases} (\partial_t + \partial_z + i\mathcal{L}\Delta_\perp)\mathcal{E}^0 = -i\beta\Lambda^0, \\ \partial_t \Lambda^0 + \frac{i}{\varepsilon}(\Lambda^0 + \mathcal{E}^0) = i\alpha\mathcal{E}^0 N^0, \\ \partial_t N^0 = \frac{2}{\varepsilon}Im(\mathcal{E}^0 \bar{\Lambda}^0). \end{cases} \quad (25)$$

It is the classical Schrödinger-Bloch system that can be found in textbooks. We have obtained it formally with our scaling. For justification and extension to the three level model see [6]. The main problem here is that this system is quite stiff since the parameter  $\varepsilon$  is of order  $5 \cdot 10^{-3}$ . It is especially difficult to make computations directly on (25) because of the factor  $\frac{1}{\varepsilon}$  in front of the nonlinear term.

### 2.3. Nonlinear change of variable

In [13], Joly, Métivier and Rauch proposed a generic change of variables in order to handle systems that satisfy a "transparency" condition. The main example considered in [13] is the Maxwell-Bloch system. In the two-level case, things are quite simple. Indeed, recall that the dimensional value  $N^*$  of  $N$  satisfies  $N^* = 1 - |C_1|^2 + |C_2|^2$  but since  $|C_1|^2 + |C_2|^2 = 1$ , one has  $N^* = 2|C_2|^2$  and  $|C_2|^2 = N^*/2$ . Besides  $|\Lambda^*|^2 = |C_1|^2|C_2|^2 = (1 - |C_2|^2)|C_2|^2 = (1 - N^*/2)N^*/2$  and  $N^*$  is a solution of the second order equation

$$X^2 - 2X + 4|\Lambda^*|^2 = 0,$$

which solutions are

$$X = 1 \pm \sqrt{1 - 4|\Lambda^*|^2}.$$

Since we expect the process to be weak ( $N^* \ll 1$ ), we have

$$N^* = 1 - \sqrt{1 - 4|\Lambda^*|^2}.$$

For the dimensionless variables, we get:

$$N = \frac{1 - \sqrt{1 - 4\Lambda_{ref}^2|\Lambda|^2}}{2\Lambda_{ref}^2}$$

But from the definition of  $\Lambda_{ref}$  and  $\alpha$ , one has  $\Lambda_{ref}^2 = \alpha\varepsilon/2$  and

$$N = \frac{1 - \sqrt{1 - 2\alpha\varepsilon|\Lambda|^2}}{\alpha\varepsilon}.$$

It follows that (25) is replaced by

$$\begin{cases} (\partial_t + \partial_z + i\mathcal{L}\Delta_\perp) \mathcal{E}^0 = -i\beta\Lambda^0, \\ \partial_t \Lambda^0 + \frac{i}{\varepsilon}(\Lambda^0 + \mathcal{E}^0) = i\mathcal{E}^0 \frac{1 - \sqrt{1 - 2\alpha\varepsilon|\Lambda^0|^2}}{\varepsilon}, \end{cases} \quad (26)$$

which is not stiff anymore. Of course we can directly verify that

$$\partial_t ((\alpha\varepsilon N^0 - 1)^2 + (1 - 2\alpha\varepsilon|\Lambda^0|^2)) = 0.$$

For the analysis of the next section, we will simplify the nonlinear term as  $i\alpha|\Lambda^0|^2\mathcal{E}^0$  and we consider (dropping the  $^0$ ):

$$\begin{cases} (\partial_t + \partial_z + i\mathcal{L}\Delta_\perp) \mathcal{E} = -i\beta\Lambda, \\ \partial_t \Lambda + \frac{i}{\varepsilon}(\Lambda + \mathcal{E}) = i\alpha|\Lambda|^2\mathcal{E}. \end{cases} \quad (27)$$

Moreover  $\varepsilon_1^2 = \frac{\nu}{2\mathcal{L}}$  and  $\mathcal{L} \sim 10^{-2}$ . We therefore write  $\mathcal{L} = \delta\varepsilon$  with  $\delta = O(1)$ . The final form of the system is:

$$\begin{cases} (\partial_t + \partial_z + i\delta\varepsilon\Delta_\perp)\mathcal{E} = -i\beta\Lambda, \\ \partial_t\Lambda + \frac{i}{\varepsilon}(\Lambda + \mathcal{E}) = i\alpha|\Lambda|^2\mathcal{E}. \end{cases} \quad (28)$$

This system (28) will be also used in the following form:

$$\partial_t\mathcal{U} + \mathcal{A}\partial_z\mathcal{U} + \delta\varepsilon\mathcal{B}\Delta_\perp\mathcal{U} + \mathcal{C}\mathcal{U} = \mathcal{S}(\mathcal{U}) \quad (29)$$

where

$$\mathcal{U} = \begin{pmatrix} \mathcal{E} \\ \Lambda \end{pmatrix}, \quad \mathcal{S}(\mathcal{U}) = \begin{pmatrix} 0 \\ i\alpha\mathcal{E}\mathcal{F}(|\Lambda|^2) \end{pmatrix},$$

$$\mathcal{A} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{B} = \begin{pmatrix} i & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{C} = \begin{pmatrix} 0 & i\beta \\ \frac{i}{\varepsilon} & \frac{i}{\varepsilon} \end{pmatrix}.$$

For the simplified system, the nonlinear function is given by  $\mathcal{F}(|\Lambda|^2) = |\Lambda|^2$ . However, in the general formulation we have  $\mathcal{F}(|\Lambda|^2) = \frac{1 - \sqrt{1 - 2\alpha\varepsilon|\Lambda|^2}}{\alpha\varepsilon}$ .

For applications of interest, the characteristic propagation distance is  $Z_{max} \sim 100$  (about  $1km$ ) and the time of propagation is  $T_{max} \sim 100$  (about  $2 \cdot 10^{-6}s$ ). The length of the domain in the transverse direction is  $\rho_{ref} \sim 10^{-2}$  (about  $10cm$ ). An other important remark on this system is that the polarization coefficient  $\beta$  is of order  $\sim 1$ , due to the fact that the gas is diluted ( $\mathcal{N} \sim 10^{18} At/m^3$ ). Consequently the coupling is not stiff. This has to be put in contrast with the solid medium ( $\mathcal{N} \sim 10^{23} At/m^3$ ) where the polarization strength is  $\beta \sim \frac{1}{\varepsilon}$ . The numerical approach we have proposed in [9] for stiff coupling ( $\beta \sim \frac{1}{\varepsilon}$ ) between the polarization and the electric field is inefficient here. In order to develop an efficient numerical approach we now analyze the asymptotic behavior of the model (28).

### 3. Asymptotic behavior

The techniques used here are inspired from the works of Joly, Métivier and Rauch, see for example [13]. However, it is not a straightforward consequence of [13]. Therefore we present the complete analysis of the problem as  $\varepsilon \rightarrow 0$ .

#### 3.1. Linear analysis

Let us consider the linear part of (28) where we neglect the  $\Delta_\perp$  term. We look for traveling waves in the form:

$$\mathcal{E} = \mathcal{E}_w e^{i(wt - \xi z)} \quad \text{and} \quad \Lambda = \Lambda_w e^{i(wt - \xi z)},$$

where  $w$ ,  $\xi$ ,  $\mathcal{E}_w$  and  $\Lambda_w$  are constants. Substituting this ansatz in (28) we find that  $\mathcal{E}_w$  and  $\Lambda_w$  satisfy the linear system

$$\begin{cases} (w - \xi)\mathcal{E}_w + \beta\Lambda_w = 0, \\ \frac{1}{\varepsilon}\mathcal{E}_w + (w + \frac{1}{\varepsilon})\Lambda_w = 0. \end{cases}$$

The existence of nontrivial traveling waves is possible if and only if the matrix associated with the system is singular. Therefore, we find that the frequency  $w$  should satisfy the following dispersion relation:

$$w^2 + \left(\frac{1}{\varepsilon} - \xi\right) w - \frac{\beta + \xi}{\varepsilon} = 0.$$

The two roots of this equation, denoted by  $w_1$  and  $w_2$ , can be approximated as follows:

$$w_1 = \beta + \xi + O(\varepsilon) \quad \text{and} \quad w_2 = -\frac{1}{\varepsilon} - \beta + O(\varepsilon).$$

There are two types of traveling waves, the first one (associated with  $w_1$ ) with a frequency of order  $\beta$  and a group velocity nearly equal to one; the second one with a frequency of order  $-\frac{1}{\varepsilon} - \beta$  and a group velocity nearly equal to zero. Since  $\beta \sim 1$ , the frequency  $-\frac{1}{\varepsilon}$  governs the oscillating component of the solution of the linear and consequently, that of the nonlinear system.

### 3.2. Formal expansion and profile equations

According to the structure of the traveling waves for the linear system the oscillating component of the solution is dominated by the frequency  $-\frac{1}{\varepsilon}$ . Therefore the solution of the nonlinear system expands as follows:

$$\mathcal{U} \simeq \mathcal{V}_\varepsilon(x, y, z, t, \theta) = \mathcal{V}_0 + \varepsilon \mathcal{V}_1 \quad \text{where} \quad \mathcal{U} = \mathcal{V} = \begin{pmatrix} \mathcal{E} \\ \Lambda \end{pmatrix}. \quad (30)$$

The functions  $\mathcal{V}_0$  and  $\mathcal{V}_1$  have Fourier series (with respect to the variable  $\theta = \frac{-t}{\varepsilon}$ ):

$$\mathcal{V}_l(x, y, z, t, \theta) = \sum_j \mathcal{V}_{lj}(x, y, z, t) e^{ij\theta} \quad \text{for} \quad l \in \{0, 1\}.$$

We assume that the functions  $\mathcal{V}_{lj}$  are sufficiently smooth. These profiles are then substituted into system (28) and the terms are collected according to the power of  $\varepsilon$ .

- **At the order  $\varepsilon^{-1}$ ,** system (28) gives

$$-\partial_\theta \mathcal{E}_0 = 0, \quad (31)$$

$$-\partial_\theta \Lambda_0 + i(\Lambda_0 + \mathcal{E}_0) = 0. \quad (32)$$

Using equation (31) we find that  $\mathcal{E}_{0p} = 0$  when  $p \neq 0$  and we conclude that  $\mathcal{E}_0 = \mathcal{E}_{00}$ . Therefore, we obtain from equation (32) that  $\Lambda_{0p} = 0$  when  $p$  is different from 0 or 1. Moreover, the following relation holds:  $\Lambda_{00} = -\mathcal{E}_{00}$ . It follows from this analysis is that the profiles of  $\mathcal{E}_0$  and  $\Lambda_0$  are given by :

$$\mathcal{E}_0 = \mathcal{E}_{00} \quad \text{and} \quad \Lambda_0 = -\mathcal{E}_{00} + \Lambda_{01} e^{i\theta}. \quad (33)$$

At this stage,  $\mathcal{E}_{00}$  and  $\Lambda_{01}$  are unknown.

