

Time Discretizations for Maxwell-Bloch Equations

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In this article we derive new time discretizations for the numerical simulation of Maxwell-Bloch equations. These discretizations decouple the equations, thus leading to improved efficiency. This approach may be combined with the fulfilment of physical properties, such as positiveness properties, which are not accounted for by classical schemes. Our time discretizations are moreover proved to be nonlinearly stable. © 2003 Wiley Periodicals, Inc. *Numer Methods Partial Differential Eq* 19: 284–300, 2003

INTRODUCTION

Transient phenomena in laser-matter interactions involving powerful and ultra-short pulse laser sources may only be modelled using a semi-classical approach in the time domain [1–3]. In this context the electromagnetic wave is described by Maxwell equations and is coupled to the Bloch model for matter *via* an expression for the polarization.

The derivation of the Maxwell-Bloch equations can be found in quantum optics textbooks (see e.g. [2, 4]), and the numerical approximation of the equations was initiated by Ziolkowski et al. [5–7] in the context of two-level atoms. The one-dimensional and two-dimensional Ziolkowski codes are based on the Yee scheme [8] for Maxwell equations together with a Crank-Nicolson scheme for the Bloch equations. The above cited results are quite good, but the method does not extend to more than two-level atoms as it would lose positiveness properties. In [9] the problem of positiveness is handled from the point of view of both physical and numerical modelling, but this study only concerns the Bloch equations. The classical coupling of the Maxwell and Bloch equations leads to a fixed-point procedure that involves both Bloch and Ampère equations, and this is more penalizing when the space dimension increases.

We compare here different ways of coupling Maxwell and Bloch equations in time. The weakly coupled splitting scheme that we introduce has the advantage of preserving positiveness properties and of decoupling equations, thus yielding more efficient codes and a straightforward parallelization of large parts of the code. However, the comparison with existing or other new schemes remains an important issue because we lack experimental measures at the atomic scale with which to compare our results.

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Martin et al. [10] show a way for modelling the Maxwell-Bloch equations in the paraxial approximation. The method also leads to partially decoupled equations at each time step thanks to a leap-frog scheme. This setting for the equations could be generalized to more than two-level atoms and even to the Yee scheme for the Maxwell equations, but it would never lead either to totally decoupled methods or to methods which preserve positiveness. Their idea of treating diagonal and off-diagonal elements differently is also present in our relaxation scheme.

In Section 1 we present the Maxwell-Bloch model and its restriction to one and two-dimensional models that are used in practical computations. A remark on a way for taking the polarization into account is made which proves useful for deriving weakly coupled schemes. The local in time Cauchy Problem and a priori estimates for the Maxwell-Bloch equations are proved in Section 2. Section 3 is devoted to the presentation of existing numerical schemes and the derivation of new weakly coupled schemes. The latter are shown to be nonlinearly stable using the a priori estimates of Section 2. They are also compared from the point of view of efficiency in Section 4. Because the weakly coupled splitting scheme turns out to be the most efficient one in our context, we end this section with some further comments on first and second order splitting schemes.

1. MAXWELL-BLOCH EQUATIONS

A. Description of the Model

In the semi-classical description of laser-matter interaction, the electromagnetic wave is modelled in a classical way using the Maxwell equations, namely,

$$\begin{cases} \partial_t \mathbf{B} + \text{curl } \mathbf{E} = \mathbf{0}, \\ \partial_t \mathbf{E} - c^2 \text{curl } \mathbf{B} = -\frac{1}{\varepsilon} \partial_t \mathbf{P}, \end{cases}$$

where we set $\mathbf{E} = \mathbf{E}(\mathbf{x}, t) = (E_x, E_y, E_z) \in \mathbb{R}^3$ and use similar notations for \mathbf{B} and \mathbf{P} . This system is closed via an expression for the polarization \mathbf{P} .

In the framework of classical models for the interaction \mathbf{P} is often supposed to be a function of \mathbf{E} and its derivatives. The semi-classical model involves a less phenomenological description of the interaction and matter is described using the quantum mechanical theory via the density matrix formalism. We refer to [9] or the physics literature (e.g., [2]) for a complete derivation of the model. Schematically the density matrix $\rho = \rho(t, \mathbf{x})$ is a $N \times N$ complex matrix that describes the states and transitions in matter. Its diagonal elements ρ_{jj} (also called populations) are the probability for an atom to be in the quantum state $|j\rangle$. Only N states are supposed to be relevant, which means that $\text{Tr}(\rho) = \sum_{j=1}^N \rho_{jj} = 1$. This fact will be called the *trace property* in the sequel. The off-diagonal elements ρ_{jk} are called coherences and basically describe transitions between states $|j\rangle$ and $|k\rangle$. The matrix ρ is Hermitian and its time evolution is given by the Bloch equations:

$$\partial_t \rho_{jk} = -i\omega_{jk}\rho_{jk} + i\frac{\mathbf{E}}{\hbar} \cdot [\mathbf{p}, \rho]_{jk} + Q(\rho)_{jk}.$$

In these equations $\omega_{jk} = \omega_j - \omega_k$ where $\mathcal{E}_j = \hbar\omega_j$ is the energy of the level $|j\rangle$. The constant $N \times N$ matrix \mathbf{p} is the dipole moment matrix. Its coefficients $\mathbf{p}_{jk} \in \mathbb{C}^3$ are the ability of the transition from $|j\rangle$ to $|k\rangle$ to give rise to a contribution to the polarization. The matrix \mathbf{p} is

Hermitian, and its diagonal elements are zero. The commutator $[\mathbf{p}, \rho]$ is defined by $\mathbf{p} \rho - \rho \mathbf{p}$. Finally, $Q(\rho)$ is a phenomenological relaxation term, the introduction of which is discussed from a mathematical point of view in [9]. The main point for the present study is that $Q(\rho)_{jk} = -\gamma_{jk}\rho_{jk}$ for $j \neq k$. We choose the Pauli master equation model for diagonal relaxations, namely $Q(\rho)_{jj} = \sum_{k \neq j} W_{jk}\rho_{kk} - \sum_{k \neq j} W_{kj}\rho_{jj}$. In [9] conditions are given on the relaxation rates γ_{jk} and W_{jk} to ensure that ρ is a positive matrix. In what follows, this property has two useful corollaries: $\rho_{jj} \in [0, 1]$ (we recall they are probabilities) and $|\rho_{jk}|^2 \leq \rho_{jj}\rho_{kk}$.

To simplify expressions we will denote by Rn the relaxation-nutation operator given by

$$Rn(\rho)_{jk} = -i\omega_{jk}\rho_{jk} + Q(\rho)_{jk}.$$

Thus the Bloch equations simply read

$$\partial_t \rho = Rn(\rho) + i \frac{\mathbf{E}}{\hbar} \cdot [\mathbf{p}, \rho].$$

Finally, the Bloch equations are coupled to the Maxwell equations, writing the polarization:

$$\mathbf{P} = N_a \text{Tr}(\mathbf{p}\rho),$$

where N_a is the atom density.

