Nonstandard finite difference schemes for the two-level Bloch model

Marc E. Songolo, Brigitte Bidégaray-Fesquet

Nonstandard finite difference schemes for the two-level Bloch model

Marc E. Songolo[a**] and Brigitte Bidégaray-Fesquet[b]
[a]Département de Mathématiques et Informatique,
Université de Lubumbashi, Lubumbashi, RD Congo;
[b]Univ. Grenoble Alpes, Grenoble INP[††], LJK, 38000 Grenoble, France

Abstract

In this paper, we present splitting schemes for the two-level Bloch model. After proposing two ways to split the Bloch equation, we show that it is possible in each case to generate exact numerical solutions of the obtained sub-equations. These exact solutions involve matrix exponentials which can be expensive to compute. Here, for 2×2 matrices we develop equivalent formulations which reduce the computational cost. These splitting schemes are nonstandard ones and conserve all the physical properties (Hermicity, positiveness and trace) of Bloch equations. In addition, they are explicit, making effective their implementation when coupled with the Maxwell equations.

Keywords: Bloch equation, Exponential of a matrix, Exact finite difference schemes, Nonstandard finite difference schemes, Splitting method.

1 Introduction

Bloch equation describes the time evolution of the density matrix. It is derived from the Schrödinger equation or the Heisenberg formalism, see for example [4, 5, 6, 9, 15]. The density matrix is a quantum observable (unlike the wave function) and is used to describe the probability of presence of electrons in the quantized energy levels (diagonal entries of the matrix) and the coherence between these levels (off-diagonal entries). Its size depends on the number of considered atom energy levels. In many references, the derivation of the Bloch equation is presented only in the case of two-level atoms. Coherent control of a quantum mechanical two-level system is at the heart of magnetic resonance imaging, quantum information processing, and quantum optics [8].

The analytical and exact numerical solutions of the Bloch equation involve the calculation of matrix exponentials, which would be very time consuming,

**Corresponding author. Email: marc.songolo@gmail.com
††Institute of Engineering Univ. Grenoble Alpes

thus leading to the search for approximate numerical solutions. It takes two forms [4]: either generic robust schemes or dedicated schemes to this equation. In the context of two-level atoms, the approach of the generic scheme was tested for the first time by R.W. Ziolkowski *et al.* at the University of Tucson [17, 18, 19]. They use a Crank–Nicolson scheme, which is second order. This scheme theoretically preserves all the physical properties (Hermicity, positiveness and trace), but in practice, it accumulates fixed point errors. This defect does not appear explicitly in [17], because the choice of modified variables used to implement the scheme does not enable to detect this problem. However, due to the accumulation of errors, the Crank–Nicolson scheme does not preserve the physical properties of the Bloch equation.

To overcome this problem, Bidégaray *et al.* introduced in [3] a splitting scheme of order two, named after Strang, based on the decomposition of the Bloch equation into a relaxation–nutation equation and an equation describing the interaction with an electromagnetic field (which is a Liouville equation). These two sub-equations have exact solutions, which are then combined by the splitting method. The resulting scheme is explicit and preserves all the physical properties of the Bloch equation. An essential feature of this scheme is that the calculation of matrix exponentials is approximated by a Crank–Nicolson method. Moreover, its explicitness makes effective the implementation when coupled with the Maxwell equations. We can find the same ingredients but with a different centering of variables in [1, 2], thus allowing a weak coupling, which is therefore algorithmically less expensive. Following these studies, Uwizeye presented in her Master thesis [14], a fourth-order Runge–Kutta method, which also preserves some physical properties.

The aim of this article is to improve the splitting schemes for the two-level Bloch model by incorporating exact numerical solutions of sub-equations. To this aim, we explore two different ways to split the Bloch equation, and then follow the same approach as in Bidégaray *et al.* [3], except that the calculations of matrix exponentials in the exact numerical solution of the Liouville equation are given by equivalent formulations and not approximations. In each case, it leads to numerical models that are consistent with the methodology of nonstandard finite difference (NSFD) schemes developed by Mickens [10]. Moreover, the obtained NSFD schemes are of variable time step-size.

The sequel of this paper is organized as follows: we present the Bloch model in Section 2. Section 3 provides the construction rules of NSFD schemes. Section 4 presents the various sub-equations, their explicit solutions and the principle of splitting. Two decompositions of the Bloch model are discussed in Section 5 and 6. Section 7 treats optical Bloch equations. Finally, numerical simulations applied to self-induced transparency are gathered in Section 8.

2 The Bloch model

We consider the Bloch equation [4, 5, 6, 9, 15]

$$\partial_t \rho_{jk} = -\frac{i}{\hbar}[H, \rho]_{jk} + Q(\rho)_{jk} \tag{1}$$

where ρ is the density matrix, H the Hamiltonian of the system, and $[H, \rho] = H\rho - \rho H$ is the commutator of H and ρ.
We can give an interpretation of the coefficients of the matrix ρ. Its diagonal entries are called *populations*. The population of level j, denoted ρ_{jj}, is the occupancy probability of the quantum state j. Off-diagonal entries are called *coherences*. The coherence ρ_{jk} between levels j and k is a complex number which modulus can be interpreted as a conditional probability of transition between levels j and k.
The Hamiltonian H can be decomposed into $H(t) = H_0 + V(t)$ where H_0 is the free electron Hamiltonian and $V(t) = -E(t)p$ expresses the (Hermitian) potential resulting from the interaction with an electromagnetic wave $E(t)$. The polarizability matrix p has a zero diagonal and transmits this property to $V(t)$. The Hamiltonian H_0 is a diagonal matrix $\mathrm{diag}(\hbar\omega_j)_{j=1,\dots,n}$.
The relaxation terms $Q(\rho)_{jk}$ take into account phenomena like spontaneous emission, collisions, vibrations in a crystal lattice, etc.

2.1 Relaxation

One distinguishes the terms that affect the coherences, called transverse relaxations, $Q(\rho)_{jk}$ with $j \neq k$, from terms affecting populations, $Q(\rho)_{jj}$, called longitudinal relaxations.

For longitudinal relaxations, we choose the Pauli master equation

$$Q(\rho)_{jj} = \sum_{k \neq j} [W_{jk}\rho_{kk}(t) - W_{kj}\rho_{jj}(t)], \tag{2}$$

where $W_{kj}\rho_{jj}(t)$ expresses the transition from level j to level k. The model chosen for transverse relaxations is more phenomenological and therefore simpler than for longitudinal relaxations. We introduce the relaxation rate $\gamma_{jk} > 0$, for $j \neq k$, and we have

$$Q(\rho)_{jk} = -\gamma_{jk}\rho_{jk}, \tag{3}$$

where $\gamma_{jk} = \gamma_{kj}$ is necessary to ensure the Hermicity of the density matrix.
This relaxation model and others are compared in Bidégaray *et al.* [3] from the point of view of the preservation of some symmetry and positivity properties of the density matrix. In particular,

1. Hermicity of ρ;
2. positiveness of ρ as an operator, which for two-level atoms reduces to conditions

(a) $\rho_{jj} \geq 0$,

(b) $|\rho_{jk}|^2 \leq \rho_{jj}\rho_{kk}$.

3. trace conservation, $\mathrm{Tr}(\rho) = \sum_j \rho_{jj} = 1$, which ensures that the number of electron is conserved through time evolution.