- **At the order  $\varepsilon^0$**  : the equations are

$$-\partial_\theta \mathcal{E}_1 + (\partial_t + \partial_z) \mathcal{E}_0 = -i\beta \Lambda_0, \quad (34)$$

$$-\partial_\theta \Lambda_1 + i(\Lambda_1 + \mathcal{E}_1) + \partial_t \Lambda_0 = i\alpha \mathcal{E}_0 |\Lambda_0|^2. \quad (35)$$

Using the relations (33), the nonlinear term  $\mathcal{E}_0 |\Lambda_0|^2$  is computed by:

$$\begin{aligned} \mathcal{E}_0 |\Lambda_0|^2 &= \mathcal{E}_{00} \left( |\mathcal{E}_{00}|^2 - \mathcal{E}_{00} \bar{\Lambda}_{01} e^{-i\theta} - \Lambda_{01} \bar{\mathcal{E}}_{00} e^{i\theta} + |\Lambda_{01}|^2 \right), \\ &= -\mathcal{E}_{00}^2 \bar{\Lambda}_{01} e^{-i\theta} + \mathcal{E}_{00} (|\mathcal{E}_{00}|^2 + |\Lambda_{01}|^2) - |\mathcal{E}_{00}|^2 \Lambda_{01} e^{i\theta}. \end{aligned}$$

The  $(e^{i\theta})^0$  component of (34)-(35) is:

$$(e^{i\theta})^0 \begin{cases} (\partial_t + \partial_z) \mathcal{E}_{00} &= i\beta \mathcal{E}_{00}, \\ i(\Lambda_{10} + \mathcal{E}_{10}) - \partial_t \mathcal{E}_{00} &= i\alpha \mathcal{E}_{00} (|\mathcal{E}_{00}|^2 + |\Lambda_{01}|^2). \end{cases} \quad (36)$$

The first equation gives the evolution of  $\mathcal{E}_{00}$ .

The component of the system associated with  $(e^{i\theta})^1$  is :

$$(e^{i\theta})^1 \begin{cases} -i\mathcal{E}_{11} &= -i\beta \Lambda_{01}, \\ i\mathcal{E}_{11} + \partial_t \Lambda_{01} &= -i\alpha |\mathcal{E}_{00}|^2 \Lambda_{01}. \end{cases}$$

It follows that the evolution of  $\Lambda_{01}$  is coupled to the evolution of  $\mathcal{E}_{00}$  by the following ordinary differential equation:

$$\partial_t \Lambda_{01} + i\beta \Lambda_{01} = -i\alpha |\mathcal{E}_{00}|^2 \Lambda_{01}. \quad (37)$$

Finally, the system associated with  $(e^{i\theta})^{-1}$  is a single relation:

$$2\Lambda_{1(-1)} + \mathcal{E}_{1(-1)} = -\alpha \mathcal{E}_{00}^2 \bar{\Lambda}_{01}.$$

For the other component of the system, associated with  $(e^{i\theta})^{-p}$ ,  $|p| > 1$ , we obtain that

$$\Lambda_{1p} = \mathcal{E}_{1p} = 0 \quad \text{for } |p| > 1.$$

Therefore, we have  $\mathcal{V}_\varepsilon = \mathcal{V}_0 + \varepsilon \mathcal{V}_1$  with

$$\mathcal{V}_0 = \mathcal{V}_{00} + \mathcal{V}_{01} e^{i\theta} \quad \text{and} \quad \mathcal{V}_1 = \mathcal{V}_{1(-1)} e^{-i\theta} + \mathcal{V}_{10} + \mathcal{V}_{11} e^{i\theta}, \quad (38)$$

where

$$\begin{aligned} \mathcal{V}_{00} &= \begin{pmatrix} \mathcal{E}_{00} \\ -\mathcal{E}_{00} \end{pmatrix}, \quad \mathcal{V}_{01} = \begin{pmatrix} 0 \\ \Lambda_{01} \end{pmatrix}, \quad \mathcal{V}_{1(-1)} = \begin{pmatrix} \mathcal{E}_{1(-1)} \\ \frac{-\alpha \mathcal{E}_{00}^2 \bar{\Lambda}_{01} - \mathcal{E}_{1(-1)}}{2} \end{pmatrix}, \\ \mathcal{V}_{10} &= \begin{pmatrix} \mathcal{E}_{10} \\ \mathcal{T}_{10}(\mathcal{E}_{00}, \Lambda_{01}) - \mathcal{E}_{10} \end{pmatrix}, \quad \mathcal{V}_{11} = \begin{pmatrix} \beta \Lambda_{01} \\ \Lambda_{11} \end{pmatrix}, \end{aligned}$$

where  $\mathcal{T}_{10}(\mathcal{E}_{00}, \Lambda_{01}) = -i\partial_t \mathcal{E}_{00} + \alpha \mathcal{E}_{00}(|\mathcal{E}_{00}|^2 + |\Lambda_{01}|^2)$ . The variables  $\mathcal{E}_{00}$  and  $\Lambda_{01}$  satisfy the following system:

$$(\partial_t + \partial_z)\mathcal{E}_{00} = i\beta \mathcal{E}_{00}, \quad (39)$$

$$\partial_t \Lambda_{01} + i\beta \Lambda_{01} = -i\alpha |\mathcal{E}_{00}|^2 \Lambda_{01}. \quad (40)$$

At this stage, we can assume that the variables  $\mathcal{E}_{1(-1)}$ ,  $\mathcal{E}_{10}$ , and  $\Lambda_{11}$  are equal to zero since they do not play any role in the expansion. Then, it is easy to check as usual that:

$$\partial_t \mathcal{V}_0 + \mathcal{A} \partial_z \mathcal{V}_0 + \delta \varepsilon \mathcal{B} \Delta_{\perp} \mathcal{V}_0 + \mathcal{C} \mathcal{V}_0 - \mathcal{S}(\mathcal{V}_0) = \varepsilon \mathcal{R}^{\varepsilon}, \quad (41)$$

with

$$\mathcal{A} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{S}(\mathcal{V}) = \begin{pmatrix} 0 \\ i\alpha \mathcal{E} |\Lambda|^2 \end{pmatrix}, \quad \mathcal{C} = \begin{pmatrix} 0 & i\beta \\ \frac{i}{\varepsilon} & \frac{i}{\varepsilon} \end{pmatrix}, \quad \mathcal{B} = \begin{pmatrix} i & 0 \\ 0 & 0 \end{pmatrix}$$

where  $\mathcal{R}^{\varepsilon}$  is bounded.

### 3.3. Rigorous results

The aim of this section is to prove the following theorem:

**Theorem 1.** *Let  $a$  and  $b$  be two functions in  $H^s(\mathbf{R}^3)$  for  $s$  large enough.*

*Let  $(\mathcal{E}_{00}(x, y, z, t), \Lambda_{01}(x, y, z, t))$  be the solution of the following Cauchy problem:*

$$\begin{cases} (\partial_t + \partial_z)\mathcal{E}_{00} = i\beta \mathcal{E}_{00} \\ \partial_t \Lambda_{01} + i\beta \Lambda_{01} = -i\alpha |\mathcal{E}_{00}|^2 \Lambda_{01} \end{cases} \quad \text{with} \quad \begin{pmatrix} \mathcal{E}_{00}(x, y, z, 0) \\ \Lambda_{01}(x, y, z, 0) \end{pmatrix} = \begin{pmatrix} a \\ b + a \end{pmatrix}.$$

*Then, there exists  $T > 0$  and a unique solution  $\mathcal{U}_{\varepsilon} \in \mathcal{C}([0, T]; H^s)$  of the system (29) satisfying the initial condition  $\mathcal{U}_{\varepsilon}(t=0) = \begin{pmatrix} a \\ b \end{pmatrix}$  and such that*

$$|\mathcal{U}_{\varepsilon} - \mathcal{V}_0|_{L^{\infty}(0, T; H^{s-2} \times H^{s-2})} = O(\varepsilon) \quad \text{where} \quad \mathcal{V}_0 = \begin{pmatrix} \mathcal{E}_{00} \\ -\mathcal{E}_{00} + \Lambda_{01} e^{-i\frac{t}{\varepsilon}} \end{pmatrix}.$$

**Proof:** By usual techniques, it is easy to show that there exists a solution  $\mathcal{U}_{\varepsilon}(t)$  of (29), defined for  $t \in [0, T_{\varepsilon}]$ . The first step is to prove that  $\exists T > 0$  such that  $T_{\varepsilon} \geq T$  and that  $\mathcal{U}_{\varepsilon}$  is bounded uniformly on  $[0, T]$  independently of  $\varepsilon$ . We first consider the linear system in Fourier form:

$$\partial_t \widehat{\mathcal{U}} = M(\xi) \widehat{\mathcal{U}} \quad \text{where} \quad M(\xi) = -i\xi \mathcal{A} - \mathcal{C},$$

and  $i\xi$  is the symbol of  $\partial_z + i\delta \varepsilon \Delta_{\perp}$ . We now write explicitly the spectral decomposition of  $M(\xi)$  in order to solve (34)-(35). The eigenvalues of  $M(\xi)$  are given by

$$\lambda_{\pm} = -\frac{i}{2\varepsilon} \left( 1 + \varepsilon \xi \pm \sqrt{\delta} \right), \quad (42)$$

where  $\delta = \delta(\xi, \varepsilon) = (1 - \varepsilon \xi)^2 + 4\varepsilon \beta$  is a real positive function. The spectral projectors  $\Pi_+$  and  $\Pi_-$  are given by:

$$\Pi_+ = \frac{M - \lambda_-}{\lambda_+ - \lambda_-} \quad \text{and} \quad \Pi_- = \frac{M - \lambda_+}{\lambda_- - \lambda_+}.$$

Let us denote by  $I$  the identity matrix and define the matrix  $J$  by:

$$J = \begin{pmatrix} \frac{\varepsilon\xi - 1}{2} & \varepsilon\beta \\ 1 & \frac{1 - \varepsilon\xi}{2} \end{pmatrix}.$$

Using these matrices, the projectors  $\Pi_+$  and  $\Pi_-$  are given by:

$$\Pi_+ = \frac{1}{2}I + \frac{1}{\sqrt{\delta}}J \quad \text{and} \quad \Pi_- = \frac{1}{2}I - \frac{1}{\sqrt{\delta}}J. \quad (43)$$

The difficulty here is that  $\delta(\xi, \varepsilon)$  is not bounded from below uniformly in  $\xi$  and  $\varepsilon$ . It is therefore not possible to obtain an uniform bound for the solution  $\mathcal{U}_\varepsilon$  of (29), such that

$$|\mathcal{U}_\varepsilon(., t)| \leq C|\mathcal{U}_\varepsilon(., 0)|,$$

with  $C$  independent of  $\varepsilon$  and  $\xi$ . Nevertheless, the particular structure of the nonlinear terms of (34)-(35) allows to obtain some bounds.

The solution  $\mathcal{U}_\varepsilon$  of system (29) satisfies:

$$\Pi_+\mathcal{U}_\varepsilon(t) = e^{\lambda_+t}\Pi_+\mathcal{U}_\varepsilon(0) + \int_0^t e^{\lambda_+(t-s)}\Pi_+\mathcal{S}(\mathcal{U}_\varepsilon(s))ds$$

and

$$\Pi_-\mathcal{U}_\varepsilon(t) = e^{\lambda_-t}\Pi_-\mathcal{U}_\varepsilon(0) + \int_0^t e^{\lambda_-(t-s)}\Pi_-\mathcal{S}(\mathcal{U}_\varepsilon(s))ds,$$

where  $\Pi_\pm$  and  $\lambda_\pm$  now denotes the Fourier multipliers which symbols are defined by the equations (43) and (42).

$$\mathcal{U}_\varepsilon(t) = (e^{\lambda_+t}\Pi_+ + e^{\lambda_-t}\Pi_-)\mathcal{U}_\varepsilon(0) + \int_0^t (e^{\lambda_+(t-s)}\Pi_+ + e^{\lambda_-(t-s)}\Pi_-)\mathcal{S}(\mathcal{U}_\varepsilon(s))ds. \quad (44)$$

The proof of Theorem 1 now goes through three lemmas.