The mathematical model and the numerical scheme are analyzed on the whole space with some initial data at time $t = 0$. Practical numerical simulations involve a finite domain and a given incident electromagnetic field.

B. Dimensionless Equations and Formulation for $\partial_t \mathbf{P}$

For the mathematical study and also numerical simulations of this system we use dimensionless equations. Our choice for characteristic values for the different quantities is guided by specific applications (see [11, 12]) where the intensity of the field is high. This may be accounted for by the fact that the Rabi frequency $\omega_R = E_c p_c / \hbar$ (where E_c and p_c are characteristic values for \mathbf{E} and \mathbf{p} , respectively) is of the same order as the transition frequencies in atoms. We use this Rabi frequency to obtain dimensionless frequencies, times, and relaxation coefficients. Space and magnetic fields are treated taking into account the light velocity in the vacuum. The density matrix elements remain untouched because they are already dimensionless and of order one.

This procedure is only valid if relaxation rates involve larger time scales than the leading frequency, which is a reasonable hypothesis. Otherwise an asymptotic model that does not take into account coherences (in the first place) should be studied. From now on all variables are dimensionless (but we use the same notation as before) and of order one except one parameter $\zeta = N_a p_c \epsilon_0 E_c$ that occurs in the coupling relation, namely $\mathbf{P} = \zeta \text{Tr}(\mathbf{p}\rho)$. This parameter is typically equal to 10^{-4} , which implies that the coupling is not stiff. The dimensionless Maxwell-Bloch equations finally read:

$$\begin{cases} \partial_t \mathbf{B} + \text{curl } \mathbf{E} = 0, \\ \partial_t \mathbf{E} - \text{curl } \mathbf{B} = -\partial_t \mathbf{P}, \\ \mathbf{P} = \zeta \text{Tr}(\mathbf{p}\rho), \\ \partial_t \rho = Rn(\rho) + i \mathbf{E} \cdot [\mathbf{p}, \rho]. \end{cases} \quad (1.1)$$

In practice we only have to compute $\partial_t \mathbf{P}$ and not \mathbf{P} . The former reads

$$\partial_t \mathbf{P} = \zeta \operatorname{Tr}(\mathbf{p} \partial_t \rho) = \zeta \operatorname{Tr}(\mathbf{p} R n(\rho)) + i \zeta \operatorname{Tr}(\mathbf{p} \mathbf{E} \cdot [\mathbf{p}, \rho]). \quad (1.2)$$

Now, because numerical simulations nowadays involve only one and two-dimensional models, we give below the precise formulations we use in these contexts. This discussion only concerns the Maxwell equations and the expression of the polarization, because the Bloch equations depend only on space in their coefficients (via the electromagnetic field \mathbf{E}).

C. One-dimensional Maxwell Equations

Most numerical simulations involve a one-dimensional model. There is indeed no need for higher dimensions to account adequately for most physical phenomena. To derive a one-dimensional model we first suppose that the unknowns depend only on the time and the space variable z . Therefore the system decouples yielding

$$(a) \quad \begin{cases} \partial_t B_x - \partial_z E_y = 0, \\ \partial_t E_y - \partial_z B_x = -\partial_t P_y, \end{cases} \quad (b) \quad \begin{cases} \partial_t B_y + \partial_z E_x = 0, \\ \partial_t E_x + \partial_z B_y = -\partial_t P_x. \end{cases} \quad (1.3)$$

In the one-dimensional context a second hypothesis is often imposed, namely $\mathbf{p} = (p_x, 0, 0)$. This leads to the fact that $\mathbf{P} = (P_x, 0, 0)$ and we only consider system (1.3)(b). To simplify notations in this context we will set $E = E_x$, $B = B_y$, $P = P_x$ and $p = p_x$. Under this condition formula (1.2) yields

$$\partial_t P = \zeta \operatorname{Tr}(p R n(\rho)).$$

D. Two-dimensional Maxwell Equations

Because the goal of multidimensional simulations is to account for multidimensional effects, the second hypothesis for the one-dimensional case is not always relevant. Sometimes two polarization directions, but only a dependence in z , is sufficient to model the physical phenomena. If this is not the case, we may suppose that unknowns only depend on time and the space variables x and y , which also decouples the system. Setting $\vec{E} = (E_x, E_y)$ and $E = E_z$, with similar notations for the other vector valued variables, we have

$$\begin{cases} \partial_t \vec{B} + \operatorname{curl} \vec{E} = 0, \\ \partial_t \vec{E} - \overrightarrow{\operatorname{curl}} B = -\partial_t \vec{P}, \end{cases} \quad \begin{cases} \partial_t \vec{B} + \overrightarrow{\operatorname{curl}} E = 0, \\ \partial_t E - \operatorname{curl} \vec{B} = -\partial_t P, \end{cases}$$

where $\operatorname{curl} \vec{V} = -\partial_y V_x + \partial_x V_y$ and $\overrightarrow{\operatorname{curl}} \phi = (\partial_y \phi, -\partial_x \phi)$. These two systems describe, respectively, the transverse electric (TE) and transverse magnetic (TM) modes. They are coupled *via* the polarization. Indeed $\vec{P} = \zeta \operatorname{Tr}(\vec{p} \rho)$ and $P = \zeta \operatorname{Tr}(p \rho)$ are both expressed in terms of ρ , which is computed using \vec{E} and E .

2. THE CAUCHY PROBLEM AND A PRIORI ESTIMATES

In order to study the nonlinear stability of the numerical schemes, we will need a priori estimates that are valid both for the continuous model and the discretized models. For this aim—and more

specifically for L^2 estimates—we need to express the system in terms of variables that will vanish at infinity. This is the case for the electromagnetic fields, but the trace of the density matrix is one everywhere, so it cannot vanish. The solution to the system $Rn(\rho^e) = 0$ is the thermodynamic equilibrium state for the Bloch equations (see [9]). Its off-diagonal elements are zero. Because the diagonal elements of \mathbf{p} are zero, we may state that $\text{Tr}(\mathbf{p}\rho^e) = 0$. This implies that \mathbf{P} will also vanish at infinity. Setting $\sigma = \rho - \rho^e$ we find that system (1.1) becomes

$$\begin{cases} \partial_t \mathbf{B} + \text{curl } \mathbf{E} = 0, \\ \partial_t \mathbf{E} - \text{curl } \mathbf{B} = -\partial_t \mathbf{P}, \\ \mathbf{P} = \zeta \text{Tr}(\mathbf{p}\sigma), \\ \partial_t \sigma = Rn(\sigma) + i\mathbf{E} \cdot [\mathbf{p}, \sigma] + i\mathbf{E} \cdot [\mathbf{p}, \rho^e]. \end{cases} \quad (2.1)$$

Equation (2.1) may be cast as an equation governing a real vector valued variable $U \in \mathbb{R}^d$, where $d = 2m + 2N^2 - N$ (with space dimension m),

$$\partial_t U = \sum_{\mu=1}^m A_\mu \partial_\mu U + F(U), \quad (2.2)$$

where the matrices A_μ are symmetric and the function $F(U)$ is a polynomial involving only first- and second-order monomials and therefore vanishes for $U = 0$. Classical arguments from semi-linear hyperbolic theory lead to the following theorem.