Conditions on the transverse and longitudinal relaxation coefficients can be found in [3] to ensure these properties. A sufficient and often fulfilled condition is $2\gamma_{jk} > \sum_l W_{lj} + \sum_l W_{lk}$.

2.2 Dimensionless equations

We want to use dimensionless equations for two reasons, first this leads to simpler equations and second this allows to exhibit the Rabi frequency which drives the behavior of the system. We introduce the following characteristic quantities:

- the characteristic frequency ω_c,
- the characteristic electric field E_c,
- the characteristic polarizability p_c.

Rescaling variables and matrices as follows:

$$H_0 = \hbar\omega_c \tilde{H}_0,\ t = \frac{1}{\omega_c}\tilde{t},\ E = E_c\tilde{E},\ p = p_c\tilde{p},\ Q = \omega_c\tilde{Q},\ \tilde{V} = \tilde{E}\tilde{p}$$

and defining the dimensionless Rabi frequency

$$\tilde{\Omega}_R = \frac{E_c p_c}{\hbar\omega_c},$$

we can rewrite equation (1) in the dimensionless form:

$$\partial_{\tilde{t}}\rho = -i[\tilde{H}_0, \rho] - i\tilde{\Omega}_R[\tilde{V}, \rho] + \tilde{Q}(\rho).$$

From now on we drop the tilde signs and can consider without loss of generality for the description of numerical methods that $\Omega_R = 1$:

$$\partial_t\rho = -i[H_0, \rho] - i[V, \rho] + Q(\rho). \tag{4}$$

2.3 The two-level case

In this study, we restrict ourselves to the case of matrices of order 2 for which

$$H_0 = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} \text{ and } V(t) = \begin{pmatrix} 0 & v_{12}(t) \\ \overline{v_{12}(t)} & 0 \end{pmatrix}, \tag{5}$$

where $\overline{v_{12}(t)}$ is the conjugate of $v_{12}(t)$.

3 NSFD methodology

In this section, we present the rules for the construction of NSFD schemes as proposed by Mickens [10].

Rule 1. *The order of the discrete derivatives must be exactly equal to the order of the corresponding derivatives of the differential equations.*

Rule 2. *Denominator functions for the discrete derivatives must, in general, be expressed in terms of more complicated functions of the step-sizes than those conventionally used. For example,*

$$\frac{\mathrm{d}u}{\mathrm{d}t} \simeq \frac{u^{n+1} - \varphi(\Delta t)u^n}{\phi(\Delta t)}$$

where φ and ϕ are the functions of the step-size Δt and have the properties:

$$\varphi(\Delta t) = 1 + \mathcal{O}(\Delta t^2) \text{ and } \phi(\Delta t) = \Delta t + \mathcal{O}(\Delta t^2) \text{ when } \Delta t \to 0.$$

Rule 3. *Nonlinear terms must, in general, be modeled non-locally on the computational grid or lattice.*

Rule 4. *Special solutions of the differential equations should also be special (discrete) solutions of the finite difference models.*

Rule 5. *The finite difference equations should not have solutions that do not correspond exactly to solutions of the differential equations.*

Definition 3.1. [12] A nonstandard finite difference scheme is any discrete representation of a system of differential equations that is constructed based on the above rules.

In addition to these five usual rules, Mickens stated a sixth rule in [11], which applies only to complex equations.

Rule 6. *For differential equations having N (≥ 3) terms, it is generally useful to construct finite difference schemes for various sub-equations composed of M terms, where $M < N$, and then combine all the schemes together in an overall consistent finite difference model.*

Given this last rule, it is first necessary to fragment the equation (4) into two sub-equations, then solve sub-equations by exact methods, and finally, connect solutions of sub-equations through a single consistent solution. In this way, we will split equation (4) in two ways: the pure relaxation equation and the raw Bloch equation in a first place; and the evolution of relaxation–nutation and the evolution with interaction of electromagnetic field in a second place. And in each case, we will see how to construct consistent finite difference model by using Strang splitting method.

4 Splitting and exact solutions

4.1 Linear operators on matrix entries

The Bloch equation is linear in the entries of the density matrix. However we want to treat the density matrix as a matrix and not its single entries. From this point of view the Bloch equation contains three types of linear operators.

4.1.1 The Liouville equation

Part of the equation is in Liouville form, i.e.

$$\partial_t \rho = [A(t), \rho].$$

This equation can be solved analytically in

$$\rho(t) = \exp\left(\int_0^t A(\tau)\mathrm{d}\tau\right) \rho(0) \exp\left(-\int_0^t A(\tau)\mathrm{d}\tau\right).$$

The computation of these exponentials is at the core of this paper.

4.1.2 Hadamard exponentials

The transverse relaxations are in the form

$$\partial_t \rho_{jk} = \beta_{jk}\rho_{jk}, \tag{6}$$

which solution is of course simply $\rho_{jk}(t) = \exp(\beta_{jk}t)\rho_{jk}(0)$. These entry-wise exponentials are gathered in a single operator, the Hadamard exponential. Let $B = (\beta_{jk})_{jk}$ where we have extended the definition to $\beta_{jj} = 0$, then the solution to equation (6) is denoted

$$\rho(t) = e^{\circ Bt} \circ \rho(0).$$

Remark 1. *The nutation part of the equation can be considered in two ways. Either as a Liouville equation, using $-iH_0$ as matrix A, or as linear equation on single entries taking $\beta_{jk} = -i(\omega_j - \omega_k)$. They each lead to one of the decomposition considered in this paper.*

4.1.3 The master equation

The longitudinal relaxation induce a master equation on populations which are easy to solve exactly in the two-level context. The equations read

$$\begin{aligned} \partial_t \rho_{11} &= W_{12}\rho_{22} - W_{21}\rho_{11}, \\ \partial_t \rho_{22} &= W_{21}\rho_{11} - W_{12}\rho_{22}. \end{aligned}$$

Denoting $W_\pm = W_{12} \pm W_{21}$, after straightforward calculations

$$\begin{aligned}\rho_{11}(t) &= \frac{1}{2} + \frac{1}{2}\left(e^{-W_+ t}(\rho_{11}(0) - \rho_{22}(0)) + (1 - e^{-W_+ t})W_-\right), \\ \rho_{22}(t) &= \frac{1}{2} - \frac{1}{2}\left(e^{-W_+ t}(\rho_{11}(0) - \rho_{22}(0)) + (1 - e^{-W_+ t})W_-\right).\end{aligned}$$

To be able to denote this solution, which would be described by an order 4 tensor if applied to the whole matrix, we define the linear application $\mathcal{M}(t)$ which is applied to the whole matrix ρ but only involve diagonal elements:

$$\rho(t) = \mathcal{M}(t)\rho(0).$$

4.2 Some results for 2×2 matrix exponentials

Theorem 4.1. *Let $A \in \mathcal{M}_2(\mathbb{C})$. Its annihilator polynomial is*

$$A^2 - \mathrm{Tr}(A)A + \det(A)I = 0 \tag{7}$$

and its eigenvalues are roots of this polynomial

$$\lambda_{1,2} = \frac{\mathrm{Tr}(A) \pm \sqrt{(\mathrm{Tr}(A))^2 - 4\det(A)}}{2}.$$