**Lemma 1.**  $\exists C_1 > 0$  such that for all  $g \in H^s(\mathbf{R}^3)$ , we have

$$\left| \Pi_\pm \begin{pmatrix} 0 \\ g \end{pmatrix} \right|_{H^s} \leq C_1 |g|_{H^s}.$$

**Proof:** Taking the Fourier transform leads to:

$$\begin{aligned} \Pi_\pm \begin{pmatrix} 0 \\ \hat{g} \end{pmatrix} &= \frac{1}{2} \begin{pmatrix} 0 \\ \hat{g} \end{pmatrix} \pm \frac{1}{\sqrt{\delta}} J \begin{pmatrix} 0 \\ \hat{g} \end{pmatrix}, \\ &= \frac{1}{2} \begin{pmatrix} 0 \\ \hat{g} \end{pmatrix} \pm \frac{\varepsilon\beta}{\sqrt{\delta}} \begin{pmatrix} \hat{g} \\ 0 \end{pmatrix} \pm \frac{1-\varepsilon\xi}{2\sqrt{\delta}} \begin{pmatrix} 0 \\ \hat{g} \end{pmatrix}. \end{aligned}$$

Now recall that  $\delta = (1 - \varepsilon\xi)^2 + 4\varepsilon\beta$  so that  $\frac{\varepsilon\beta}{\sqrt{\delta}}$  and  $\frac{1 - \varepsilon\xi}{2\sqrt{\delta}}$  are uniformly bounded with respect to  $\varepsilon$  and  $\xi$ . The result follows. ■

**Lemma 2.** For all  $\varepsilon \leq 1/2$ ,  $\exists C_2 > 0$  such that for all  $f$  and  $g$  in  $H^s(\mathbf{R}^3)$ , with the support of  $\hat{f}$  and the support of  $\hat{g}$  included in  $\left\{|\xi| \leq \frac{1}{\sqrt{\varepsilon}}\right\}$ , we have

$$\left| \Pi_{\pm} \begin{pmatrix} f \\ g \end{pmatrix} \right|_{H^s} \leq C_2 (|f|_{H^s} + |g|_{H^s}).$$

**Proof:** Taking the Fourier transform leads to:

$$\begin{aligned} \Pi_{\pm} \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix} &= \frac{1}{2} \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix} \pm \frac{1}{\sqrt{\delta}} J \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix}, \\ &= \frac{1}{2} \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix} \pm \frac{\varepsilon\beta}{\sqrt{\delta}} \begin{pmatrix} \hat{g} \\ 0 \end{pmatrix} \pm \frac{1}{\sqrt{\delta}} \begin{pmatrix} 0 \\ \hat{f} \end{pmatrix} \pm \frac{1-\varepsilon\xi}{2\sqrt{\delta}} \begin{pmatrix} -\hat{f} \\ \hat{g} \end{pmatrix}. \end{aligned} \quad (45)$$

For  $|\xi| \leq \frac{1}{\sqrt{\varepsilon}}$  and  $\varepsilon \leq 1/2$ , we have

$$\sqrt{\delta} \geq \sqrt{(1 - \sqrt{\varepsilon})^2 + 4\varepsilon\beta} \geq 1/2.$$

Moreover,  $\frac{\varepsilon\xi - 1}{\sqrt{\delta}}$  and  $\frac{\varepsilon\beta}{\sqrt{\delta}}$  are bounded. Lemma 2 follows. ■

**Lemma 3.**  $\exists C_3 > 0$  such that for all  $f$  and  $g$  in  $H^s(\mathbf{R}^3)$ , for all  $\varepsilon \leq 1/2$  with the support of  $\hat{f}$  and the support of  $\hat{g}$  included in  $\left\{|\xi| \geq \frac{1}{\sqrt{\varepsilon}}\right\}$ , we have

$$\left| \Pi_{\pm} \begin{pmatrix} f \\ g \end{pmatrix} \right|_{H^s} \leq C_3 (|f|_{H^{s+1}} + |g|_{H^{s+1}}).$$

**Proof:** Using again (45) and writing

$$\sqrt{\delta} = \sqrt{(1 - \varepsilon\xi)^2 + 4\varepsilon\beta} \geq \sqrt{4\beta}\sqrt{\varepsilon}$$

we get

$$\left| \Pi_{\pm} \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix} \right| \leq C_3 \left(1 + \frac{1}{\sqrt{\varepsilon}}\right) (|\hat{f}| + |\hat{g}|) \leq C_3 (1 + |\xi|) (|\hat{f}| + |\hat{g}|).$$

The last inequality is satisfied thanks to the condition on the support of  $\hat{f}$  and  $\hat{g}$ . It follows that

$$\left| \Pi_{\pm} \begin{pmatrix} f \\ g \end{pmatrix} \right|_{H^s} \leq C_3 (|f|_{H^{s+1}} + |g|_{H^{s+1}}).$$

This ends the proof of Lemma 3. ■

Let us come back to equation (44). We have

$$\begin{aligned} |\mathcal{U}_\varepsilon(t)|_{H^s} &\leq |\Pi_+ \mathcal{U}_\varepsilon(0)|_{H^s} + |\Pi_- \mathcal{U}_\varepsilon(0)|_{H^s} \\ &\quad + \int_0^t (|\Pi_+ \mathcal{S}(\mathcal{U}_\varepsilon)|_{H^s} + |\Pi_- \mathcal{S}(\mathcal{U}_\varepsilon)|_{H^s}) d\tau. \end{aligned}$$

Using Lemma 2 and 3 and writing

$$\hat{\mathcal{U}}_\varepsilon(0) = \hat{\mathcal{U}}_\varepsilon(0) \mathbf{1}_{\{|\xi| \leq \frac{1}{\sqrt{\varepsilon}}\}} + \hat{\mathcal{U}}_\varepsilon(0) \mathbf{1}_{\{|\xi| > \frac{1}{\sqrt{\varepsilon}}\}},$$

we obtain

$$|\Pi_+ \mathcal{U}_\varepsilon(0)|_{H^s} + |\Pi_- \mathcal{U}_\varepsilon(0)|_{H^s} \leq (C_2 + C_3) |\mathcal{U}_\varepsilon(0)|_{H^{s+1}}.$$

Now using Lemma 1, we have

$$\left| \Pi_\pm \begin{pmatrix} 0 \\ i\alpha \mathcal{E}^\varepsilon |\Lambda^\varepsilon|^2 \end{pmatrix} \right|_{H^s} \leq C_1 |\mathcal{E}|_{H^s} |\Lambda|_{H^s}^2 \leq C_1 |\mathcal{U}_\varepsilon|_{H^s}^3,$$

provided  $s > d/2$ . Finally, equation (44) leads to the following estimate

$$|\mathcal{U}_\varepsilon(t)|_{H^s} \leq C |\mathcal{U}_\varepsilon(0)|_{H^{s+1}} + C \int_0^t |\mathcal{U}_\varepsilon|_{H^s}^3 ds.$$

This implies that there exists  $T > 0$  and  $C_0$  such that

$$T_\varepsilon \geq T \quad \text{and} \quad |\mathcal{U}_\varepsilon|_{L^\infty(0,T;H^s)} \leq C_0.$$

Now in order to prove Theorem 1, we define  $\tilde{\mathcal{U}}$  by:

$$\mathcal{U}_\varepsilon = \mathcal{V}_0 + \varepsilon \tilde{\mathcal{U}}.$$

According to equations (29) and (41) satisfied respectively by  $\mathcal{U}_\varepsilon$  and  $\mathcal{V}_\varepsilon$ , the system satisfied by  $\tilde{\mathcal{U}}$  is

$$\partial_t \tilde{\mathcal{U}} + \mathcal{A} \partial_z \tilde{\mathcal{U}} + \delta \varepsilon \mathcal{B} \Delta_\perp \tilde{\mathcal{U}} + \mathcal{C} \tilde{\mathcal{U}} = -\mathcal{R}^\varepsilon + \frac{\mathcal{S}(\mathcal{U}_\varepsilon) - \mathcal{S}(\mathcal{V}_0)}{\varepsilon} = -\mathcal{R}^\varepsilon + \begin{pmatrix} 0 \\ i\alpha \end{pmatrix} \frac{\delta \mathcal{S}}{\varepsilon}, \quad (46)$$

where  $\delta \mathcal{S} = |\mathcal{U}_{\varepsilon,2}|^2 \mathcal{U}_{\varepsilon,1} - |\mathcal{V}_{0,2}|^2 \mathcal{V}_{0,1}$ . What we need now is to control  $\frac{\delta \mathcal{S}}{\varepsilon}$  uniformly in  $\varepsilon$ . We have:

$$\begin{aligned} \delta \mathcal{S} &= \left( |\mathcal{U}_{\varepsilon,2}|^2 - |\mathcal{V}_{0,2}|^2 \right) \mathcal{U}_{\varepsilon,1} + \varepsilon |\mathcal{V}_{0,2}|^2 \tilde{\mathcal{E}}, \\ &= \left( \varepsilon (\mathcal{U}_{\varepsilon,2} + \mathcal{V}_{0,2}) \bar{\tilde{\Lambda}} + \mathcal{U}_{\varepsilon,2} \bar{\mathcal{V}}_{0,2} - \bar{\mathcal{U}}_{\varepsilon,2} \mathcal{V}_{0,2} \right) \mathcal{U}_{\varepsilon,1} + \varepsilon |\mathcal{V}_{0,2}|^2 \tilde{\mathcal{E}}, \\ &= \varepsilon \left( \mathcal{U}_{\varepsilon,2} \bar{\tilde{\Lambda}} + \mathcal{V}_{0,2} \bar{\tilde{\Lambda}} + \bar{\mathcal{V}}_{0,2} \tilde{\Lambda} - \mathcal{V}_{0,2} \bar{\tilde{\Lambda}} \right) \mathcal{U}_{\varepsilon,1} + \varepsilon |\mathcal{V}_{0,2}|^2 \tilde{\mathcal{E}}, \\ &= \varepsilon \left( \left( \mathcal{U}_{\varepsilon,2} \bar{\tilde{\Lambda}} + \bar{\mathcal{V}}_{0,2} \tilde{\Lambda} \right) \mathcal{U}_{\varepsilon,1} + |\mathcal{V}_{0,2}|^2 \tilde{\mathcal{E}} \right) = \varepsilon f(\tilde{\mathcal{U}}), \end{aligned}$$

where  $f(\tilde{\mathcal{U}}) = \frac{\delta \mathcal{S}}{\varepsilon}$  is a linear function in  $\tilde{\mathcal{U}}$  with uniformly bounded coefficients. The integral form of the differential equation (46) is

$$\begin{aligned} \tilde{\mathcal{U}} = & \left( e^{\lambda_+ t} \Pi_+ + e^{\lambda_- t} \Pi_- \right) \tilde{\mathcal{U}}(0) - \int_0^t \left( e^{\lambda_+(t-\tau)} \Pi_+ + e^{\lambda_-(t-\tau)} \Pi_- \right) \mathcal{R}^\varepsilon d\tau \\ & + \int_0^t \left( e^{\lambda_+(t-\tau)} \Pi_+ + e^{\lambda_-(t-\tau)} \Pi_- \right) \begin{pmatrix} 0 \\ i\alpha f(\tilde{\mathcal{U}}) \end{pmatrix} d\tau. \end{aligned}$$

Using Lemma 2 and 3 for the first two terms and Lemma 3 for the last one yields:

$$|\tilde{\mathcal{U}}|_{H^s} \leq C|\tilde{\mathcal{U}}(0)|_{H^{s+1}} + \int_0^t C|\mathcal{R}|_{H^{s+1}} d\tau + \int_0^t C|f(\tilde{\mathcal{U}})|_{H^s} d\tau.$$

Now since the function  $f(\tilde{\mathcal{U}})$  is linear and since  $|\tilde{\mathcal{U}}|_{L^\infty(0,T;H^s)} \leq C$ , Gronwall's lemma implies that  $\tilde{\mathcal{U}}$  is bounded in  $[0, T]$ , in fact as long as  $\mathcal{U}_\varepsilon$  exists. This ends the proof of Theorem 1.  $\blacksquare$

### 3.4. Long time expansion

Let us consider the case when  $\Lambda_{01}(x, y, z, 0) = 0$ ; then according to equation (37) for all time  $\Lambda_{01}(x, y, z, t) = 0$ . We introduce the variable  $\tau = \varepsilon t$  and we suppress the variable  $\theta$ :

$$\mathcal{U} \simeq \mathcal{V}_\varepsilon = \mathcal{V}_0 + \varepsilon \mathcal{V}_1 + \varepsilon^2 \mathcal{V}_2 \quad \text{with} \quad \Lambda_0 = -\mathcal{E}_0. \quad (47)$$