Theorem 2.1. *Let $s > m/2$ be real and $U(0, \cdot) \in H^s(\mathbb{R}^m)^d$, then there exists a time $T_* \in]0, \infty]$ such that equation (2.2) with the Cauchy data $U(0, \cdot)$ has a unique solution $U \in \mathcal{C}([0, T_*]; H^s(\mathbb{R}^m)^d)$. Moreover, this solution is continuous with respect to the initial data.*

In [13] or [14] global existence results are given for an analogous system. But, in opposition to what the title of this second article suggests, they do not address Maxwell-Bloch equations but different forms of Maxwell-Lorentz equations. It is not straightforward to generalize their H^1 results to the Maxwell-Bloch system. Namely, it is possible to derive L^2 estimates due to cancellations that follow from Lemma 2.2 below, but such cancellations do not always appear when we consider higher derivatives in the equations.

We now show two estimates for the solutions to system (2.1). They are interesting in themselves but Estimate 2.3 is also used to show the convergence of the numerical schemes in Section 3.

Lemma 2.2. *Let $V_1, V_2 \in \mathcal{M}_{N,N}(\mathbb{C})$, then $\text{Tr}([V_1, V_2]V_1) = 0$.*

Proof. The proof of this lemma is straightforward and follows from a permutation on indices once the products are made explicit. ■

Estimate 2.3. L^∞ estimate for Bloch variables. *Let ρ be the solution of the Bloch equations; then,*

$$\frac{1}{N} \leq \text{Tr}(\rho^2) \leq 1 \quad \text{and} \quad \text{Tr}(\rho^2) - 2 + \frac{1}{N} \leq \text{Tr}(\sigma^2) \leq \text{Tr}(\rho^2) + 1.$$

Proof. The first estimate follows from the different properties of the matrix ρ that are recalled above.

$$\mathrm{Tr}(\rho^2) = \sum_{j,k} |\rho_{jk}|^2 \leq \sum_{j,k} \rho_{kk} \rho_{jj} = \left(\sum_j \rho_{jj} \right)^2 = 1.$$

This estimate is optimal because if $\rho_{jk} = \sqrt{\rho_{jj}\rho_{kk}}$, we have exactly $\mathrm{Tr}(\rho^2) = 1$. Besides it does not involve any special form of the relaxation coefficients (which have however to be positive as shown in [9]). The minimum for $\mathrm{Tr}(\rho^2)$ is $1/N$ and is obtained for the configuration where coherences are zero and the populations are equal to $1/N$. The second estimate follows from $\mathrm{Tr}(\sigma^2) = \mathrm{Tr}(\rho^2) - 2 \mathrm{Tr}(\rho\rho^e) + \mathrm{Tr}(\rho^{e2})$. ■

Let us now define the pseudo-energy:

$$\mathcal{E}(t) = \int_{\mathbb{R}^m} (|\mathbf{E}(t, \mathbf{x})|^2 + |\mathbf{B}(t, \mathbf{x})|^2 + \mathrm{Tr}(\sigma^2)(t, \mathbf{x})) d\mathbf{x},$$

then we have the estimate

Estimate 2.4. L^2 estimate for all the variables. *There exists a constant C , that depends only on the matrices W , \mathbf{p} , on γ_{jk} and the parameter ζ , such that $\mathcal{E}(t) \leq e^{Ct}\mathcal{E}(0)$.*

This result is certainly not optimal since we do not expect this pseudo-energy to soar but instead to be more or less constant.

Proof. Taking the scalar product of the Faraday and Ampère equations with \mathbf{B} and \mathbf{E} , respectively, we obtain

$$\frac{1}{2} \partial_t |\mathbf{E}|^2 + \frac{1}{2} \partial_t |\mathbf{B}|^2 + \mathrm{div}(\mathbf{E} \wedge \mathbf{B}) = -\partial_t \mathbf{P} \cdot \mathbf{E}.$$

Moreover using Lemma 2.2 with $V_1 = \mathbf{p} \cdot \mathbf{E}$ and $V_2 = \sigma$ or ρ^e , we obtain

$$\partial_t \mathbf{P} \cdot \mathbf{E} = \zeta \mathrm{Tr}(\mathbf{p} \cdot \mathbf{E} R n(\sigma)).$$

Using once more Lemma 2.2 with $V_1 = \sigma$ and $V_2 = \mathbf{p} \cdot \mathbf{E}$, we obtain the equality

$$\partial_t \mathrm{Tr}(\sigma^2) = -2 \sum_{j,k} \gamma_{jk} |\sigma_{jk}|^2 + 2 \sum_j \sigma_{jj} \left(\sum_{k \neq j} W_{jk} \sigma_{kk} \right) + i \sum_{jk} \sigma_{jk} \mathbf{p}_{kj} \cdot \mathbf{E} [\rho_{jj}^e - \rho_{kk}^e].$$

Setting $\mathbf{p}_{jk}^e = (i/2) \mathbf{p}_{jk} [\rho_{jj}^e - \rho_{kk}^e]$, which is also an Hermitian matrix, and using Cauchy-Schwarz estimates, we find that

$$\frac{1}{2} \partial_t \mathcal{E}(t) \leq \int_{\mathbb{R}^m} \left(\zeta \mathrm{Tr}(\mathbf{p} \cdot \mathbf{E} R n(\sigma)) + \sum_{jk} \sigma_{jj} W_{jk} \sigma_{kk} + \mathrm{Tr}(\sigma(\mathbf{p}^e \cdot \mathbf{E})) \right) d\mathbf{x} \leq C \mathcal{E}(t).$$

The constant C depends a priori on W , \mathbf{p} , γ_{jk} , ζ and the equilibrium state, but this state depends only on the matrix W and therefore we have proved Estimate 2.4. ■

3. NUMERICAL TIME COUPLING

The classical finite difference scheme to discretise the Maxwell-Bloch equations is based on the Yee method [8]. This method has the advantage of being nondiffusive but is dispersive. The coupling we perform here displays the same accuracy limitations as those of the Yee method. It is second order, but not satisfactory for computations over long time intervals. We do not make explicit the space discretization and want to be able to treat complex geometries. What follows does not only apply to the Yee scheme, but also to finite volume formulations (see [11, 15]) that use dual Delaunay-Voronoi meshes. We are not interested in using finite element methods for two reasons: the variational formulation would be different when the form of the relaxation operator $Q(\rho)$ changes for the populations, and the mass matrix would be unnecessarily difficult to invert.