Due to the existence of this annihilator polynomial of degree 2, any analytic function of A can be written as a linear combination of A and I. In particular

$$\exp(A) = \alpha(\lambda_1, \lambda_2)I + \beta(\lambda_1, \lambda_2)A,$$

where

$$\begin{aligned}\alpha(\lambda_1, \lambda_2) &= \frac{\lambda_1 \exp(\lambda_2) - \lambda_2 \exp(\lambda_1)}{\lambda_1 - \lambda_2}, \\ \beta(\lambda_1, \lambda_2) &= \frac{\exp(\lambda_1) - \exp(\lambda_2)}{\lambda_1 - \lambda_2}.\end{aligned}$$

Proof. Suppose that the linear combination is written as

$$\exp(A) = \alpha I + \beta A$$

and A has two distinct eigenvalues. Defining $D = \mathrm{diag}(\lambda_1, \lambda_2)$, we can write $D = P^{-1}AP$ and diagonalize the system:

$$P^{-1}\exp(A)P = \alpha I + P^{-1}\beta A P,$$

$$\exp(D) = \alpha I + \beta D,$$

$$\begin{pmatrix} \exp(\lambda_1) & 0 \\ 0 & \exp(\lambda_2) \end{pmatrix} = \alpha \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \beta \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$

Therefore we have the system

$$\begin{cases} \exp(\lambda_1) = \alpha + \beta\lambda_1, \\ \exp(\lambda_2) = \alpha + \beta\lambda_2, \end{cases}$$

which solution is $\alpha = \alpha(\lambda_1, \lambda_2)$ and $\beta = \beta(\lambda_1, \lambda_2)$. □

Remark 2. *For any complex $\gamma \in \mathbb{C}$, applying the same argument to γA which eigenvalues are $\gamma\lambda_j$*

$$\exp(\gamma A) = \alpha_\gamma(\lambda_1, \lambda_2) I + \beta_\gamma(\lambda_1, \lambda_2) A,$$

with

$$\begin{aligned} \alpha_\gamma(\lambda_1, \lambda_2) &= \frac{\lambda_1 \exp(\gamma\lambda_2) - \lambda_2 \exp(\gamma\lambda_1)}{\lambda_1 - \lambda_2}, \\ \beta_\gamma(\lambda_1, \lambda_2) &= \frac{\exp(\gamma\lambda_1) - \exp(\gamma\lambda_2)}{\lambda_1 - \lambda_2}. \end{aligned}$$

Remark 3. *Such an approach is only possible if $\lambda_1 \neq \lambda_2$, which is not a case we have to deal with for our application.*

4.3 Strang splitting

We define a regular time step Δt and discretize the equations at times $t_n = n\Delta t$.

We will decompose the Bloch equation into a sum of two contributions

$$\partial_t \rho = M_1 \rho + M_2 \rho,$$

where M_1 and M_2 are order 4 tensors. To each tensor is associated evolution operators $\mathcal{M}_1(t)$ and $\mathcal{M}_2(t)$. The solution is approximated thanks to a combination of these two evolution operators on subintervals of length Δt. Strang splitting [13] is chosen in order to achieve second order precision. It consists in approximating $\rho(t_n) = (\mathcal{M}_1(t_n) + \mathcal{M}_2(t_n))\rho(0)$ by

$$\rho^n = \left(\mathcal{M}_1(\frac{\Delta t}{2}) \mathcal{M}_2(\Delta t) \mathcal{M}_1(\frac{\Delta t}{2}) \right)^n \rho(0).$$

This method is consistent (see [7], for details) according to Rule 6. So, if $\mathcal{M}_1$ and $\mathcal{M}_2$ preserve properties of the density matrix, then these iterations of both operators will also preserve naturally the same properties. Here the Liouville equation and the combination of transverse and longitudinal relaxations (provided some conditions on the γ_{jk} and W_{jk} are fulfilled, see [3]) both preserve the Hermicity of the density matrix, its positiveness as an operator and its trace. This will therefore also be true for the derived splitting scheme.

5 Relaxation/raw Bloch decomposition

We decompose equation (4) into a pure relaxation equation:

$$\partial_t \rho_{jk} = Q(\rho)_{jk}, \tag{8}$$

and the raw Bloch equation

$$\partial_t \rho_{jk} = -i[H, \rho]_{jk}. \tag{9}$$

5.1 Exact discretization of the raw Bloch equation

Let $V^{n+1/2}$ be the average of the interaction Hamiltonian V on the interval $[t_n, t_{n+1}]$:

$$V^{n+1/2} = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} V(\tau)\mathrm{d}\tau.$$

On this time interval an exact evolution of the Liouville equation is given by

$$\rho^{n+1} = \exp(-i\Delta t(H_0 + V^{n+1/2}))\rho^n \exp(i\Delta t(H_0 + V^{n+1/2})).$$

We can use the results of Section 4.2 to compute the matrix exponentials. Let $\lambda_{1,2}^{n+1/2}$ be the eigenvalues of the matrix $H^{n+1/2} = H_0 + V^{n+1/2}$, then

$$\exp(i\Delta t H^{n+1/2}) = \alpha^{n+1/2} I + \beta^{n+1/2} H^{n+1/2}, \tag{10}$$

where with the notations of remark 2,

$$\begin{aligned} \alpha^{n+1/2} &= \alpha_{i\Delta t}(\lambda_1^{n+1/2}, \lambda_2^{n+1/2}), \\ \beta^{n+1/2} &= \beta_{i\Delta t}(\lambda_1^{n+1/2}, \lambda_2^{n+1/2}). \end{aligned}$$

Therefore

$$(\alpha^{n+1/2} I + \beta^{n+1/2} H^{n+1/2})\rho^{n+1} = \rho^n(\alpha^{n+1/2} I + \beta^{n+1/2} H^{n+1/2}).$$

We can rewrite this in an explicit form

$$\rho^{n+1} = (\alpha^{n+1/2} I + \beta^{n+1/2} H^{n+1/2})^{-1}\rho^n(\alpha^{n+1/2} I + \beta^{n+1/2} H^{n+1/2}). \tag{11}$$

5.2 Non-standard interpretation of the raw Bloch equation

The scheme (11) can also be written

$$\alpha^{n+1/2}(\rho^{n+1} - \rho^n) = \beta^{n+1/2}(\rho^n H^{n+1/2} - H^{n+1/2}\rho^{n+1}).$$

If Δt is small enough, we can ensure that $\beta^{n+1/2}$ is nonzero and

$$i\frac{\alpha^{n+1/2}}{\beta^{n+1/2}}(\rho^{n+1} - \rho^n) = -i(H^{n+1/2}\rho^{n+1} - \rho^n H^{n+1/2}),$$

or equivalently

$$\begin{cases} (\Phi^{n+1/2}(\Delta t))^{-1}(\rho^{n+1} - \rho^n) = -i(H^{n+1/2}\rho^{n+1} - \rho^n H^{n+1/2}), \\ \Phi^{n+1/2}(\Delta t) = -i\dfrac{\beta^{n+1/2}}{\alpha^{n+1/2}} I. \end{cases} \tag{12}$$

In the right-hand side, we recognize a nonlocal discretization of the right-hand side of the Bloch equation (9) (see Rule 3). In the left-hand side, we have a nonstandard discretization of the time derivative of ρ according to Rules 1 and 2, setting

$$\phi(\Delta t) = \Phi^{n+1/2}(\Delta t) \text{ and } \varphi(\Delta t) = I.$$

We can check easily that

$$\phi(\Delta t) = \Delta t I + \mathcal{O}(\Delta t^2) \text{ when } \Delta t \to 0.$$