At the order  $\varepsilon^0$ , the equations are:

$$\begin{cases} (\partial_t + \partial_z) \mathcal{E}_0 &= -i\beta \Lambda_0, \\ i(\Lambda_1 + \mathcal{E}_1) + \partial_t \Lambda_0 &= i\alpha \mathcal{E}_0 |\Lambda_0|^2. \end{cases}$$

Therefore, we obtain

$$\begin{cases} (\partial_t + \partial_z) \mathcal{E}_0 &= i\beta \mathcal{E}_0, \\ \partial_t \mathcal{E}_0 - i(\Lambda_1 + \mathcal{E}_1) &= -i\alpha \mathcal{E}_0 |\mathcal{E}_0|^2. \end{cases} \quad (48)$$

At the order  $\varepsilon^1$ , we obtain:

$$\begin{cases} \partial_\tau \mathcal{E}_0 + (\partial_t + \partial_z) \mathcal{E}_1 + i\delta \Delta_\perp \mathcal{E}_0 &= -i\beta \Lambda_1, \\ i(\Lambda_2 + \mathcal{E}_2) + \partial_t \Lambda_1 - \partial_\tau \mathcal{E}_0 &= i\alpha \mathcal{E}_1 |\Lambda_0|^2 + 2i\alpha \mathcal{E}_0 \text{Re}(\bar{\Lambda}_0 \Lambda_1). \end{cases} \quad (49)$$

Using the value of  $(\Lambda_1 + \mathcal{E}_1)$ , given by the order  $\varepsilon^0$  expansion, leads to

$$\partial_\tau \mathcal{E}_0 + \left( \partial_t + \partial_z - i\beta \right) \mathcal{E}_1 + i\delta \Delta_\perp \mathcal{E}_0 = -\beta \left( \partial_t \mathcal{E}_0 + i\alpha |\mathcal{E}_0|^2 \mathcal{E}_0 \right).$$

In order to avoid secular terms, we have to impose:

$$\left( \partial_t + \partial_z - i\beta \right) \mathcal{E}_1 = 0$$

and therefore

$$\partial_\tau \mathcal{E}_0 + i\delta \Delta_\perp \mathcal{E}_0 = -\beta \left( \partial_t \mathcal{E}_0 + i\alpha |\mathcal{E}_0|^2 \mathcal{E}_0 \right)$$

and we take  $\mathcal{E}_1 = 0$ . Then  $\Lambda_1$  is then given by the second equation of (48) and  $\Lambda_2$  by the second equation of (49). We obtain the following proposition.

**Proposition 1.** *Let us consider an approximate solution  $\mathcal{U}_0$  of system (29), defined on  $[0, T/\varepsilon]$  with the initial condition  $\Lambda_0(0) = -\mathcal{E}_0(0)$ . Then  $\mathcal{E}_0$  satisfies the equations:*

$$(\partial_t + \partial_z)\mathcal{E}_0 = i\beta\mathcal{E}_0, \quad (50)$$

$$\partial_\tau\mathcal{E}_0 + i\delta\Delta_\perp\mathcal{E}_0 - \beta\partial_z\mathcal{E}_0 = -i\beta^2\mathcal{E}_0 - i\alpha\beta|\mathcal{E}_0|^2\mathcal{E}_0. \quad (51)$$

The phase associated with equation (50) is  $\beta$ . If we disregard the transverse direction, the phase associated with equation (51) one is  $-(\beta^2 + \beta\alpha|\mathcal{E}_0|^2)$ , therefore, the oscillatory frequency given by this expansion is  $\omega_l \simeq \beta - \varepsilon(\beta^2 + \beta\alpha|\mathcal{E}_0|^2)$ . Moreover, it easy to see thanks to equation (50), that  $|\mathcal{E}_0|$  is simply transported. We do not know how to prove a convergence result yet, because the estimates of the previous section are not valid on a time interval of the form  $[0, T/\varepsilon]$ . However, we have:

**Proposition 2.** *Let  $\mathcal{E}_0$  be the solution of system (50)-(51) with a smooth enough initial data  $a$ . Take  $s$  large enough. Then there exists  $T_0 > 0$  independent of  $\varepsilon$  and a unique solution  $\mathcal{U}^\varepsilon$  of (29) with initial data  $(a, -a)$  defined on  $[0, T_0|\log(\varepsilon)|]$ . Moreover there exists  $K > 0$  and  $A > 0$  such that:*

$$|\mathcal{U}^\varepsilon - (\mathcal{V}_0 + \varepsilon\mathcal{V}_1)|_{H^s} \leq K\varepsilon^2(e^{At} - 1) \text{ for all } t \in [0, T_0|\log(\varepsilon)|]$$

This proposition implies that

$$|\mathcal{E} - \mathcal{E}_0|_{H^s} \leq K\varepsilon^2(e^{At} - 1) \text{ for all } t \in [0, T_0|\log(\varepsilon)|]$$

This proposition is a consequence of the work by D. Lannes and J. Rauch [14]. It implies that for bounded time this approximation is better than the previous one since it is of order  $\varepsilon^2$ .

#### 4. Numerical Method

In the previous section, we proved that at first order, the electric field moves with velocity 1 and has time frequency  $\beta$ . It is therefore important that our numerical method enables us to obtain this behavior. The best way to achieve this is to use a splitting strategy in three steps. The first step is the resolution of  $(\partial_t + \partial_z)\mathcal{E} = 0$  (propagation with velocity 1). The second step is the computation of the remaining of the linear part of the system, that is:

$$\begin{cases} (\partial_t + i\delta\varepsilon\Delta_\perp)\mathcal{E} = -i\beta\Lambda, \\ \partial_t\Lambda + \frac{i}{\varepsilon}(\Lambda + \mathcal{E}) = 0. \end{cases}$$

Asymptotically, this gives the right frequency  $\beta$  for  $\mathcal{E}$ . The last step is the nonlinear one. More precisely: we are concerned with the propagation of localized wave packets (pulses) over a large distance. In order to reduce the computer resources needed to compute the entire region of interest, the system is formulated with the arbitrary Lagrangian Eulerian (ALE) approach. Given a moving window with the velocity  $\mathbf{u}$  the ALE formulation of the system is:

$$\partial_t\mathcal{U} + \mathcal{A}\partial_z\mathcal{U} + \delta\varepsilon\mathcal{B}\Delta_\perp\mathcal{U} + \mathcal{C}\mathcal{U} = \mathcal{S}(\mathcal{U}), \quad (52)$$

where  $\mathcal{A}$  is now a function of the velocity  $\mathbf{u}$ :

$$\mathcal{A} = \begin{pmatrix} 1 - \mathbf{u} & 0 \\ 0 & -\mathbf{u} \end{pmatrix}.$$

In the sequel we assume that  $\mathbf{u}$  is constant during a time step. In practice, the window velocity is  $\mathbf{u} = 0$  until the pulse is completely in the computational domain. Then, the window velocity is set to  $\mathbf{u} = 1$  until the end of the computation.

The field equations are discretized in the standard finite-difference staggered grid in conjunction with an explicit time-marching method. In order to simplify the presentation of the numerical approach we assume that the spatial dimension is two. Let us consider a Cartesian grid and denote by  $\delta z$ ,  $\delta x$  the grid size in the propagation direction and in the transverse direction respectively and by  $\delta t$  the time step. The discrete variables are defined by:

$$\mathcal{U}_{j,k}^n = \mathcal{U}(n\delta t, j\delta x, k\delta z),$$

for  $0 \leq j \leq N_x$ ,  $0 \leq k \leq N_z + 1$  and  $0 \leq n \leq N_t$ . We denote by  $L_x = N_x\delta x$  and by  $L_z = N_z\delta z$ . In the sequel, we assume, without loss of generality, that the solution is periodic in the transverse direction. Indeed, the pulse is always localized in the transverse direction. Then if the computational domain is sufficiently large, the solution on the transverse boundary is always zero and we can assume periodicity.

It is classical in optics applications to use Crank-Nicolson implicit schemes for the nonlinear Schrödinger equation [11,10,1] because of its non-diffusive property. However, this kind of scheme suffers phase errors for large propagation distance [3]. For high frequency wave propagation over longer distances, the grid requirement (in order to avoid the phase error) becomes excessive, leading to unreachable processing time and memory requirements. This is the most penalizing aspect of the Crank-Nicolson method especially when the space dimension increases. However, our system has a stiff coupling for the linear terms but only a weak coupling with regard to the nonlinearity. Then we can use a splitting technique, based on the fact that the (linear) propagation and the linear interaction can be solved exactly. The numerical resolution consists in three steps: propagation, linear interaction and nonlinear interaction.

- **Propagation step:** The system solved in this step is the hyperbolic system defined by  $\partial_t \mathcal{U} + \mathcal{A} \partial_z \mathcal{U} = 0$  where the initial condition, inside the domain, is the solution  $(\mathcal{U}_{j,k}^n)$  computed at the previous time step. When  $\mathbf{u} = 0$ , we only have to define the electric amplitude at the left boundary of the computational domain. The incoming wave at the left boundary, is defined by a function  $\mathcal{I}(t, x)$  where  $x$  is the transverse coordinate. Therefore we have:

$$\mathcal{E}_{j,0}^n = \mathcal{I}(t^n, x_j).$$

The index  $k = 0$  is associated with the left boundary of the vapor when the computational window is fixed ( $\mathbf{u} = 0$ ). On the other hand, when  $\mathbf{u} = 1$ , we have to set the value of the polarization field or the right boundary of the computational window (associated with the index  $k = N_z + 1$ ). As the atoms behind the computational

window are in the ground state and the electric field is equal to zero, it is natural to set this polarization to zero on the right boundary:  $\Lambda_{j,N_z+1}^n = 0$ .

For  $0 \leq j \leq N_x$  and  $1 \leq k \leq N_z$ , the propagation is performed as follows:

$$\mathcal{U}_{j,k}^{n+\frac{1}{3}} - \mathcal{U}_{j,k}^n + \frac{\delta t}{\delta z} \left( -\mathcal{A}^+ \mathcal{U}_{j,k-1} + |\mathcal{A}| \mathcal{U}_{j,k} + \mathcal{A}^- \mathcal{U}_{j,k+1} \right) = 0,$$

where  $|\mathcal{A}| = \mathcal{A}$  if  $\mathbf{u} = 0$  and  $|\mathcal{A}| = -\mathcal{A}$  if  $\mathbf{u} = 1$ ,  $\mathcal{A}^+ = \frac{\mathcal{A}+|\mathcal{A}|}{2}$ ,  $\mathcal{A}^- = \frac{\mathcal{A}-|\mathcal{A}|}{2}$ . It is easy to see that the stability condition of this numerical scheme is  $\delta t \leq \delta z$  and that the amplitude error is optimal when  $\delta t = \delta z$  (the normalized light speed here is equal to equal one). For all the tests cases, the time step is chosen in order to give a Courant number of equal to 1.