In this method \mathbf{E} and \mathbf{B} are computed on staggered grids in space and time. We only make the time dependence explicit, because we are interested in the time coupling: given a time step δt , \mathbf{E}^n and $\mathbf{B}^{n-1/2}$ are the computed values for $\mathbf{E}(n\delta t)$ and $\mathbf{B}((n + \frac{1}{2})\delta t)$. The Faraday and Ampère equations are discretized respectively at time $n\delta t$ and $(n + \frac{1}{2})\delta t$ by

$$\frac{\mathbf{B}^{n+1/2} - \mathbf{B}^{n-1/2}}{\delta t} + \text{curl } \mathbf{E}^n = 0, \quad (3.1)$$

$$\frac{\mathbf{E}^{n+1} - \mathbf{E}^n}{\delta t} - \text{curl } \mathbf{B}^{n+1/2} = -(\partial_t \mathbf{P})^{n+1/2}. \quad (3.2)$$

In the sequel we compare different methods for the Bloch equations; these have already been compared in the zero-dimensional case (see [9]), that is for a forced electromagnetic field. The coupling, however, leads to new considerations. Indeed the point is now to choose the time of discretization for ρ . In any case it is natural to take the same space locations as for \mathbf{E} for the Yee scheme and the same mesh as \mathbf{E} for finite volume approximations.

A. Classical Crank-Nicolson Schemes

The literature [5–7, 11] only uses what we call here *strongly coupled methods*. The common property for strongly coupled methods is that ρ is computed at time $n\delta t$, and the Bloch equations are written at time $(n + \frac{1}{2})\delta t$. In both the cases that we present here, the classical Crank-Nicolson scheme reads

$$\frac{\rho^{n+1} - \rho^n}{\delta t} = Rn \left(\frac{\rho^{n+1} + \rho^n}{2} \right) + i \frac{\mathbf{E}^{n+1} + \mathbf{E}^n}{2} \cdot \left[\mathbf{p}, \frac{\rho^{n+1} + \rho^n}{2} \right].$$

The two schemes differ from the expression for the coupling.

In [11] (and also [16] for rate equations), the coupling with the Maxwell equations is performed using a value for \mathbf{P} at times $n\delta t$ and computing

$$(\partial_t \mathbf{P})^{n+1/2} = \frac{\mathbf{P}^{n+1} - \mathbf{P}^n}{\delta t} = \zeta \operatorname{Tr} \left(\mathbf{p} \frac{\rho^{n+1} - \rho^n}{\delta t} \right).$$

In [5–7], the coupling with the Maxwell equations is done using the formulation (1.2) for $\partial_t \mathbf{P}$. The right-hand side in the Ampère equation reads

$$-\zeta \operatorname{Tr} \left(\mathbf{p} Rn \left(\frac{\rho^{n+1} + \rho^n}{2} \right) \right) - i\zeta \operatorname{Tr} \left(\mathbf{p} \frac{\mathbf{E}^{n+1} + \mathbf{E}^n}{2} \cdot \left[\mathbf{p}, \frac{\rho^{n+1} + \rho^n}{2} \right] \right).$$

In both cases the nonlinear semi-implicit term involving $(\mathbf{E}^{n+1} + \mathbf{E}^n)(\rho^{n+1} + \rho^n)$ in the Bloch equation is solved using a predictor-corrector scheme or a fixed-point procedure and couples all the spatial discretization points *via* the Ampère equation.

B. Weakly Coupled Methods

A simple but new way to decouple the Ampère and Bloch equations is to discretise ρ at time $(n + \frac{1}{2})\delta t$. Hence in the Ampère equation the right-hand side, which we always base on formulation (1.2), reads

$$-\zeta \operatorname{Tr}(\mathbf{p} Rn(\rho^{n+1/2})) - i\zeta \operatorname{Tr} \left(\mathbf{p} \frac{\mathbf{E}^{n+1} + \mathbf{E}^n}{2} \cdot [\mathbf{p}, \rho^{n+1/2}] \right), \quad (3.3)$$

and $\rho^{n+1/2}$ has already been computed when we have to evaluate this quantity.

A Crank-Nicolson scheme for the Bloch equations now reads

$$\frac{\rho^{n+1/2} - \rho^{n-1/2}}{\delta t} = Rn \left(\frac{\rho^{n+1/2} + \rho^{n-1/2}}{2} \right) + i\mathbf{E}^n \cdot \left[\mathbf{p}, \frac{\rho^{n+1/2} + \rho^{n-1/2}}{2} \right].$$

We still have to perform a fixed-point procedure to solve the Ampère equation in the two- and three-dimensional cases. This is not necessary in the one-dimensional case. Besides at each time step, the Bloch equations associated with each discretization point evolve separately (and are very small systems to invert). They may be computed using a parallel implementation, which is even more useful for two and three-dimensional codes.

As shown in [9] Crank-Nicolson schemes have the drawback that they lead to the nonconservation of positiveness properties. For example, populations may not remain in the interval $[0, 1]$. Nevertheless we may estimate the Bloch variables on a time interval $[0, T]$. Namely, for example for the weakly coupled Crank-Nicolson scheme, the following lemma holds true.

Lemma 3.1. *There exist δt_0 and C that depend only on the matrix W , such that for all $\delta t \leq \delta t_0$ and all n such that $n\delta t \leq T$,*

$$\operatorname{Tr}(\rho^{n+1/2})^2 \leq e^{CT} \operatorname{Tr}(\rho^{1/2})^2.$$

Proof. From the definition of this scheme and using Lemma 2.2,

$$\operatorname{Tr}(\rho^{n+1/2})^2 - \operatorname{Tr}(\rho^{n-1/2})^2 = 2\delta t \operatorname{Tr} \left(Rn \left(\frac{\rho^{n+1/2} + \rho^{n-1/2}}{2} \right) \frac{\rho^{n+1/2} + \rho^{n-1/2}}{2} \right).$$

In this formula the trace may be decomposed in a negative part that mainly comes from the off-diagonal terms and a part that is estimated by $C(W)(\text{Tr}(\rho^{n+1/2})^2 + \text{Tr}(\rho^{n-1/2})^2)$, where the constant $C(W)$ depends only on the matrix W (and the number of energy levels N). Therefore,

$$\text{Tr}(\rho^{n+1/2})^2 \leq \left(\frac{1 + 2\delta t C(W)}{1 - 2\delta t C(W)} \right) \text{Tr}(\rho^{n-1/2})^2 \leq \exp(1 + 8n\delta t C(W)) \text{Tr}(\rho^{1/2})^2,$$

if $\delta t \leq \delta t_0 = 1/(4C(W))$. The form of this condition may be interpreted by saying that the time step should be chosen in order to model diagonal relaxation effects. To approximate ρ on the time interval $[0, T]$, we always have $n\delta t \leq T$, and this yields the result. ■

This estimate will be used in the proof of the convergence for this scheme.