5.3 Exact discretization of the relaxation equation

An exact finite difference scheme for the equation (8) is straightforwardly derived from its analytic solution. We can for example first update off-diagonal entries and then diagonal entries and the solution is exactly

$$\rho(t_{n+1}) = \mathcal{M}(\Delta t) e^{\circ \Gamma \Delta t} \circ \rho(t_n)$$

where $\Gamma = (\gamma_{jk})_{jk}$ and we therefore define

$$\rho^{n+1} = \mathcal{M}(\Delta t) e^{\circ \Gamma \Delta t} \circ \rho^n \equiv \mathcal{R}(\Delta t)\rho^n. \tag{13}$$

5.4 Splitting scheme

We can now generate a splitting scheme from equations (11) and (13), and get

$$\rho^{n+1} = \mathcal{R}(\Delta t/2)(\alpha^{n+1/2} I + \beta^{n+1/2} H^{n+1/2})^{-1} \mathcal{R}(\Delta t/2)\rho^n (\alpha^{n+1/2} I + \beta^{n+1/2} H^{n+1/2}). \tag{14}$$

This scheme has a variable time step-size and preserve positiveness, because both steps (11) and (13) preserve positiveness. The trace is also conserved.

If implemented as (14) this scheme is very expensive. First there is a matrix inversion. This can be overcome either with a formula deriving from the annihilator polynomial, or with an explicit form mimicking equation (10) for $-\Delta t$. The second reason is that we have to compute (10) at each time step. This is one of the reasons why a second decomposition is proposed in the next section.

6 Relaxation–nutation/interaction decomposition

We rewrite Equation (4) in the form

$$\partial_t \rho_{jk} = -i\omega_{jk}\rho_{jk} - i[V, \rho]_{jk} + Q(\rho)_{jk},$$

where $\omega_{jk} = \omega_j - \omega_k$ is the frequency associated with the transition of the level k to level j. We decompose this equation into a relaxation–nutation evolution:

$$\partial_t \rho = L\rho, \tag{15}$$

where $(L\rho)_{jk} = -i\omega_{jk}\rho_{jk} + Q(\rho)_{jk}$ and an evolution with the interaction of electromagnetic field

$$\partial_t \rho = -i[V, \rho]. \tag{16}$$

The relaxation–nutation equation has exactly the same algebraic structure as the relaxation equation (8). We can perform the same exact resolution.

6.1 Exact discretization of the interaction equation

We can reuse the computation of the raw equation. This time we have a zero diagonal and we can give a simple formula for the eigenvalues. Indeed

$$V^{n+1/2} = \begin{pmatrix} 0 & v_{12}^{n+1/2} \\ \overline{v_{12}^{n+1/2}} & 0 \end{pmatrix}$$

and its eigenvalues are $\lambda_{1,2}^{n+1/2} = \pm|v_{12}^{n+1/2}|$. Setting $\theta^{n+1/2} = \Delta t|v_{12}^{n+1/2}|$, we have

$$\begin{aligned} \alpha^{n+1/2} &= \frac{|v_{12}^{n+1/2}|\exp\left(-i\theta^{n+1/2}\right) + |v_{12}^{n+1/2}|\exp\left(i\theta^{n+1/2}\right)}{2|v_{12}^{n+1/2}|} = \cos(\theta^{n+1/2}), \\ \beta^{n+1/2} &= \frac{\exp\left(i\theta^{n+1/2}\right) - \exp\left(-i\theta^{n+1/2}\right)}{2|v_{12}^{n+1/2}|} = \frac{i}{|v_{12}^{n+1/2}|}\sin(\theta^{n+1/2}). \end{aligned}$$

and

$$\Phi^{n+1/2}(\Delta t) = -i\frac{\beta^{n+1/2}}{\alpha^{n+1/2}}I = \frac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2})I.$$

Since $V^{n+1/2}$ is a Hermitian matrix

$$\exp\left(\pm i\Delta t V^{n+1/2}\right) = I\cos(\theta^{n+1/2}) \pm i\frac{V^{n+1/2}}{|v_{12}^{n+1/2}|}\sin(\theta^{n+1/2}). \tag{17}$$

Dividing this expression by $\cos(\theta^{n+1/2})$ (which is nonzero for sufficiently small Δt), we get

$$\rho^{n+1} = \cos^2(\theta^{n+1/2})\left(I - i\frac{V^{n+1/2}}{|v_{12}^{n+1/2}|}\tan(\theta^{n+1/2})\right)\rho^n\left(I + i\frac{V^{n+1/2}}{|v_{12}^{n+1/2}|}\tan(\theta^{n+1/2})\right). \tag{18}$$

This is an exact scheme for the evolution equation with the electromagnetic field.

6.2 NSFD schemes for the Liouville equation

Scheme 1. The scheme (18) can be cast as

$$\left(I + i\frac{V^{n+1/2}}{|v_{12}^{n+1/2}|}\tan(\theta^{n+1/2})\right)\rho^{n+1} = \rho^n\left(I + i\frac{V^{n+1/2}}{|v_{12}^{n+1/2}|}\tan(\theta^{n+1/2})\right).$$

After some algebraic manipulations, we get

$$\begin{cases} \Phi^{-1}(\theta^{n+1/2}, \Delta t)(\rho^{n+1} - \rho^n) = -i(V^{n+1/2}\rho^{n+1} - \rho^n V^{n+1/2}), \\ \Phi(\theta^{n+1/2}, \Delta t) = \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2})I, \end{cases} \tag{19}$$

where Φ is the renormalization matrix.

Remark 4. *The function Φ has the following property:*

$$\Phi(\theta^{n+1/2}, \Delta t) = \Delta t I + \mathcal{O}(\Delta t^2) \text{ when } \Delta t \to 0.$$

Scheme 2. The scheme (18) can also be written as

$$\rho^{n+1}\left(I - i\frac{V^{n+1/2}}{|v_{12}^{n+1/2}|}\tan(\theta^{n+1/2})\right) = \left(I - i\frac{V^{n+1/2}}{|v_{12}^{n+1/2}|}\tan(\theta^{n+1/2})\right)\rho^{n},$$

then

$$\begin{cases} \Phi^{-1}(\theta^{n+1/2},\Delta t)(\rho^{n+1}-\rho^{n}) = -i(V^{n+1/2}\rho^{n} - \rho^{n+1}V^{n+1/2}), \\ \Phi(\theta^{n+1/2},\Delta t) = \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2})I \end{cases} \tag{20}$$

and we notice that Φ is the same renormalization matrix as for Scheme 1.