- **Linear Interaction step:** In this section we are concerned with the integration, during the time step  $\delta t$ , of the system  $\partial_t \mathcal{U} + \mathcal{B} \Delta_\perp \mathcal{U} + \mathcal{C} \mathcal{U} = 0$ , with the initial condition  $\mathcal{U}_{j,k}^{n+\frac{1}{3}}$ . We apply the Fourier transform with respect to the transverse direction, to the system for linear interactions and to the initial data. Let us denote by  $m$  ( $m = 1 - \frac{N_x}{2}, \dots, \frac{N_x}{2}$ ) the index of the Fourier coefficient and by  $\mathcal{M}_m$  the matrix  $\mathcal{M}_m = \xi_m \mathcal{B} - \mathcal{C}$  with  $\xi_m = \mathcal{L} \left( \frac{2\pi m}{L_x} \right)^2$ . For  $0 \leq j \leq N_x$  and  $1 \leq k \leq N_z$ , the linear interaction step reads:

$$\begin{cases} \partial_t \hat{\mathcal{U}}_{m,k} - \mathcal{M}_m \hat{\mathcal{U}}_{m,k} = 0, \\ \hat{\mathcal{U}}_{m,k}(t = t^n) = \hat{\mathcal{U}}_{m,k}^{n+\frac{1}{3}}. \end{cases}$$

The index  $k$  still indicates the position in the propagation direction  $z$ . The previous system is integrated analytically and the predicted solution  $\hat{\mathcal{U}}_{m,k}^{n+\frac{2}{3}}$  is given by:

$$\hat{\mathcal{U}}_{m,k}^{n+\frac{2}{3}} = e^{(\mathcal{M}_m \delta t)} \hat{\mathcal{U}}_{m,k}^{n+\frac{1}{3}},$$

or more explicitly

$$\begin{cases} \hat{\mathcal{E}}_{m,k}^{n+\frac{2}{3}} &= -\mathcal{K}_1 (\lambda_1 \varepsilon + 1) e^{(i\lambda_1 \delta t)} - \mathcal{K}_2 (\lambda_2 \varepsilon + 1) e^{(i\lambda_2 \delta t)}, \\ \hat{\Lambda}_{m,k}^{n+\frac{2}{3}} &= \mathcal{K}_1 e^{(i\lambda_1 \delta t)} + \mathcal{K}_2 e^{(i\lambda_2 \delta t)}, \end{cases}$$

where

$$\lambda_1 = \frac{\varepsilon \xi_m - 1 - \sqrt{(\varepsilon \xi_m - 1)^2 + 4\varepsilon(\beta + \xi_m)}}{2\varepsilon}, \quad \mathcal{K}_1 = \frac{(\varepsilon \lambda_2 + 1) \hat{\Lambda}_{m,k}^{n+\frac{1}{3}} + \hat{\mathcal{E}}_{m,k}^{n+\frac{1}{3}}}{\sqrt{(\varepsilon \xi_m - 1)^2 + 4\varepsilon(\beta + \xi_m)}},$$

$$\lambda_2 = \frac{\varepsilon \xi_m - 1 + \sqrt{(\varepsilon \xi_m - 1)^2 + 4\varepsilon(\beta + \xi_m)}}{2\varepsilon}, \quad \mathcal{K}_2 = -\frac{(\varepsilon \lambda_1 + 1) \hat{\Lambda}_{m,k}^{n+\frac{1}{3}} + \hat{\mathcal{E}}_{m,k}^{n+\frac{1}{3}}}{\sqrt{(\varepsilon \xi_m - 1)^2 + 4\varepsilon(\beta + \xi_m)}}.$$

Since this integration is exact, we are computing accurately the phase of the solution.

- **Nonlinear Interaction step:** In order to compute the nonlinearity, we apply the inverse Fourier transform to the coefficients  $\hat{\mathcal{U}}_{m,k}^{n+\frac{2}{3}}$  computed in the previous step.

Then we obtain  $\mathcal{U}_{j,k}^{n+\frac{2}{3}}$  for  $0 \leq j \leq N_x$  and  $1 \leq k \leq N_z$ . We solve the system  $\partial_t \mathcal{U}_{j,k} = \mathcal{S}(\mathcal{U}_{j,k})$  with  $\mathcal{U}_{j,k}(t^n) = \mathcal{U}_{j,k}^{n+\frac{2}{3}}$ . The solution  $\mathcal{U}_{j,k}^{n+1}$  of this system at time  $t = t^n + \delta t$  is approximated by:

$$\mathcal{U}_{j,k}^{n+1} = \mathcal{U}_{j,k}^{n+\frac{2}{3}} + \delta t \mathcal{S}(\mathcal{U}_{j,k}^{n+\frac{2}{3}}),$$

for  $0 \leq j \leq N_x$  and  $1 \leq k \leq N_z$ .

In the whole the splitting technique for the simplified system is:

$$\mathcal{U}^{n+1} = \mathbb{S}_b \circ \mathbb{S}_{nl}(\delta t) \circ \mathbb{F}^{-1} \circ \hat{\mathbb{S}}_l(\delta t) \circ \mathbb{F} \circ \mathbb{S}_p(\delta t) \cdot \mathcal{U}^n, \quad (53)$$

where  $\mathbb{S}_p(\delta t)$ ,  $\hat{\mathbb{S}}_l(\delta t)$  and  $\mathbb{S}_{nl}(\delta t)$  are the semi-groups associated to the propagation, to the linear interaction and to the nonlinear interaction respectively. The boundary conditions operator is  $\mathbb{S}_b$ , and  $\mathbb{F}$  is the Fourier transform operator. The stability and the accuracy of this splitting technique for linear operators can be found in [21].

## 5. Applications

The numerical scheme introduced in the previous section is now applied to the propagation of a light pulse in a two-level atom medium. At the initial time of the computation ( $t = 0$ ), the atoms of the medium are in the ground state:  $\mathbf{C}_1 = 1$  and  $\mathbf{C}_2 = 0$ . The incoming electric field at the left boundary ( $z = 0$ ) is given by:

$$\mathcal{I}(t, \rho) = A_0 e^{-A_t(t-T_m)^2} e^{-iA_c \cos(\omega_c(t-T_m))} e^{-A_\rho(\rho-\rho_0)^{10}},$$

where  $T_m = 80ns$  and  $A_t = \frac{\ln \sqrt{2}}{T_l^2}$  with  $T_l = 20ns$ . Computations are performed for different values of  $A_0$ ,  $A_c$ ,  $\omega_c$ . The Gaussian pulses are defined by  $A_c = 0$  and  $\omega_c = 0$ . The phase-modulated Gaussian pulses are defined by  $A_c \neq 0$  and  $\omega_c \neq 0$ . For the 1D computations we have  $A_\rho = 0$  and for higher space dimensions  $A_\rho = 2 \ln \sqrt{2}$ ,  $\rho_0 = \frac{\max \rho + \min \rho}{2}$ . For the 2D computations  $\rho = x$  and for the 3D computations  $\rho = \sqrt{x^2 + y^2}$ .

From the initial time  $t = 0$  to  $t = 2T_m$ , the computations are performed in a fixed window  $z \in [0, 2R_w]$  where the radius of the window is  $R_w = cT_m = 24m$  (Fig. 1 and 2). When the parameter  $\varepsilon$  is small, the pulse at the time  $t = 2T_m$  is centered in the window. Then, for  $t > 2T_m$ , the computations are performed in a moving window  $\xi \in [0, 2R_w]$  where  $\xi = z - c(t - 2T_m)$  and the mesh size is  $\delta\xi = \delta z$ .

### 5.1. Gaussian pulse

We consider the propagation of a Gaussian pulse propagating in a two level-atom medium and assume that the transverse effects are negligible. Therefore, we consider a one dimensional problem. At the time  $t = 3.3\mu s$  the moving window is centered at the point  $z = Z_m = 984m$ . The fixed parameters are:  $\beta = 0.92$ ,  $\alpha = 0.5$ ,  $\|A_0\| = 1$  and  $\delta z = 24mm$ . For small values  $\varepsilon \leq 10^{-5}$ , the pulse is also centered in the moving window. When large values are used for the parameter  $\varepsilon$ , the pulse moves to the left. The long time expansion estimates this drift as being proportional to  $\varepsilon\beta$ . Using the results of Figure 3

we compute the position  $Z_{max}$  of the maximum value of the electric field as a function of the parameter  $\varepsilon$ :

| $\beta = 0.92, \   A_0   = 1, \ \alpha = 0.5, \ Z_m = 984m$ |                      |                         |                 |
|-------------------------------------------------------------|----------------------|-------------------------|-----------------|
| $\varepsilon$                                               | $\varepsilon\beta$   | $-\varepsilon\beta Z_m$ | $Z_{max} - Z_m$ |
| $4 \cdot 10^{-3}$                                           | $3.68 \cdot 10^{-3}$ | $-3.62m$                | $\sim -3.55m$   |
| $2 \cdot 10^{-3}$                                           | $1.84 \cdot 10^{-3}$ | $-1.81m$                | $\sim -1.80m$   |
| $10^{-3}$                                                   | $0.92 \cdot 10^{-3}$ | $-0.91m$                | $\sim -0.90m$   |
| $5 \cdot 10^{-4}$                                           | $0.46 \cdot 10^{-3}$ | $-0.45m$                | $\sim -0.45m$   |
| $2.5 \cdot 10^{-4}$                                         | $0.23 \cdot 10^{-3}$ | $-0.22m$                | $\sim -0.21m$   |
| $1.0 \cdot 10^{-5}$                                         | $0.01 \cdot 10^{-3}$ | $-0.01m$                | $\sim 0m$       |

Therefore, we have  $Z_m - Z_{max} \sim -\varepsilon\beta Z_m$  and  $|\mathcal{E}(t, \xi)|$  is preserved during the pulse propagation in the two-level atom vapor (3). These results are in accordance with the asymptotic analysis for long time expansion. This means that the numerical scheme reproduces accurately the behavior of the amplitude of the electric field. The next set of test cases is used to estimate the phase error of the numerical scheme. The fixed parameters fixed are :  $\beta = 0.92, \alpha = 0.5, \varepsilon = 10^{-2}$  and  $\delta z = 24mm$ . The computations (Fig. 4) are then performed for different values of the amplitude  $||A_0||$ . The spatial period of rotation of the electric field is given by the asymptotic analysis by:  $P_\varepsilon^0 = \frac{2\pi L_{ref}}{\beta}$  where  $L_{ref} = 10.19m$  in this context. A correction of this period is obtained by the long time expansion, so that the spatial period is estimated by:  $P_\varepsilon^1 = \frac{2\pi L_{ref}}{\beta - \varepsilon(\beta^2 + \alpha\beta||E_0||^2)}$ . We have plotted in Figure 4 the spatial evolution of the electric field at the center of the moving window. From this figure we can estimate the spatial period ( $P_\nu$ ) of the oscillation of the electric field obtained from the numerical approach:

| $\beta = 0.92, \ \varepsilon = 10^{-2}, \ \alpha = 0.5$ |                   |                   |            |
|---------------------------------------------------------|-------------------|-------------------|------------|
| $  A_0  $                                               | $P_\varepsilon^0$ | $P_\varepsilon^1$ | $P_\nu$    |
| 0.01                                                    | 69.44m            | 69.50m            | $\sim 70m$ |
| 1                                                       | 69.44m            | 69.54m            | $\sim 70m$ |
| 5                                                       | 69.44m            | 70.38m            | $\sim 71m$ |
| 10                                                      | 69.44m            | 73.16m            | $\sim 73m$ |
| 15                                                      | 69.44m            | 78.32m            | $\sim 78m$ |

The numerical period  $P_\nu$  is very close to the estimate  $P_\varepsilon^1$  obtained from the long time asymptotic expansion. For the range of parameters considered in the physical applications, we can conclude that the numerical method is accurate and efficient.