In [9] a new scheme for the Bloch equations is constructed. This handles positiveness problems and is based on a splitting procedure. The main point is that we know how to solve exactly the relaxation-nutation part

$$\partial_t \rho = Rn(\rho)$$

and the Hamiltonian part

$$\partial_t \rho = i\mathbf{E} \cdot [\mathbf{p}, \rho]$$

separately, and each part preserves positiveness. Denoting, respectively, by S_R and $S_H(\mathbf{E})$ the semi-groups associated to these equations, we obtain a second-order scheme by computing

$$\rho^{n+1/2} = S_R\left(\frac{\delta t}{2}\right) S_H(\mathbf{E}^n)(\delta t) S_R\left(\frac{\delta t}{2}\right) \rho^{n-1/2}.$$

It is both positiveness preserving and decoupled. A second-order approximation to $S_H(\mathbf{E}^n)(\delta t)$, which still ensures positiveness is given in [9], as well as specific Fadeev Formulae that lead to a very efficient evaluation of this term, which may also be computed on parallel architectures. A comment on the effective order of splitting methods is given in Section 4.

In terms of theoretical properties and of efficiency the weakly coupled splitting scheme is the best of all the methods presented here. In particular the equivalent of Lemma 3.1 is the physical estimate $\text{Tr}(\rho^{n+1/2})^2 \leq 1$. Next we also compare them from the point of view of the quality of the computed solutions.

C. Nonlinear Stability Results

In this section we show that the weakly coupled Crank-Nicolson scheme and the splitting scheme are both nonlinearly stable under suitable Courant-Friedrichs-Lewy conditions. We suppose that the Yee scheme is implemented on a uniform space grid with mesh step h .

Theorem 3.2. *The weakly coupled Crank-Nicolson and splitting schemes are nonlinearly L^2 -stable for $\delta t \leq \delta t_0$ and $\lambda^2 \equiv \delta t^2/h^2 \leq \lambda_0^2 < 1$, where δt_0 and λ_0 depend only on the coefficients of the equations.*

Remark. The CFL condition that follows from the proof below is not much more restrictive than that of the Yee scheme. Indeed, for the Yee scheme λ should be less than 1 and here we obtain a condition that reads $(1 + Ch\lambda)\lambda^2 < 1$.

Proof. In order to be able to have L^2 estimates in the whole space, we write numerical schemes introducing ρ^e and $\sigma^{n+1/2}$ with straightforward notations. In order to have shorter expressions we also set $\mathbf{E}^{n+1/2} = (\mathbf{E}^n + \mathbf{E}^{n+1})/2$ and $\sigma^n = (\sigma^{n+1/2} + \sigma^{n-1/2})/2$. We denote by $\|\cdot\|$ the L^2 norm, and by (\cdot, \cdot) the associated scalar product. We first introduce a numerical pseudo-energy $U^{n+1/2}$ which only deals with Maxwell variables, namely

$$U^{n+1/2} = \|\mathbf{B}^{n+1/2}\|^2 - \frac{\delta t^2}{4} \|\operatorname{curl} \mathbf{B}^{n+1/2}\|^2 + \|\mathbf{E}^{n+1/2}\|^2.$$

This quantity is positive provided $\delta t \leq h$, thanks to the well-known estimate

$$\|\operatorname{curl} \mathbf{B}^{n+1/2}\|^2 \leq \frac{4}{h^2} \|\mathbf{B}^{n+1/2}\|^2. \quad (3.4)$$

The field \mathbf{E}^n appears in the equations and has to be replaced by

$$\mathbf{E}^n = \frac{1}{2}(\mathbf{E}^{n+1/2} + \mathbf{E}^{n-1/2}) - \frac{1}{4}(\mathbf{E}^{n+1} - \mathbf{E}^n) + \frac{1}{4}(\mathbf{E}^n - \mathbf{E}^{n-1}), \quad (3.5)$$

and Eqs. (3.1) and (3.2) lead in a classical way to

$$\begin{aligned} U^{n+1/2} - U^{n-1/2} = & -\frac{\delta t}{2} (\mathbf{E}^{n+1/2} + \mathbf{E}^{n-1/2}, (\partial_t \mathbf{P})^{n+1/2} + (\partial_t \mathbf{P})^{n-1/2}) \\ & - \frac{\delta t^2}{4} (\operatorname{curl} \mathbf{B}^{n+1/2} + \operatorname{curl} \mathbf{B}^{n-1/2}, (\partial_t \mathbf{P})^{n+1/2} - (\partial_t \mathbf{P})^{n-1/2}). \end{aligned}$$

For the classical Maxwell equations, $\mathbf{P} = 0$, and this leads to stability under the CFL condition $\delta t \leq h$. Here we have to express $(\partial_t \mathbf{P})^{n+1/2}$ that reads for both the weakly coupled Crank-Nicolson and splitting methods:

$$(\partial_t \mathbf{P})^{n+1/2} = \zeta \operatorname{Tr}(\mathbf{p} R n(\sigma^{n+1/2})) + i\zeta \operatorname{Tr}(\mathbf{p} \mathbf{E}^{n+1/2} \cdot [\mathbf{p}, \sigma^{n+1/2}]) + i\zeta \operatorname{Tr}(\mathbf{p} \mathbf{E}^{n+1/2} \cdot [\mathbf{p}, \rho^e]).$$

This has the advantage of introducing the quantity ζ which is small. We denote by α and β the constants that depend only on \mathbf{p} and W such that

$$\|\operatorname{Tr}(\mathbf{p} R n(\sigma))\|^2 \leq \alpha \|\sigma\|^2 \quad \text{and} \quad \|\operatorname{Tr}(\mathbf{p} \mathbf{E} \cdot [\mathbf{p}, \sigma])\|^2 \leq \beta \|\mathbf{E}\|^2.$$

Careful estimates lead to

$$\begin{aligned} \|U^{n+1/2} - U^{n-1/2}\| \leq & \frac{3}{4} \zeta \delta t^3 (\|\operatorname{curl} \mathbf{B}^{n+1/2}\|^2 + \|\operatorname{curl} \mathbf{B}^{n-1/2}\|^2) \\ & + \frac{3\zeta\delta t}{8} (4 + 3\beta) (\|\mathbf{E}^{n+1/2}\|^2 + \|\mathbf{E}^{n-1/2}\|^2) + \frac{3\zeta\delta t\alpha}{4} (\|\sigma^{n+1/2}\|^2 + \|\sigma^{n-1/2}\|^2). \end{aligned}$$

We now need an estimate on $\|\sigma^{n+1/2}\|^2$, which is obtained by integrating $\text{Tr}(\sigma^{n+1/2})^2$ in space. From now on, in order to carry out the calculations, we have to distinguish between the two schemes.