Crank–Nicolson scheme. Combining schemes (19) and (20), we obtain the following Crank–Nicolson-type scheme:

$$\Phi^{-1}(\theta^{n+1/2},\Delta t)(\rho^{n+1}-\rho^{n}) = -i[V^{n+1/2}, \frac{\rho^{n}+\rho^{n+1}}{2}]. \tag{21}$$

This scheme is also exact (since (19) and (20) are). We can then establish the following explicit Crank–Nicolson model:

$$\begin{cases} \rho^{n+1} = M^{n+1/2}\rho^{n}N^{n+1/2}, \\ M^{n+1/2} = \left(I - \dfrac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)\left(I + \dfrac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)^{-1}, \\ N^{n+1/2} = \left(I + \dfrac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)\left(I - \dfrac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)^{-1}, \\ \Phi(\theta^{n+1/2},\Delta t) = \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2})I. \end{cases} \tag{22}$$

6.3 Splitting scheme

From the outset it should be noted that the form of the exact discrete model (18) (and therefore (22)) for equation of evolution with the electromagnetic field ensures the preservation of quantitative and qualitative properties such as the trace conservation, the Hermitian character and positivity of ρ as operator. To construct the splitting scheme, we use the Strang formula [13], because the coupling with the electromagnetic field is of order two [4]. Thus, by using the exact model (18) for the Liouville equation we propose the following scheme for the Bloch model for two-level atoms:

$$\begin{cases} \rho^{n+1} = \cos^{2}(\theta^{n+1/2})\mathcal{L}(\Delta t/2)M^{n+1/2}\mathcal{L}(\Delta t/2)\rho^{n}N^{n+1/2}, \\ M^{n+1/2} = I - i\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}, \\ N^{n+1/2} = I + i\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}, \\ \Phi(\theta^{n+1/2},\Delta t) = \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2}). \end{cases} \tag{23}$$

To demonstrate the performance of our splitting scheme compared to that presented in [3]:

$$\begin{cases} \rho^{n+1} = \mathcal{L}(\Delta t/2) M^{n+1/2} \mathcal{L}(\Delta t/2) \rho^n N^{n+1/2}, \\ M^{n+1/2} = \left(I - \dfrac{i}{2}\Delta t V^{n+1/2}\right)\left(I + \dfrac{i}{2}\Delta t V^{n+1/2}\right)^{-1}, \\ N^{n+1/2} = \left(I + \dfrac{i}{2}\Delta t V^{n+1/2}\right)\left(I - \dfrac{i}{2}\Delta t V^{n+1/2}\right)^{-1}, \end{cases} \tag{24}$$

we renormalise the step-size such that the discrete model for the Liouville equation becomes exact, which leads to the scheme:

$$\begin{cases} \rho^{n+1} = \mathcal{L}(\Delta t/2) M^{n+1/2} \mathcal{L}(\Delta t/2) \rho^n N^{n+1/2}, \\ M^{n+1/2} = \left(I - \dfrac{i}{2}\Phi(\theta^{n+1/2}, \Delta t) V^{n+1/2}\right)\left(I + \dfrac{i}{2}\Phi(\theta^{n+1/2}, \Delta t) V^{n+1/2}\right)^{-1}, \\ N^{n+1/2} = \left(I + \dfrac{i}{2}\Phi(\theta^{n+1/2}, \Delta t) V^{n+1/2}\right)\left(I - \dfrac{i}{2}\Phi(\theta^{n+1/2}, \Delta t) V^{n+1/2}\right)^{-1}, \\ \Phi(\theta^{n+1/2}, \Delta t) = \dfrac{\Delta t}{\theta^{n+1/2}} \tan(\theta^{n+1/2}). \end{cases} \tag{25}$$

Schemes (23) and (25) have a variable time step-size and preserve positiveness, because the solutions of sub-equations are positive. This property is still conserved when relaxation terms satisfy the conditions given in Section 2. The trace is also conserved.

We can already see that these two schemes are theoretically equivalent, because they use exact solutions of sub-equations. However, the scheme (23) is algorithmically less expensive because it uses only matrix products, whereas the scheme (25) needs a matrix inversion or an iterative method. Moreover, this last scheme is more complex than that presented in [3], because it implies to recalculate the discretization time step-size at each iteration.

The scheme (23) is of the same type than (14), because both use the exact expansion of the matrix exponential for the exact discretization of the Liouville equation. One of the advantages of (23) is that it simplifies the computations of parameters α and β, thus giving for the matrix exponential an expression that is easy to invert analytically, which effectively reduces the computational cost. Indeed, one can calculate once and for all the coherence moduli of the electric dipole matrix and recalculate at each step the eigenvalues of the electrical potential matrix by a simple multiplication.

7 Optical Bloch equations

We consider the exact scheme (19) for the evolution of interaction with the electromagnetic field and write explicitly the evolution of each entry of the

density matrix:

$$\left\{\begin{array}{rcl}
\dfrac{\rho_{11}^{n+1}-\rho_{11}^{n}}{\phi(\theta^{n+1/2},\Delta t)} &=& -i(v_{12}^{n+1/2}\rho_{21}^{n+1}-\rho_{12}^{n}\overline{v_{12}^{n+1/2}}),\\
\dfrac{\rho_{12}^{n+1}-\rho_{12}^{n}}{\phi(\theta^{n+1/2},\Delta t)} &=& -i(v_{12}^{n+1/2}\rho_{22}^{n+1}-\rho_{11}^{n}v_{12}^{n+1/2}),\\
\dfrac{\rho_{21}^{n+1}-\rho_{21}^{n}}{\phi(\theta^{n+1/2},\Delta t)} &=& -i(\overline{v_{12}^{n+1/2}}\rho_{11}^{n+1}-\rho_{22}^{n}\overline{v_{12}^{n+1/2}}),\\
\dfrac{\rho_{22}^{n+1}-\rho_{22}^{n}}{\phi(\theta^{n+1/2},\Delta t)} &=& -i(\overline{v_{12}^{n+1/2}}\rho_{12}^{n+1}-\rho_{21}^{n}v_{12}^{n+1/2}),\\
\phi(\theta^{n+1/2},\Delta t) &=& \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2}).
\end{array}\right. \tag{26}$$

We now want to transform the complex variables of the Bloch equation into real variables. To do so, we use the following change of variable

$$\left\{\begin{array}{rcl}
u_1^n &=& \rho_{21}^n+\rho_{12}^n,\\
u_2^n &=& i(\rho_{12}^n-\rho_{21}^n),\\
u_3^n &=& \rho_{11}^n-\rho_{22}^n.
\end{array}\right. \tag{27}$$

System (26) becomes

$$\left\{\begin{array}{rcl}
\dfrac{u_1^{n+1}-u_1^n}{\phi(\theta^{n+1/2},\Delta t)} &=& -2\,\mathrm{Im}(v_{12}^{n+1/2})\left(\dfrac{u_3^{n+1}+u_3^n}{2}\right),\\
\dfrac{u_2^{n+1}-u_2^n}{\phi(\theta^{n+1/2},\Delta t)} &=& -2\,\mathrm{Re}(v_{12}^{n+1/2})\left(\dfrac{u_3^{n+1}+u_3^n}{2}\right),\\
\dfrac{u_3^{n+1}-u_3^n}{\phi(\theta^{n+1/2},\Delta t)} &=& 2\,\mathrm{Re}(v_{12}^{n+1/2})\left(\dfrac{u_2^{n+1}+u_2^n}{2}\right)\\
&& +2\,\mathrm{Im}(v_{12}^{n+1/2})\left(\dfrac{u_1^{n+1}+u_1^n}{2}\right),\\
\phi(\theta^{n+1/2},\Delta t) &=& \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2}).
\end{array}\right. \tag{28}$$

Note that System (28) is an exact scheme for the evolution of interaction with the electromagnetic field in which the same variable changes are made, i.e.,

$$\left\{\begin{array}{rcl}
\partial_t u_1 &=& -2\,\mathrm{Im}(v_{12})u_3,\\
\partial_t u_2 &=& -2\,\mathrm{Re}(v_{12})u_3,\\
\partial_t u_3 &=& 2\,\mathrm{Re}(v_{12})u_2+2\,\mathrm{Im}(v_{12})u_1.
\end{array}\right. \tag{29}$$

Moreover, this scheme satisfies the Mickens rules and can be seen as a nonstandard Crank–Nicolson scheme. This justifies why the Crank–Nicolson scheme for the two-level model has good mathematical properties.