## 5.2. Phase-modulated Gaussian pulse.

We consider in this section a phase modulated pulse with  $A_c = 7.5$  and  $\omega_c = 0.4\pi 10^9 rad/s$ . This is not a monochromatic laser beam and it does not satisfy the hypotheses of the asymptotic analysis since the  $H^1$  norm of the initial value is more or less of size  $1/\sqrt{\varepsilon}$  (see below). However, computations were performed to obtain convergent numerical results at

the limit of the mesh refinement (Fig. 5-8). The temporal profile of the electric amplitude after 1km of propagation in the atomic vapor shows an envelope modification of the pulse and of the population densities (Fig. 5-8). The variation of the population densities is very small (Fig. 7 and 8). The local amplitude of the electric field progressively grows to reach saturation after  $\sim 2km$  of vapor (Fig. 9). Then the system goes into an oscillating regime (Fig. 9). We claim that this behavior of the electric field is only due to the linear interactions of the different spectral components of the initial pulse. To understand what happens, let us go back to the model and consider the linear asymptotic behavior for high frequencies. In the Fourier basis, the simplified linear model for a given frequency  $m$  is:

$$\begin{cases} \partial_t \hat{\mathcal{E}}_m &= i\zeta_m \hat{\mathcal{E}}_m - i\beta \hat{\Lambda}_m, \\ \partial_t \hat{\Lambda}_m &= -i\frac{1}{\varepsilon} \hat{\mathcal{E}}_m - i\frac{1}{\varepsilon} \hat{\Lambda}_m. \end{cases}$$

The eigenvalues of this system are given by

$$\lambda_{\pm} = -\frac{i}{2\varepsilon} \left( 1 - \varepsilon\zeta_m \pm \sqrt{(1 - \varepsilon\zeta_m)^2 + 4\varepsilon(\beta + \zeta_m)} \right).$$

For the considered test case ( $A_c = 7.5$  and  $\omega_c = 0.4\pi 10^9 \text{ rad/s}$ ), the typical frequency of the modulation is

$$\zeta_m = \omega_c T_{ref} \simeq 25 \sim \frac{1}{\sqrt{\varepsilon}}.$$

Thus we assume that  $\zeta_m = \frac{\zeta}{\sqrt{\varepsilon}}$  with  $\zeta$  of order one. In doing so we shall use the following expansion:

$$\begin{aligned} \sqrt{(1 - \varepsilon\zeta_m)^2 + 4\varepsilon(\beta + \zeta_m)} &\simeq 1 + \sqrt{\varepsilon}\zeta + 2\beta\varepsilon - 2\beta\varepsilon\sqrt{\varepsilon}\zeta + 2\beta\varepsilon^2 \left( \zeta^2 - \beta \right) \\ &\quad - \varepsilon^2 \sqrt{\varepsilon} \left( 2\beta\zeta^3 - 6\beta^2\zeta + \frac{7}{8}\zeta^5 \right). \end{aligned}$$

Then, we can derive an equation for the longtime linear self-action:

$$(i\partial_T + \partial_Z^2 - \sqrt{\varepsilon}\partial_Z^3)\mathcal{A} = 0.$$

Let us consider a permanent wave with constant amplitude and modulated phase corresponding to  $A_c = 7.5$  and  $\omega_c = 0.4\pi \text{ rad/ns}$ . The phase modulation is periodic and we focus our investigation on a period. The dynamics of the normalized shape obtained in this case (Fig. 11) is very close to the behavior that can be locally observed for computations performed with the two-level atom model (Fig. 12). It is then clear that the local compression observed on the shape of the electric field is essentially related to linear effects on a phase modulated wave. Three dimensional computations have been also performed successfully (Fig. 13). All the numerical results are in accordance with the expected physical behavior.

## 6. Conclusion

We have suggested a methodology for the derivation of simplified models for laser beams propagating in two-level atom material medium. This methodology can be extended

to other material media. In order to avoid some difficulties related to the stiffness of the model, we introduced a nonlinear change of variable inspired by the conservation properties of the physical system. A small parameter is associated with the simplified model. Using the classical ansatz for geometric optics, the stability of the asymptotic expansion was proved. Moreover, the characteristic component of the model has been identified and according to this result, a splitting numerical approximation was proposed. This numerical model has been validated in the hypothesis of asymptotic stability but also successfully applied in a more general context. However, the strategy proposed can not be applied to systems where population inversion can arise. A number of points will be investigated in further works:

- The stability of splitting schemes for systems that are singularly perturbed is not clear when the perturbation term is not skew symmetric. The symmetric case is treated in [21]. See also [2] for Schrödinger-like equations.
- The asymptotic behavior for initial data with modulated phase has to be made more precise and it is clearly not covered by geometric optics as done in Section 3.
- The numerical experiments show that the propagation of the pulse over a long distance is stable, even in the phase-modulated Gaussian case. Of course the simulation should include the other isotope  $U^{235}$  which is not considered in this work. Our purpose was only to propose a simple and efficient numerical scheme for a two-level case.

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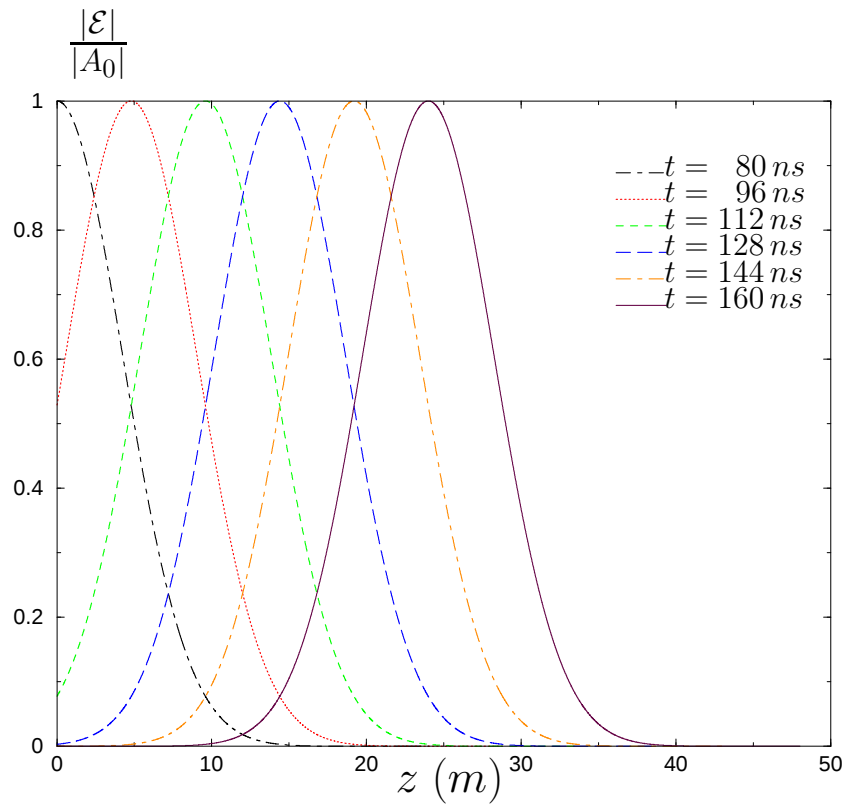


Figure 1. Evolution of the Spatial profile of the normalized amplitude of the electric field. Fixed window during the incoming pulse phase. The computation is performed with the parameters:  $\beta = 0.92$ ,  $|A_0| = 2\pi$ ,  $\varepsilon = 4 \cdot 10^{-4}$  and  $\alpha = 0.5$ .

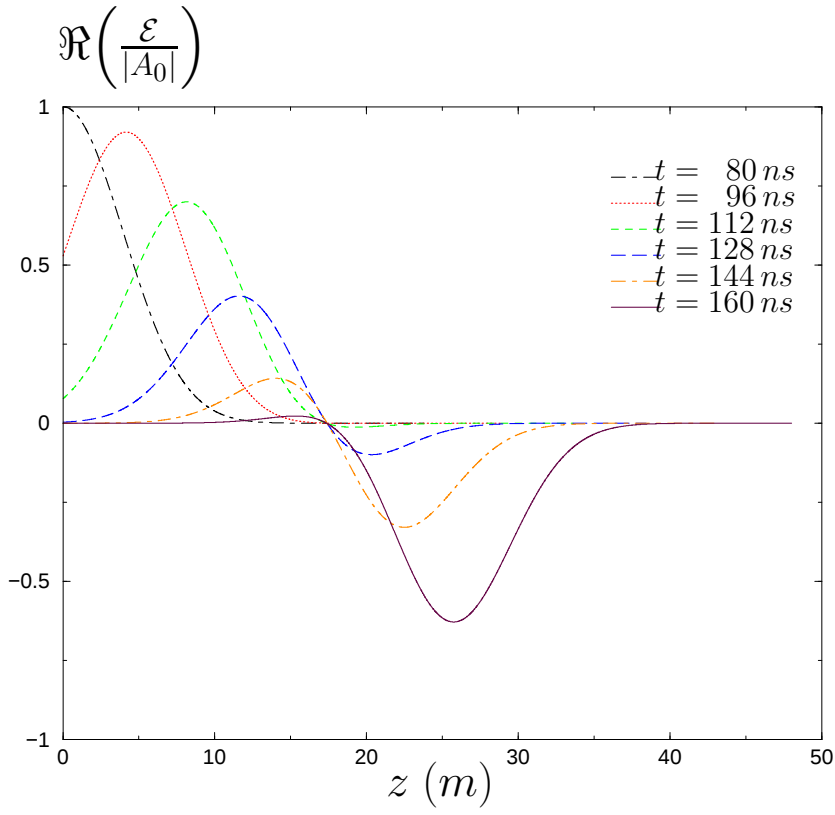


Figure 2. Evolution of the Spatial profile of the normalized real component of the electric field. Fixed window during the incoming pulse phase. The computation is performed with:  $\beta = 0.92$ ,  $|A_0| = 2\pi$ ,  $\varepsilon = 4 \cdot 10^{-4}$  and  $\alpha = 0.5$  .

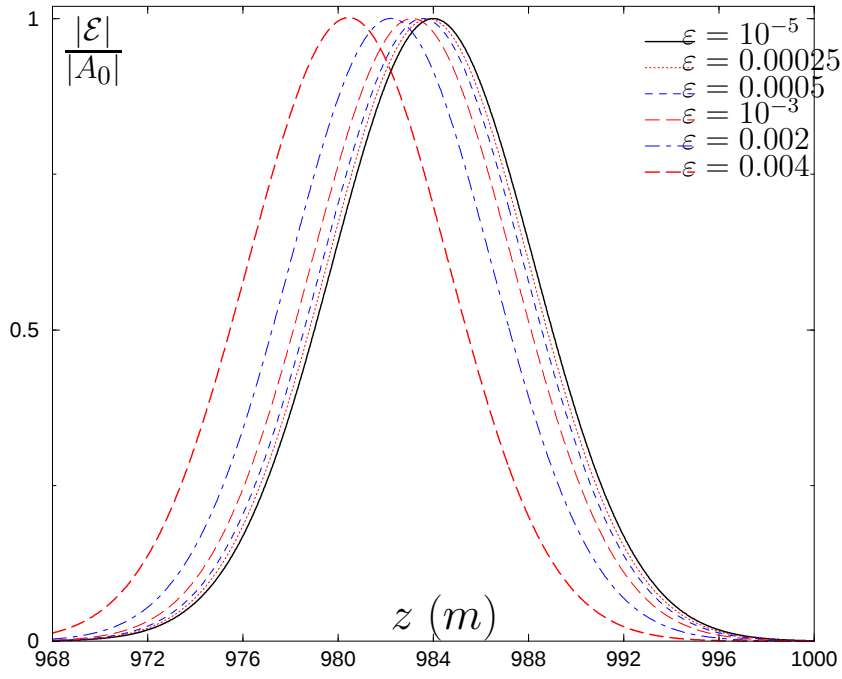


Figure 3. Spatial profile of the normalized amplitude of the electric field at time  $T = 3.3\mu s$ , for different values of  $\varepsilon$ . For these computations:  $\beta = 0.92$ ,  $|A_0| = 1$  and  $\alpha = 0.5$ .