For the Crank-Nicolson scheme, we have

$$\text{Tr}(\sigma^{n+1/2})^2 - \text{Tr}(\sigma^{n-1/2})^2 = 2\delta t \text{Tr}(Rn(\sigma^n)\sigma^n) + 2i\delta t \mathbf{E}^n \cdot \text{Tr}([\mathbf{p}, \rho^e]\sigma^n).$$

There also exist constants $\tilde{\alpha}$, which depends only on W , and $\tilde{\beta}$, which depends only on \mathbf{p} , such that

$$\text{Tr}(Rn(\sigma)\sigma) \leq \tilde{\alpha} \text{Tr}(\sigma)^2 \quad \text{and} \quad \|\text{Tr}(\mathbf{E} \cdot [\mathbf{p}, \rho^e]\sigma)\|^2 \leq \tilde{\beta}(\|\mathbf{E}\|^2 + \|\sigma\|^2).$$

Hence,

$$\begin{aligned} \|\sigma^{n+1/2}\|^2 &\leq \|\sigma^{n-1/2}\|^2 + \frac{3}{4} \delta t \tilde{\beta} (8 + 3\delta t^2 \zeta^2 \beta) (\|\mathbf{E}^{n+1/2}\|^2 + \|\mathbf{E}^{n-1/2}\|^2) \\ &\quad + \frac{3\delta t^3}{2} \tilde{\beta} (\|\text{curl } \mathbf{B}^{n+1/2}\|^2 + \|\text{curl } \mathbf{B}^{n-1/2}\|^2) + \delta t \left(\frac{3}{2} \delta t^2 \zeta^2 \alpha \tilde{\beta} + 4(\tilde{\alpha} + \tilde{\beta}) \right) (\|\sigma^{n+1/2}\|^2 + \|\sigma^{n-1/2}\|^2). \end{aligned}$$

For the splitting scheme, we analyze separately the two parts. One part requires the computing of $S_R(\delta t)\sigma$, which is solution to $\partial_t \sigma = Rn(\sigma)$. For this equation, using the Gronwall lemma, we find that

$$\|S_R(\delta t)\sigma(t)\|^2 \leq \exp(C_R \delta t) \|\sigma(t)\|^2,$$

where C_R depends only on W . The second ingredient is $\tilde{S}_H(\mathbf{E}^n)(\delta t)\sigma$, which is the solution of $\partial_t \sigma = i\mathbf{E}^n \cdot [\mathbf{p}, \sigma] + i\mathbf{E}^n \cdot [\mathbf{p}, \rho^e]$. In the same way we have

$$\|\tilde{S}_H(\mathbf{E}^n)(\delta t)\sigma(t)\|^2 \leq (\|\sigma(t)\|^2 + \delta t \|\mathbf{E}^n\|^2) \exp(C_H \delta t),$$

where C_H depends only on \mathbf{p} and ρ^e . Now we may apply this, for example, to the second-order scheme, and there exist two constants \tilde{C}_σ and \tilde{C}_E , depending on C_H and C_R , such that

$$\|\sigma^{n+1/2}\|^2 \leq (1 + \tilde{C}_\sigma \delta t) \|\sigma^{n-1/2}\|^2 + \delta t (1 + \tilde{C}_E \delta t) \|\mathbf{E}^n\|^2,$$

if $\delta t \leq \delta t_1$ (and δt_1 may be chosen arbitrarily).

For both schemes, we may define the pseudo-energy

$$\mathcal{E}^{n+1/2} = \|\mathbf{B}^{n+1/2}\|^2 - \frac{\delta t^2}{4} \|\text{curl } \mathbf{B}^{n+1/2}\|^2 + \|\mathbf{E}^{n+1/2}\|^2 + \|\sigma^{n+1/2}\|^2, \quad (3.6)$$

which now deals with all variables and is a positive quantity. Gathering the above estimates, there exist three constants C_B , C_E , and C_σ that depend only on the parameters in the Maxwell-Bloch equations such that

$$\begin{aligned} \mathcal{E}^{n+1/2} &\leq \mathcal{E}^{n-1/2} + \frac{\delta t^3}{4} C_B (\|\operatorname{curl} \mathbf{B}^{n+1/2}\|^2 + \|\operatorname{curl} \mathbf{B}^{n-1/2}\|^2) + \delta t C_E (\|\mathbf{E}^{n+1/2}\|^2 + \|\mathbf{E}^{n-1/2}\|^2) \\ &\quad + \delta t C_\sigma (\|\sigma^{n+1/2}\|^2 + \|\sigma^{n-1/2}\|^2). \end{aligned}$$

Let $\lambda^2 = \delta t^2/h^2$, then estimate (3.4) implies that

$$\begin{aligned} &\left(1 - \frac{\lambda^2}{1 - \lambda^2} \delta t C_B\right) \left(\|\mathbf{B}^{n+1/2}\|^2 - \frac{\delta t^2}{4} \|\operatorname{curl} \mathbf{B}^{n+1/2}\|^2\right) + (1 - \delta t C_E) \|\mathbf{E}^{n+1/2}\|^2 + (1 - \delta t C_\sigma) \|\sigma^{n+1/2}\|^2 \\ &\leq \left(1 + \frac{\lambda^2}{1 - \lambda^2} \delta t C_B\right) \left(\|\mathbf{B}^{n+1/2}\|^2 - \frac{\delta t^2}{4} \|\operatorname{curl} \mathbf{B}^{n+1/2}\|^2\right) + (1 + \delta t C_E) \|\mathbf{E}^{n-1/2}\|^2 \\ &\quad + (1 + \delta t C_\sigma) \|\sigma^{n-1/2}\|^2. \end{aligned} \tag{3.7}$$