If we transform the scheme (20), which is also exact, then we get a system similar to (28) but in which the right-hand sides are opposite from (28). This means that if we transform the Crank–Nicolson scheme (21) (which is also exact), then we get a system in which the right-hand sides are zero. We can also notice that the discrete nonlocal models (20) and (21) cannot be used for the

raw equation. This shows that the nonlocal discretization used in (19) is the only valid nonlocal discrete representation for the Liouville equation (for any N-level model). However, the exact numerical model for the raw equation cannot be transformed into an exact scheme for the optical Bloch equations, because of nonlocal discretization. In this case, it will be interesting to first apply the nonlocal discretization to the optical Bloch equations and then to renormalize the discretization step-size. But such an approach goes beyond the scope of this paper.

8 Numerical Simulations

In this section we present numerical simulations applied to Self-Induced Transparency (SIT) for testing the reliability of theoretical results.

8.1 Self-induced transparency

SIT is a phenomenon that can be described very well with much simpler models than the nonlinear Schrödinger equation. It is also relatively simple because it involves only two levels, and allows to quantify the performance of a scheme without being polluted by positiveness problems that occur for more than two levels. This is the test case used by Ziolkowski *et al.* [17] to test the first Bloch code. For our study, this test case qualitatively and quantitatively validates the discrete models we have derived.

SIT consists to light a matter with a wave which profile corresponds to the soliton of the cubic Schrödinger equation. This wave should transmit energy to the matter which should give it back exactly. The wave thus leaves matter unchanged, while matter experiences an integer number of inversions.
Consider the propagating field given by

$$E(t,z) = \mathcal{E}(t,z)\sin(\omega_0(t - z/v)),$$

where ω_0 is the frequency of the pulse and $\mathcal{E}(t,z)$ is the envelope of the wave, which equals to

$$\mathcal{E}(t,z) = \mathcal{E}_0 \operatorname{sech}\left(\frac{t - z/v}{\tau_p}\right),$$

where $\mathcal{E}_0 = 2/m\tau_p$ is the maximum amplitude of the wave, τ_p is the pulse duration, $m = \|p\|_\infty$ with p the dipolar moment associated to the transition. At the initial moment, all the atoms are in the ground state.

8.2 Comparison

In the following, we compare various schemes for the Bloch model without relaxation, since the relaxation terms does not have a major impact on the phenomenon we are studying and would destroy the SIT phenomenon. Therefore we consider

$$\partial_t \rho = -i[H_0 + V, \rho].$$

We perform the numerical simulations for six schemes (described below): *Crank–Nicolson method*, *NSFD Euler method 1*, *RK4 method*, *NSFD Euler method 2*, *NSFD Crank–Nicolson method*, and *SFD Crank–Nicolson method*. All these schemes are consistent. They preserve the qualitative properties of Bloch equations, except the generic methods for differential equations, namely Crank–Nicolson and RK4 methods.

All these methods give qualitatively good results for small values of the time step. To measure the time step we give an equivalent of the CFL condition based on the wave frequency ω_0, such that the schemes preserving the density matrix perform well for a CFL smaller than 1.

Then we test the robustness of the methods when the time step becomes larger, through its ability to preserve the main features of the SIT phenomenon. On the various figures we plot the population of the excited level $\rho_{11}(t)$ (red) and the real part of the coherence $\rho_{12}(t)$ (blue).

8.3 Schemes without splitting

Crank–Nicolson. The first scheme to be considered for this equation is the Crank–Nicolson approach which is of order two, tested for the first time on the Bloch equation by R.W. Ziolkowski *et al.* [17]:

$$\rho^{n+1} = \rho^n - i\Delta t[H_0 + V^{n+1/2}, \frac{\rho^{n+1} + \rho^n}{2}]. \tag{30}$$

This method is resolved by a fixed point procedure.

NSFD Euler method 1. We consider in the second place the exact scheme that should be written in the form of a NSFD model:

$$\begin{cases} \rho^{n+1} = (I + i\phi^{n+1/2}(H_0 + V^{n+1/2}))^{-1}\rho^n(I + i\phi^{n+1/2}(H_0 + V^{n+1/2})), \\ \phi^{n+1/2} = -i\dfrac{\beta^{n+1/2}}{\alpha^{n+1/2}}. \end{cases} \tag{31}$$

We observe that if $\phi^{n+1/2} = \Delta t$, then we get the first order Euler approximation of the matrix exponential, so this method will be called *NSFD Euler method 1*.

RK4. To construct the fourth-order Runge–Kutta scheme (RK4), we rewrite the Bloch equation in the form:

$$\partial_t \rho = f(\rho).$$

We define regular time step Δt and discretize the equation at times $t_n = n\Delta t$. The RK4 method is written [14]:

$$\begin{cases} \rho^{n+1} = \rho^n + \dfrac{\Delta t}{6}(K_1 + 2K_2 + 2K_3 + K_3), \\ K_1 = f(t_n, \rho^n), \\ K_2 = f(t_n + \dfrac{\Delta t}{2}, \rho^n + \dfrac{\Delta t}{2}K_1), \\ K_3 = f(t_n + \dfrac{\Delta t}{2}, \rho^n + \dfrac{\Delta t}{2}K_2), \\ K_4 = f(t_n + \Delta t, \rho^n + \Delta t K_3). \end{cases} \tag{32}$$

By construction all the methods perform relatively well for a CFL less than 1 as shows Figure 1. The divergence from the correct SIT phenomenon first shows small ripples in the coherence after the interaction the the wave (already visible for the Crank–Nicolson scheme at CFL=0.5) and these small ripples become a thick queue when the time step grows. Then an effect on the final value of the population is visible, at CFL=2. for the Crank–Nicolson and RK4 schemes, and CFL=5. for the NSFD Euler method 1. For CFL=7. the Crank-Nicolson methods is even unstable and does not produce a plotable result. We can conclude that none of these methods really perform well for large values of Δt. We are able to overcome this using splitting.

8.4 Schemes with splitting

To write the other schemes, we split the Hamiltonian into two matrices, describing respectively the nutation and the interaction