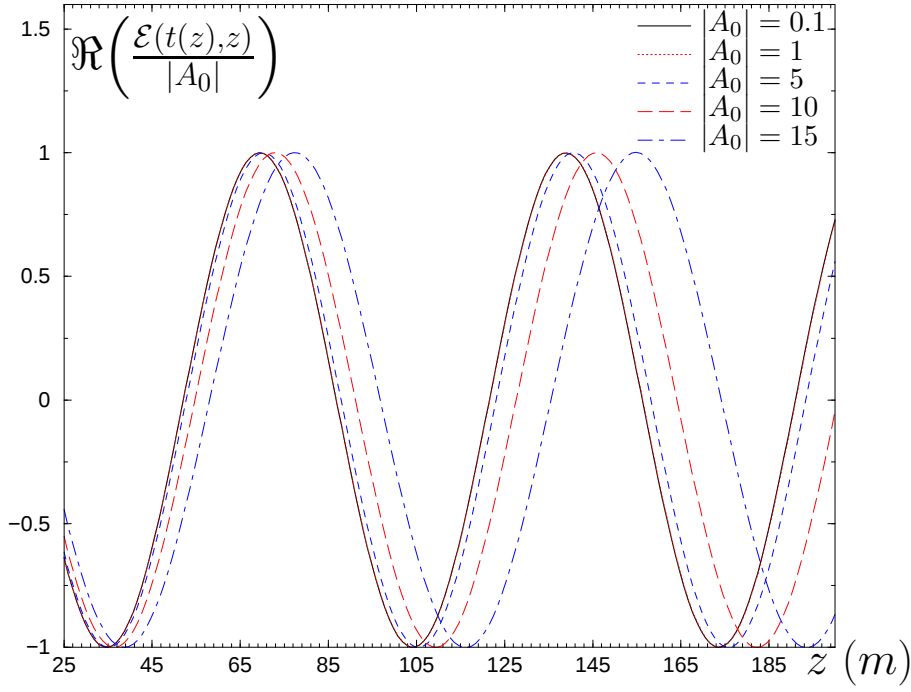


Figure 4. Rotation of the real component of the electric field at the middle of the moving window  $(t(z) = 2T_m + \frac{z-R_w}{c})$ , for different values of  $|A_0|$ . For these computations:  $\beta = 0.92$ ,  $\varepsilon = 10^{-3}$  and  $\alpha = 0.5$ .

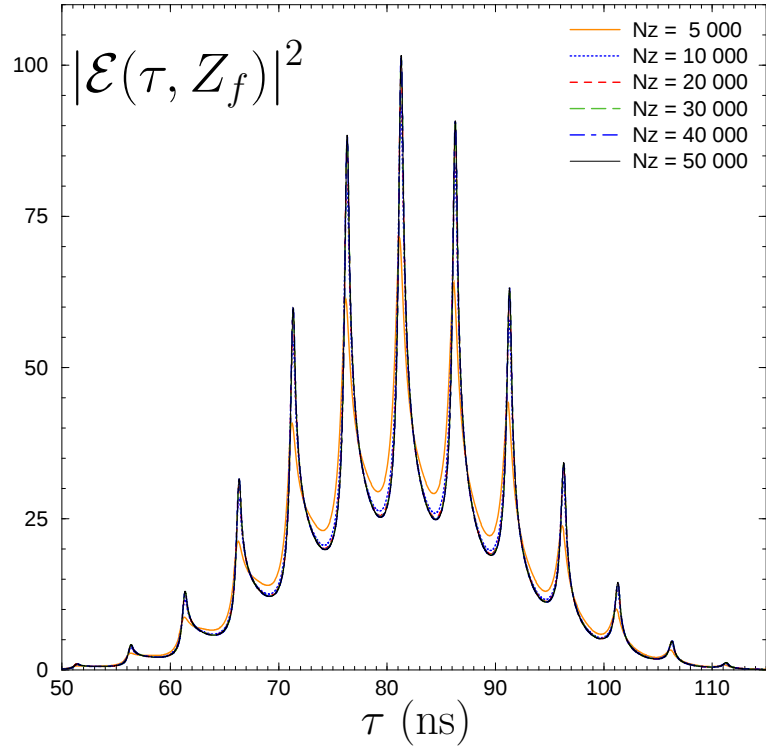


Figure 5. Temporal profile of the norm of the electric field at the point  $z = Z_f = 1km$ :  $\tau = t - \frac{Z_f}{c}$ . For these computations:  $\beta = 0.92$ ,  $\varepsilon = 10^{-3}$ ,  $\alpha = 0.5$ ,  $A_0 = 6.93$ ,  $A_\omega = 7.5$  and  $w_c = 0.4\pi rad/ns$ .

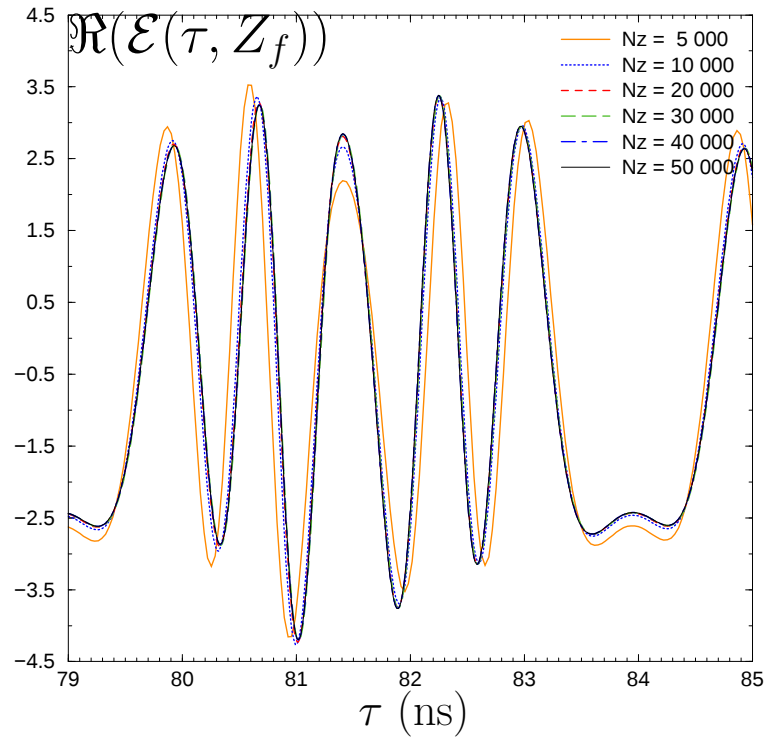


Figure 6. Zoom on the temporal profile of the real component of the electric field at the point  $z = Z_f = 1\text{km}$ :  $\tau = t - \frac{Z_f}{c}$ . For these computations:  $\beta = 0.92$ ,  $\varepsilon = 4 \cdot 10^{-4}$ ,  $\alpha = 0.5$  and  $A_0 = 6.93$ .

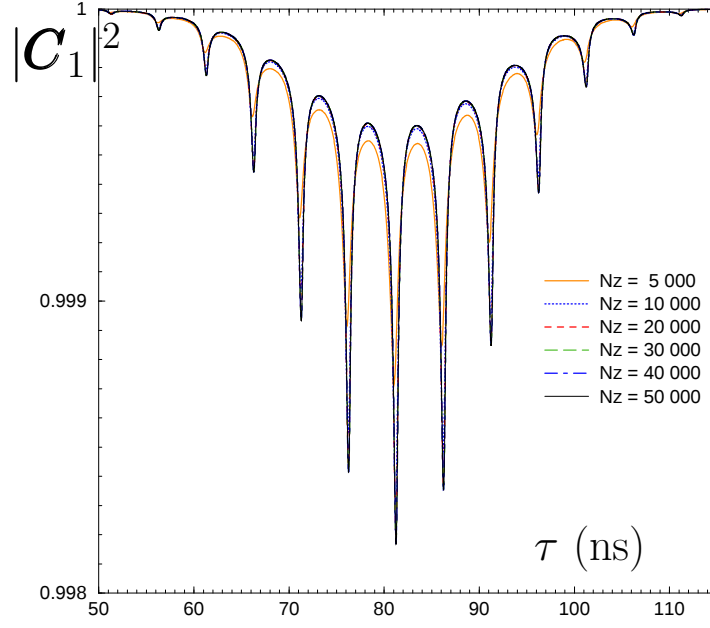


Figure 7. Temporal profile of the density population  $|\mathbf{C}_1|^2$  at the point  $z = Z_f = 1km$ :  $\tau = t - \frac{Z_f}{c}$ . For these computations:  $\beta = 0.92$ ,  $\varepsilon = 10^{-3}$ ,  $\alpha = 0.5$ ,  $A_0 = 6.93$ ,  $A_\omega = 7.5$  and  $w_c = 0.4\pi rad/ns$ .

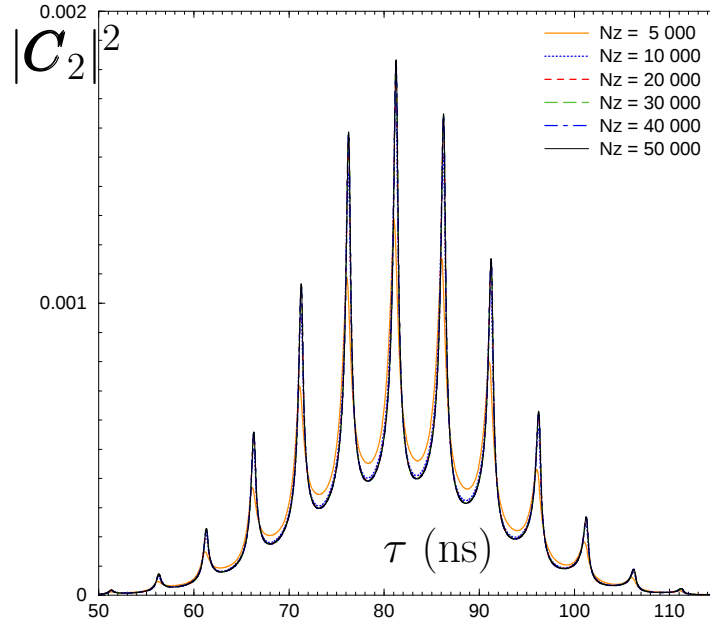


Figure 8. Temporal profile of the density population  $|\mathbf{C}_2|^2$  at the point  $z = Z_f = 1km$ :  $\tau = t - \frac{Z_f}{c}$ . For these computations :  $\beta = 0.92$ ,  $\varepsilon = 10^{-3}$ ,  $\alpha = 0.5$ ,  $A_0 = 6.93$ ,  $A_\omega = 7.5$  and  $w_c = 0.4\pi rad/ns$ .

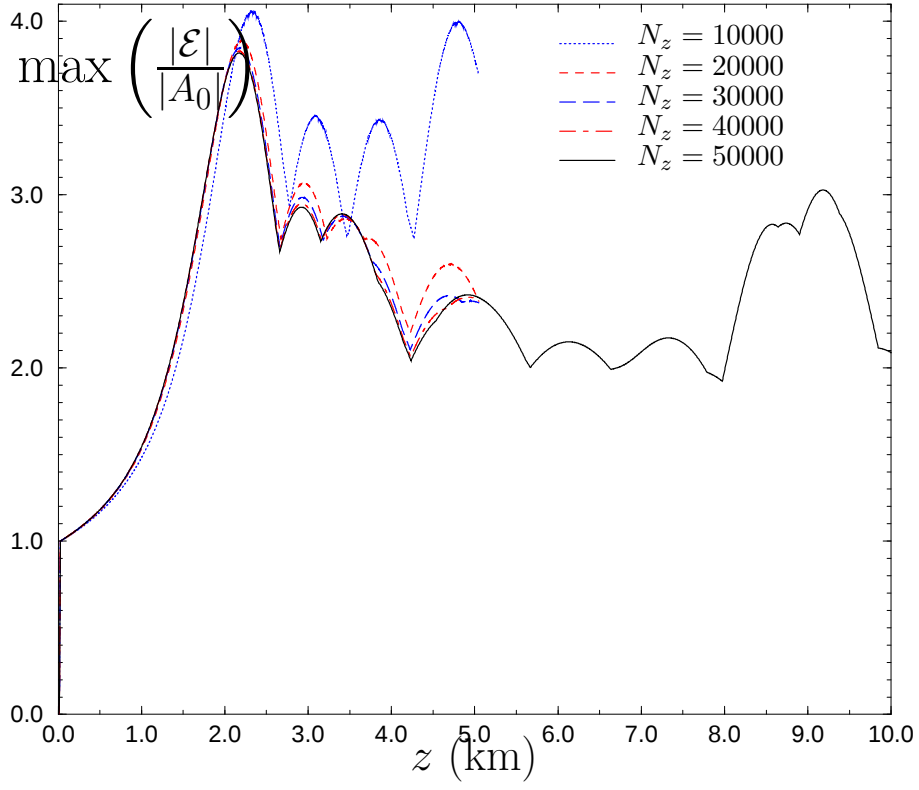


Figure 9. Evolution of the normalized maximum amplitude in the atomic vapor. For these computations we have used:  $\beta = 0.92$ ,  $\varepsilon = 4 \cdot 10^{-4}$ ,  $\alpha = 0.5$ ,  $A_0 = 6.93$ ,  $A_\omega = 7.5$  and  $w_c = 0.4\pi \text{ rad/ns}$ .