Provided that $(1 + \delta t C_B) \delta t^2/h^2 < 1$ and $\delta t < 1/\max(C_E, C_\sigma) \equiv \delta t_0$, the left-hand side of Eq. (3.7) is a positive quantity. To have positive coefficients we suppose that $\lambda^2 \leq \lambda_0^2 = 1/(1 + \delta t_0 C_B) < 1$ and set

$$C = \max\left(\frac{\lambda_0^2}{1 - \lambda_0^2} C_B, C_E, C_\sigma\right)$$

and

$$\mathcal{E}^{n+1/2} \leq \frac{1 + C \delta t}{1 - C \delta t} \mathcal{E}^{n-1/2} \leq \left(\frac{1 + C \delta t}{1 - C \delta t}\right)^n \mathcal{E}^{1/2} \leq C s t,$$

for all n and $\delta t \leq \delta t_0$ such that $n \delta t \leq T$. This ensures the L^2 nonlinear stability for both weakly coupled schemes under the CFL condition $\delta t^2/h^2 \leq \lambda_0^2 = 1/(1 + \delta t_0 C_B)$ and for $\delta t \leq \delta t_0$. ■

4. NUMERICAL COMPARISON OF METHODS

The schemes we present here, together with a relaxation scheme, have already been compared in [9] but with no coupling issues because the electromagnetic field was supposed to be given (and monochromatic). The two points that are illustrated in that reference are positiveness results and the trace property. Dynamics are also compared with a rough qualitative point of view. As the theoretical analysis predicts, only the splitting scheme conserves positiveness and the trace property.

Now, to address coupling issues we only present 1D simulations and consider a self-induced transparency (SIT) test that has first been used by Ziolkowski et al. [7] and has the advantage of not being polluted by positiveness problems that only occur for more than two levels. In this test case which involves what is called a 4π -pulse, the medium is supposed to undergo four inversions and to stabilize eventually in the initial state.

It is very important to compare different numerical methods because we do not have any physical experiment with which to compare our results. The point is not to display here physical tests but to find hints that would lead us to choose one of our schemes for further more demanding simulations. Examples of applications are given, e.g., in [11, 12]).

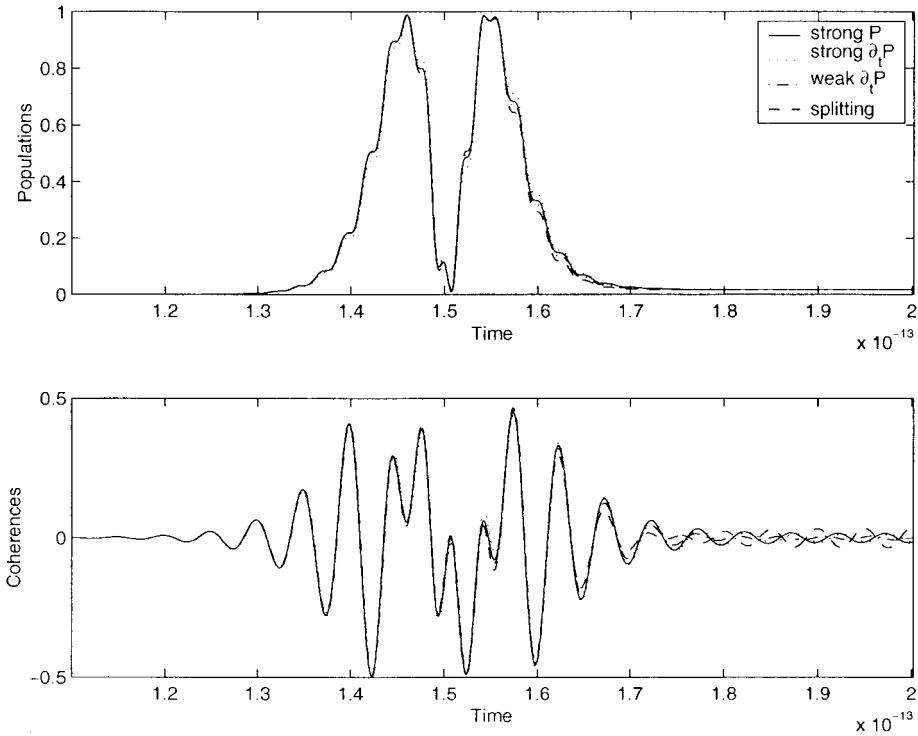


FIG. 1. SIT. Comparison of the different schemes on a 20 points per wavelength grid. Time evolution of ρ_{11} and $|\rho_{12}|$.

The plots present the time evolution of the population ρ_{11} and the coherence $|\rho_{12}|$ for the different schemes. In this SIT experiment the incident electromagnetic field is a wave packet that is not much perturbed by the interaction and therefore we do not plot it.

A. General Comparison

The methods that are presented above are compared in Fig. 1. These simulations give very comparable results. We may however recall that weakly coupled methods are much more efficient. Besides the gain in efficiency is even more important with a parallel implementation. The main difference between the methods is the amplitude of the remaining coherences. No physical argument may discriminate between the different plots. Therefore, we perform convergence experiments for weakly coupled methods.

B. Convergence and Higher Order Splitting Schemes

The Shannon sampling theorem tells us that we need at least 6 points per wavelength to model correctly the evolution of the electromagnetic field and consequently the coherences. Because we want typically to observe cubic nonlinearities in isotropic media, we use at least 20 points per wavelength. Convergence tests have been performed with 20 and 100 points per wavelength grids and we have plotted the results on Fig. 2.

For 20 points per wavelength the main difference between the schemes may be seen on the coherence tail, whereas for 100 points per wavelength, all the methods give similar results.

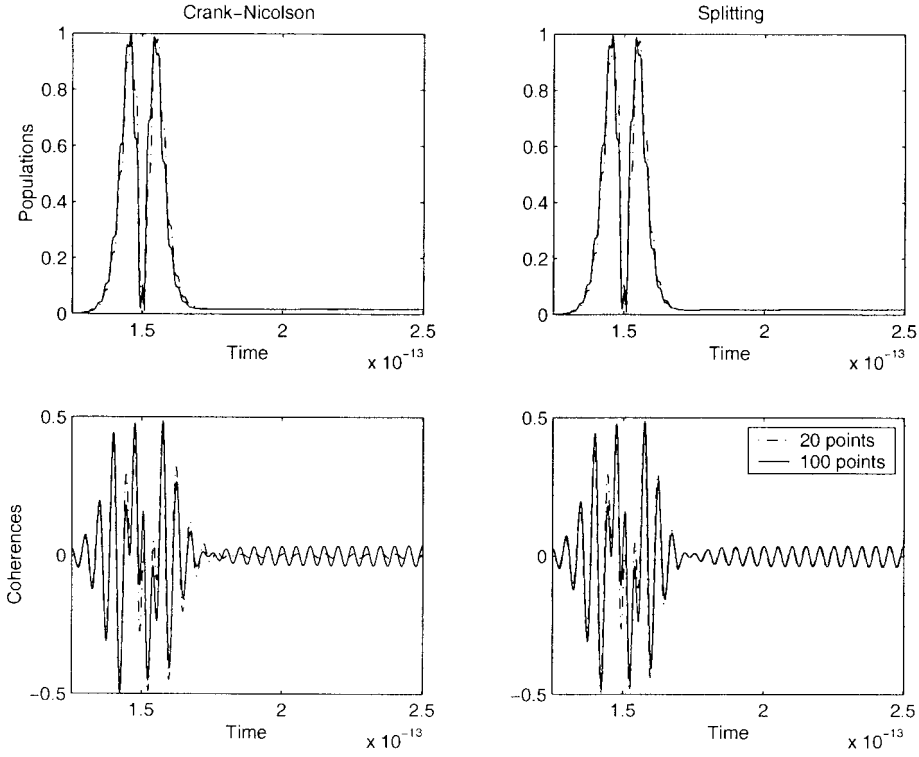


FIG. 2. SIT. Convergence of the Crank-Nicolson and splitting methods. Time evolution of ρ_{11} and $|\rho_{12}|$.