$$\partial_t \rho = -i[H_0, \rho] - i[V, \rho].$$

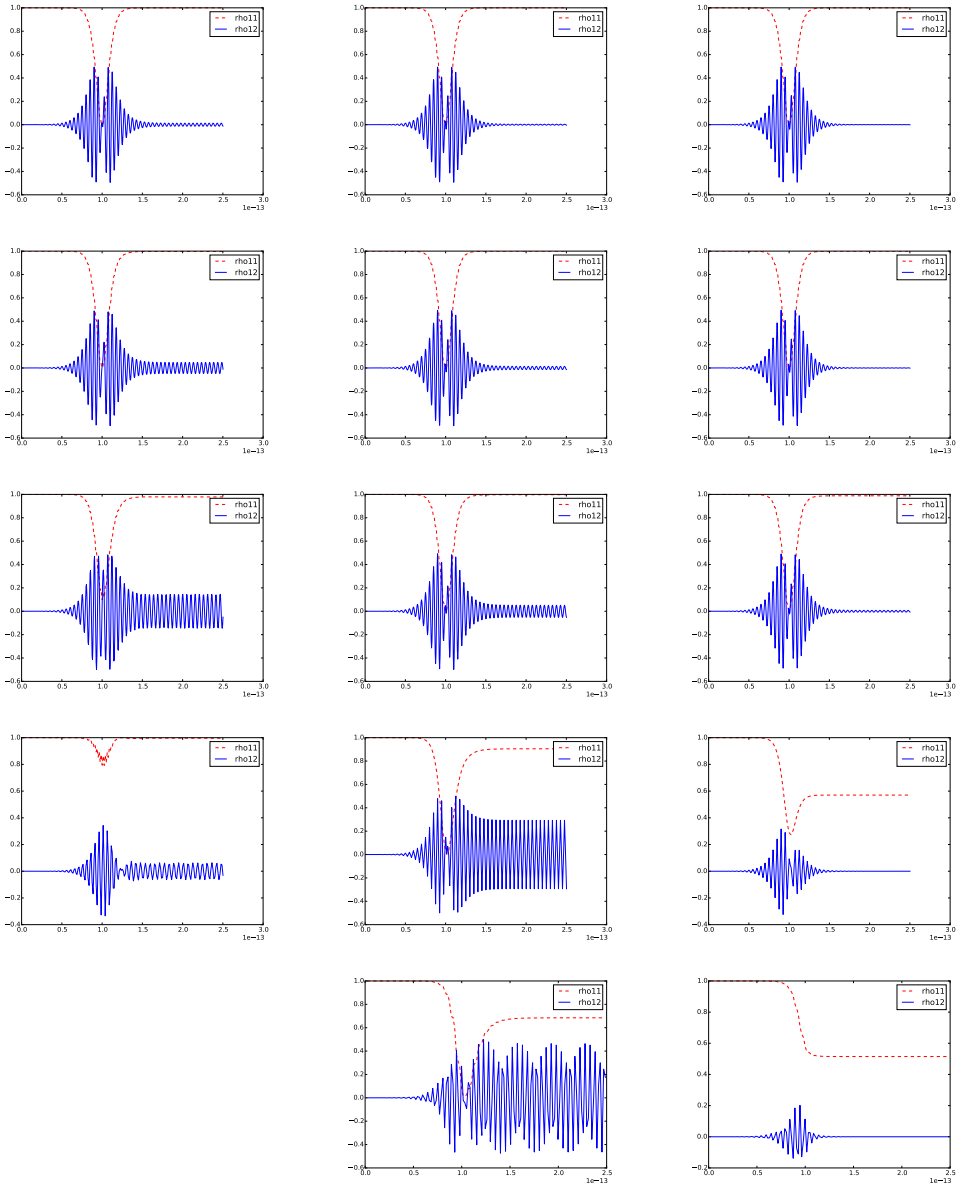
In the following, we present Strang-type schemes which only differ by the method of calculating the matrix exponential of the exact solution to the Liouville equation. We systematically end with the nutation step, which is stiffer especially when the electric field is small.

NSFD Euler method 2. For this splitting we recover the schemes defined in Section 6.3

$$\begin{aligned} \rho^{n+1} = \exp(-iH_0\frac{\Delta t}{2})\exp(-iV^{n+1/2}\Delta t)\exp(-iH_0\frac{\Delta t}{2})\rho^n \\ \exp(iH_0\frac{\Delta t}{2})\exp(iV^{n+1/2}\Delta t)\exp(iH_0\frac{\Delta t}{2}). \end{aligned} \tag{33}$$

It is more convenient to write this scheme as

$$\begin{cases} \rho^{n+1} = \cos^2(\theta^{n+1/2})\exp(-iH_0\frac{\Delta t}{2})M^{n+1/2}\exp(-iH_0\frac{\Delta t}{2})\rho^n \exp(iH_0\frac{\Delta t}{2})N^{n+1/2}\exp(iH_0\frac{\Delta t}{2}), \\ M^{n+1/2} = I - i\phi(\theta^{n+1/2}, \Delta t)V^{n+1/2}, \\ N^{n+1/2} = I + i\phi(\theta^{n+1/2}, \Delta t)V^{n+1/2}, \\ \phi(\theta^{n+1/2}, \Delta t) = \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2}). \end{cases} \tag{34}$$



Crank-Nicolson NSFD Euler method 1 RK4

Figure 1: Methods without splitting for CFL= 0.5, 1., 2., 5., and 7. (top to bottom).

Let us also observe that $\phi(\theta^{n+1/2}, \Delta t) = \Delta t$ would give the first order Euler approximation of the matrix exponential. This scheme will be called *NSFD Euler method 2*.

NSFD Crank–Nicolson method. We can use the nonstandard Crank–Nicolson approximation to evaluate the matrix exponential and write:

$$\left\{\begin{array}{l} \rho^{n+1} = \exp(-iH_0\frac{\Delta t}{2})M^{n+1/2}\exp(-iH_0\frac{\Delta t}{2})\rho^n\exp(iH_0\frac{\Delta t}{2})N^{n+1/2}\exp(iH_0\frac{\Delta t}{2}), \\ M^{n+1/2} = \left(I - \frac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)\left(I + \frac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)^{-1}, \\ N^{n+1/2} = \left(I + \frac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)\left(I - \frac{i}{2}\Phi(\theta^{n+1/2},\Delta t)V^{n+1/2}\right)^{-1}, \\ \phi(\theta^{n+1/2},\Delta t) = \dfrac{\Delta t}{\theta^{n+1/2}}\tan(\theta^{n+1/2}). \end{array}\right. \tag{35}$$

This method will be called *NSFD Crank–Nicolson method*.