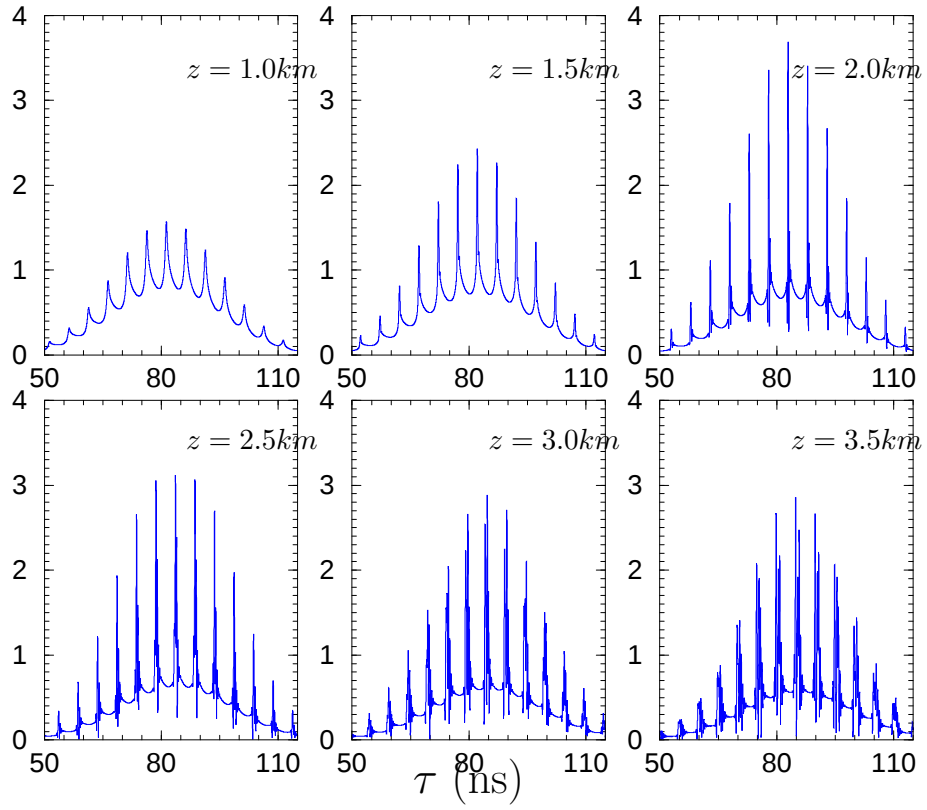


Figure 10. Temporal profile of the normalized amplitude  $\frac{|\mathcal{E}|}{|A_0|}$  at the points  $z = 1km$ ,  $z = 1.5km$ ,  $z = 2km$ ,  $z = 2.5km$ ,  $z = 3km$  and  $z = 3.5km$ . For these computations we have used:  $\beta = 0.92$ ,  $\varepsilon = 4 \cdot 10^{-4}$ ,  $\alpha = 0.5$ ,  $A_0 = 6.93$ ,  $A_c = 7.5$  and  $w_c = 0.4\pi \text{ rad/ns}$ .

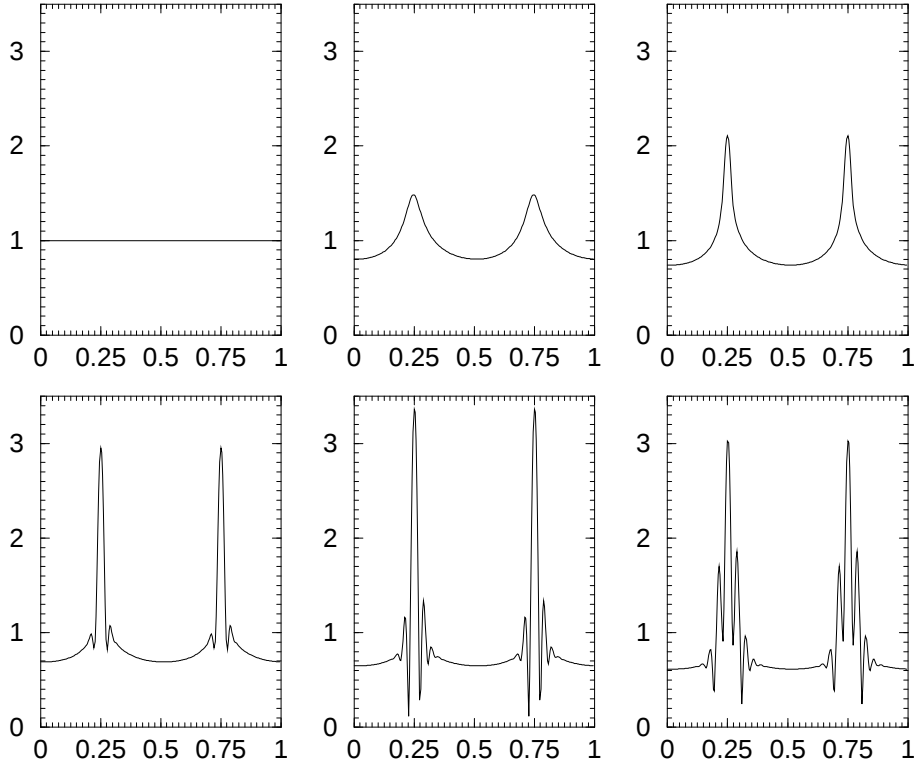


Figure 11. Evolution of the temporal profile of the amplitude when solving the equation:  $(i\partial_T + \partial_Z^2 + \sqrt{\varepsilon}\partial_Z^3)\mathcal{A} = 0$ . For these computations the initial spatial profile has a constant amplitude and a modulated phase corresponding to  $A_c = 7.5$  and  $w_c = 0.4\pi \text{ rad/ns}$ .

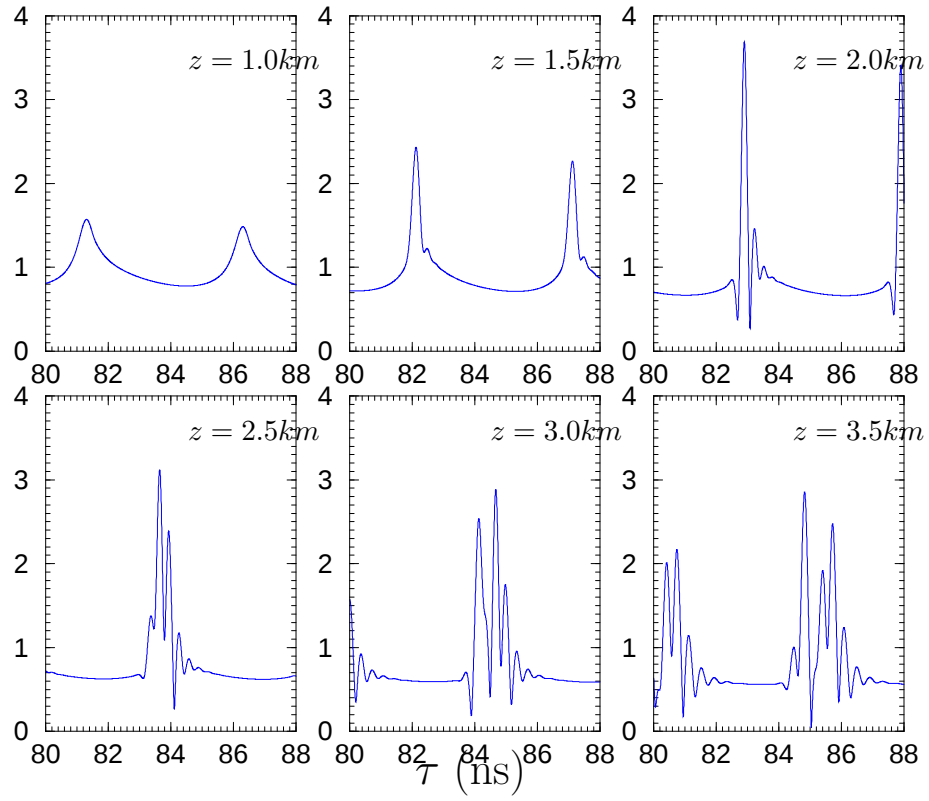


Figure 12. Zoom on the temporal profile of the normalized amplitude  $\frac{|\varepsilon|}{|A_0|}$  at the points  $z = 1km$ ,  $z = 1.5km$ ,  $z = 2km$ ,  $z = 2.5km$ ,  $z = 3km$  and  $z = 3.5km$ . For these computations:  $\beta = 0.92$ ,  $\varepsilon = 4 \cdot 10^{-4}$ ,  $\alpha = 0.5$ ,  $A_0 = 6.93$ ,  $A_c = 7.5$  and  $w_c = 0.4\pi rad/ns$ .

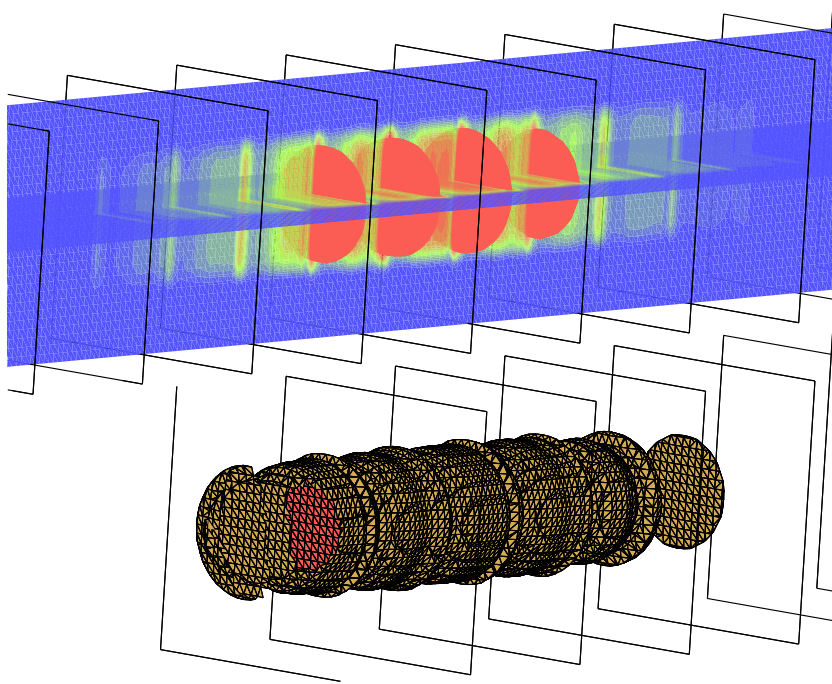


Figure 13. Modulated laser pulse propagating in a two-level atom medium: Spatial profile of the shape of the Numerical solution after  $100m$  in the atomic vapor. For these computations:  $\mathcal{L} = 10^{-6}$ ,  $\beta = 0.92$ ,  $\varepsilon = 4 \cdot 10^{-4}$ ,  $\alpha = 0.5$ ,  $A_0 = 6.93$ ,  $A_c = 7.5$  and  $w_c = 0.4\pi \text{ rad/ns}$ .