Another advantage of the splitting method arises from this point of view. The coherence tail has indeed the right amplitude with a small number of points per wavelength. Rougher meshes may be used for the splitting scheme than for the other schemes.

A first order splitting scheme, namely,

$$\rho^{n+1/2} = S_R(\delta t) S_H(\mathbf{E}^n)(\delta t) \rho^{n-1/2},$$

has been used to compute the solutions plotted in Figs. 1 and 3 and gives good results compared to the other methods, which are second-order ones. We compared the results for Lie splitting methods, the former one (H-R) but also the one that consists in computing the relaxation-nutation step first (R-H) and Strang formulae [17] (H-R-H) and (R-H-R). The steps that are doubled are taken on half time-steps (as described in Section 3 for the (R-H-R) scheme). Results for the SIT test are very similar and to see the differences we have to zoom on the end of the last inversion. The results for 20 points per wavelength are shown on Fig. 3. At first sight it may seem strange that the (H-R-H) scheme, which is usually called a second-order scheme, should give worse results than a first-order scheme. This is explained using arguments that may be found in [18]. Indeed we deal with a set of variables that evolve with different time scales. The dimensionless equations that we compute are not stiff, but some coefficients are of order 1 and others are smaller. More precisely, we choose the frequency ω_0 and the amplitude of the incident field such that

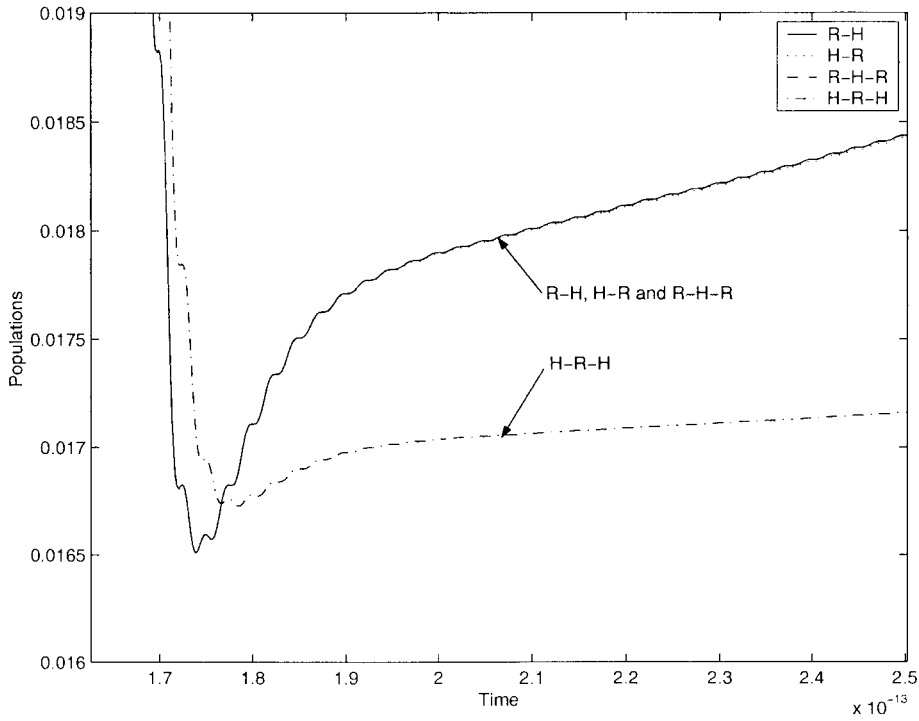


FIG. 3. SIT. Comparison of splitting schemes on a 20 points per wavelength grid. Time evolution of ρ_{11} .

$$\omega_0 = \omega_{21} = \omega_R.$$

Therefore, the relaxation-nutation coefficient for the coherences is of order 1 but is much smaller for the populations. The end of the last inversion is a time when the amplitude of the field is much smaller than the maximum amplitude of the incident field. Therefore, the Bloch equations may be written as

$$\partial_t \rho = (Rn_0(\rho) + \varepsilon Rn_1(\rho)) + \varepsilon H(\rho).$$

On a large time scale $T = \varepsilon t$, this leads to

$$\partial_T \rho = \left(\frac{1}{\varepsilon} Rn_0(\rho) + Rn_1(\rho) \right) + H(\rho),$$

and our findings coincide with the conclusions of [18], which are that the stiff part (i.e., the relaxation-nutation part in our case) has to be computed last and therefore the (H-R) and (R-H-R) are better schemes in our context.

To enhance the accuracy we may think about higher-order schemes. We should consider higher-order schemes for both the Maxwell and the Bloch equations. This is a priori possible in the context of Yee type schemes for the Maxwell equations (see e.g., [19]) and also for the splitting schemes for the Bloch equations (see [20]). In this reference it is shown that it is impossible to write a splitting scheme of order three or more with only positive coefficients. This

is great restriction in the case of the Bloch equations because it would be difficult to preserve positiveness properties.

5. CONCLUSION

The lack of experimental measures at such small scales makes it all the more difficult to justify that numerical schemes are adequate to simulate the Maxwell-Bloch model. It is therefore important to compare different methods. Some schemes yield disastrous results, such as the relaxation scheme for the Bloch equations presented in [9]. The ones we display in this article yield very similar results. Nevertheless the weakly coupled methods we introduce allow some gain in computational time, which may be further improved using parallel computing. Among them, the splitting method allows a factor 5 gain on the space step and this of course also has repercussions on the time step *via* the CFL condition. We chose the SIT test case in order that positiveness difficulties do not interfere but we recall (see [9]) that, in contrast to Crank-Nicolson schemes, the splitting schemes give physically relevant solutions with respect to positiveness whatever the test case. The weakly coupled splitting schemes seem therefore to be the relevant scheme for further simulations, especially for long time computations, although difficulties connected to the dispersive character of the Yee scheme remain. This may not be remedied by using higher order schemes which would spoil the positiveness properties of splitting schemes.

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