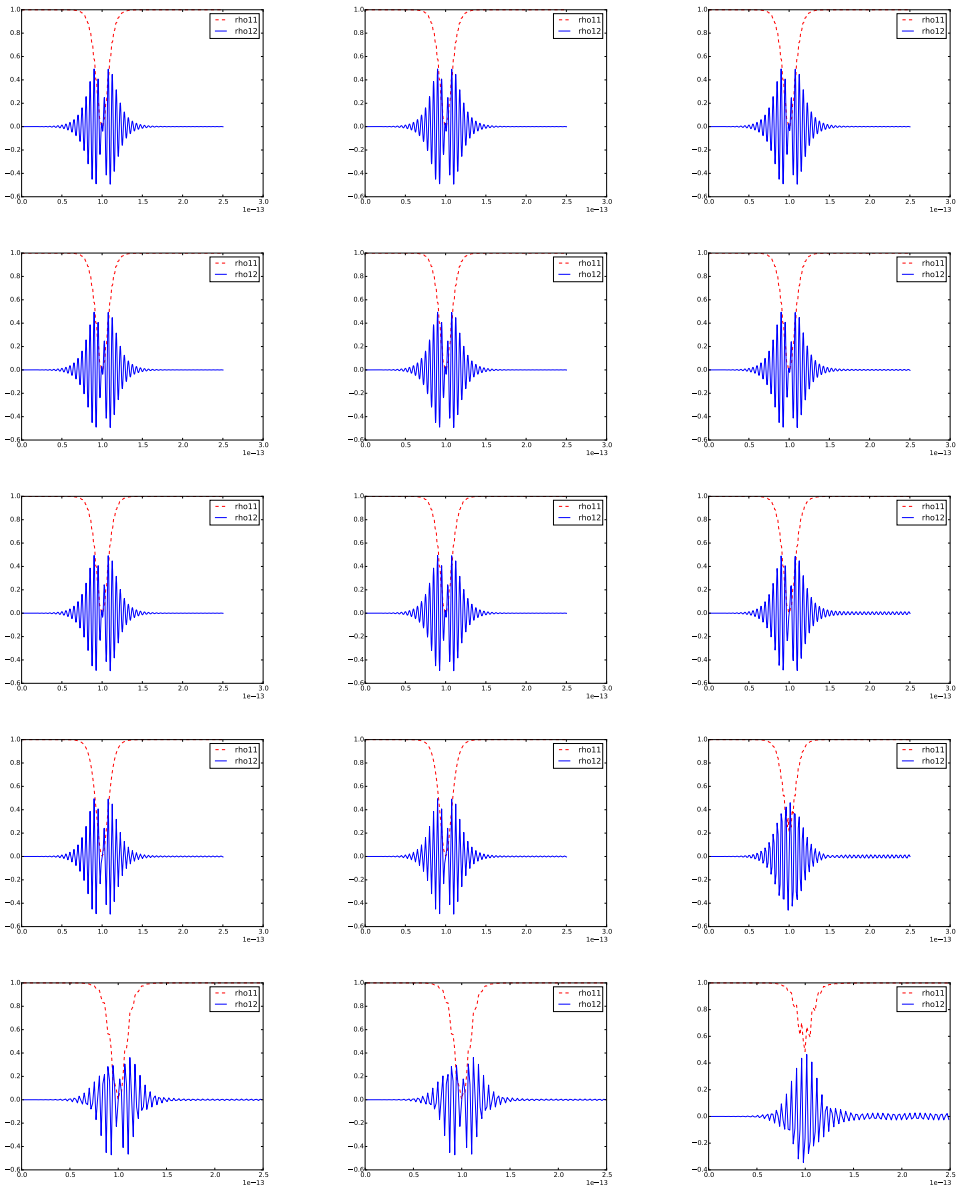
SFD Crank–Nicolson method. Replacing $\phi(\theta^{n+1/2}, \Delta t)$ by Δt in the previous scheme, we obtain the splitting scheme derived by Bidégaray *et al.* in [3] that we call *SFD Crank–Nicolson method*.

Globally the SIT phenomenon is much well preserved when splitting is applied. The NSFD methods give very good results. Even for large CFLs the population are relatively well described. We observe for CFL=7. that the population inversion is complete but slower. The standard Crank-Nicolson method yields a good final value for the population but the inversion is not complet for CFLs larger than 2. We also observe ripples in the population.

9 Conclusion

In this paper, we presented splitting schemes for the two-level Bloch model. To do this, we have proposed two ways to decompose the Bloch equation in sub-equations. First, into a pure relaxation equation and the raw Bloch equation, second into a relaxation–nutation evolution and the interaction with an electromagnetic field. Having solved exactly sub-equations in each case, we constructed splitting schemes of order two. These schemes are of variable time step sizes and satisfy the rules of nonstandard discretization of Mickens. Furthermore, they preserve the qualitative and quantitative properties of the Bloch equations (Hermicity, trace, and positiveness) and can be coupled with the Yee method [16] for the numerical study of the radiation–matter interaction.

At the end of this study, it appears that the splitting schemes are more robust for large time-steps. High accuracy methods such as RK4 which do not preserve the physical properties of the Bloch equation are a solution to achieve this robustness. The two phenomena of nutation and interaction with the wave are intimately intricate in the SIT experiment but only when the wave is significant. To associate them when the nutation term is really stiffer is a bad



NSFD Euler method 2 NSFD Crank-Nicolson SFD Crank-Nicolson

Figure 2: Methods with splitting for CFL= 0.5, 1., 2., 5., and 7. (top to bottom).

idea and this is why the splitting methods perform better. Despite its complexity compared to the SFD Crank–Nicolson method, the NSFD Crank–Nicolson method is an interesting choice from the point of view of the conservation of physical properties whatever the discretization step-size. However, this method is theoretically equivalent to NSFD Euler method 2 and produces similar numerical simulations. Thus, the simplicity of implementation of the NSFD Euler method 2 selects it as the best method from every point of view.

The gain related to the two-level Bloch model approximation by the splitting method allows to consider the numerical resolution of N-level model. It will then be essential to generalize to the matrices of order $N \geq 3$ the equivalent formulations for matrix exponentials developed for the exact numerical solution of the Liouville equation. This is the object of our future research.

References

[1] Jonathan Andreasen and Hui Cao. *Finite-difference time–domain formulation of stochastic noise in macroscopic atomic systems.* Journal of Lightwave Technology, 27(20):4530–4535, 2009.

[2] Brigitte Bidégaray. *Time discretizations for Maxwell–Bloch equations.* Numerical Methods for Partial Differential Equations, 19(3):284–300, 2003.

[3] Brigitte Bidégaray, Antoine Bourgeade, and Didier Reignier. *Introducing relaxation terms in Bloch equations.* Journal of Computational Physics, 170(2): 603–613, 2001.

[4] Brigitte Bidégaray-Fesquet. *Hiérarchie de modèles en optique quantique. De Maxwell–Bloch à Schrödinger non–linéaire.* volume 49 in Mathématiques et Applications, Springer, 2006.

[5] Karl Blum. *Density Matrix. Theory and Applications.* 3rd Edition, Springer, New York, 2012.

[6] Robert W. Boyd. *Nonlinear Optics.* 3rd Edition, Academics Press, 2008.

[7] Istvan Farago and Agnes Havasi. *Consistency Analysis of Operator Splitting Methods for C_0-Semigroups.* Semigroup Forum, 74 , pp. 125–139, 2007.

[8] Martin Frimmer and Lukas Novotny. *The classical Bloch equations.* American Journal of Physics, 82(10):947–954, 2014.

[9] Rodney Loudon. *The Quantum Theory of Light.* 3rd Edition, Oxford University Press, New York, 2000.

[10] Ronald E. Mickens. *Nonstandard finite difference models of differential equations.* World scientific, 1994.

[11] Ronald E. Mickens. *Nonstandard finite difference schemes.* In R. E. Mickens (ed), Applications of Nonstandard Finite Difference Schemes, World scientific, pp. 1–54, 2000.

[12] Ronald E. Mickens. *Nonstandard finite difference Methods.* In R. E. Mickens (ed), Advanced in the applications of Nonstandard Finite Difference Schemes, World scientific, pp. 1–9, 2005.

[13] Gilbert Strang. *On the construction and comparison of difference schemes.* SIAM Journal on Numerical Analysis, 5(3):506–517, 1968.

[14] Clarisse Uwizeye. *Asymptotic preserving scheme for Bloch equations.* Master Thesis, Université Joseph Fourier, June 2015.

[15] John Weiner and P.-T. Ho. *Light–Matter interaction. Fundamentals and Applications.* Wiley-Interscience, 2003.

[16] Kane S. Yee. *Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media.* IEEE Transactions on Antennas and Propagation, 14(3):302–307, 1966.

[17] Richard W. Ziolkowski, John M. Arnold, and Daniel M. Gogny. *Ultrafast pulse interaction with two-level atoms.* Physical Review A, 53(4): 3082–3094, 1995.

[18] Richard W. Ziolkowski. *Realization of an all-optical triode and diode with a two-level atom loaded diffraction grating.* Applied Optics, 36(33):8547–8556, 1997.

[19] Richard W. Ziolkowski. *The incorporation of microscopic material models into the FDTD approach for ultrafast optical pulse simulations.* IEEE Transactions on Antennas and Propagation, 45(3):375–391, 1997.