Chapter 4

ODE-PDE modeling and numerical analysis in quantum optics

When the Hamiltonian of the system is time-varying, it can be difficult or even impossible to formally or practically find solution to the evolution equation of the system state. We therefore turn to numerical solutions.

We are here interested in systems which are exited by or in interaction with an electromagnetic field, which is time dependent.

The properties of quantum channels that preserve properties of the states is something we also want to achieve at the numerical level.

4.1 Numerical resolution of the von Neumann equation

4.1.1 Modelling

We consider $\mathcal{H} = \mathbb{C}^d$, and a state $\rho \in \mathrm{DM}(\mathcal{H})$ which is governed by the von Neumann equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [H(t), \rho(t)],$$

where $H(t)$ is a sum of a constant Hamiltonian, H_0, that we can consider to be a diagonal matrix (up to a convenient choice of the basis) and a time-varying Hamiltonian $V(t)$. From the physics point of view, and regardless of the dimensions that are omitted here, the diagonal entries of H_0 are the discrete energy levels of the system and the potential V is the scalar product of the polarizability $\mathbf{p}$, a $d \times d$ matrix (with entries in $\mathbb{C}^3$) that depend on the symmetries of the states, and $\mathbf{E}(t) \in \mathbb{R}^3$ is the electromagnetic field: $V(t) = \mathbf{p} \cdot \mathbf{E}(t)$. Here, we first consider that the electromagnetic field $\mathbf{E}(t)$ is given.

There is also a certain number of physical phenomena that are hard to describe precisely and they are simply gathered in a phenomenological term, called relaxation term. Hence we study

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i[H(t), \rho(t)] + Q(\rho(t)).$$

4.1.2 Preservation of the density matrix property at the continuous level

Even with a time-varying Hamiltonian $H(t)$, the density matrix property is preserved through the time evolution for the relaxation-free equation. Indeed $H(t)$ is still Hermitian ($\mathbf{p}$ is Hermitian with a vanishing diagonal).

Let us now consider also relaxation terms

$$
\begin{aligned}
(\frac{\mathrm{d}}{\mathrm{d}t}\rho(t))^* &= (-i[H(t),\rho(t)] + Q(\rho(t)))^* = i(H(t)\rho(t) - \rho(t)H(t))^* + Q(\rho(t))^*,\\
\frac{\mathrm{d}}{\mathrm{d}t}\rho^*(t) &= -i[H^*(t),\rho^*(t)] + Q(\rho(t))^*,\\
\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) &= -i[H(t),\rho(t)] + Q(\rho(t))^*.
\end{aligned}
$$

In the sequel we will have to distinguish diagonal terms in the density matrix, also called *populations*, and the off-diagonal terms, called *coherences*.

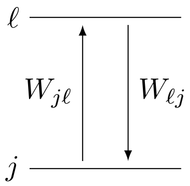
To preserve Hermicity, we should have $Q(\rho(t))^* = Q(\rho(t))$ and the off-diagonal terms have to check $Q(\rho(t))_{kj} = \overline{Q(\rho(t))_{jk}}$. This is ensured by simply setting $Q(\rho)_{jk} = -\gamma_{jk}\rho_{jk}$ with $\gamma_{jk} = \gamma_{kj} \in \mathbb{R}$.

We also want to preserve positiveness and the trace. To preserve trace

$$
Q(\rho)_{jj} = \sum_{\ell \neq j} W_{\ell j}\rho_{\ell\ell} - \sum_{\ell \neq j} W_{j\ell}\rho_{jj} = \sum_{\ell \neq j} W_{\ell j}\rho_{\ell\ell} - \Gamma_j \rho_{jj},
$$

where $\Gamma_j = \sum_{\ell \neq j} W_{j\ell}$. By convention $W_{jj} = 0$ for all $j = 1,\dots,d$. Clearly $\sum\limits_{j=1}^{d} Q(\rho)_{jj} = 0$ and this preserves the trace.

This form describes transitions according to the following diagram



which means that $W_{j\ell}$ is a $W_{j\to\ell}$, and justifies the (unusual) order of the subscripts.

We also have a relation between the coefficients:

$$
W_{j\ell} = W_{\ell j} e^{\beta(\varepsilon_j - \varepsilon_\ell)},
$$

which ensures that the system $\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = Q(\rho(t))$ ultimately (in absence of forcing, i.e. $V(t) = 0$) tends to an equilibrium state, which is a Gibbs state. Indeed, if we only consider the equations involving relaxation (master equation)

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\rho_{jj} &= \sum_{\ell \neq j} W_{j\ell} e^{-\beta(\varepsilon_j - \varepsilon_\ell)}\rho_{\ell\ell} - \sum_{\ell \neq j} W_{j\ell}\rho_{jj},\\
\frac{\mathrm{d}}{\mathrm{d}t} e^{\beta\varepsilon_j}\rho_{jj} &= \sum_{\ell \neq j} W_{j\ell} e^{\beta\varepsilon_\ell}\rho_{\ell\ell} - \sum_{\ell \neq j} W_{j\ell} e^{\beta\varepsilon_j}\rho_{jj} = \sum_{\ell \neq j} W_{j\ell}\left(e^{\beta\varepsilon_\ell}\rho_{\ell\ell} - e^{\beta\varepsilon_j}\rho_{jj}\right)
\end{aligned}
$$

In the limit we want $\frac{\mathrm{d}}{\mathrm{d}t} e^{\beta\varepsilon_j}\rho_{jj}(t) \to 0$ and all the limits of $e^{\beta\varepsilon_\ell}\rho_{\ell\ell}(t)$ are equal. Since the trace is conserved

$$
\lim_{t\to+\infty} \rho_{jj}(t) = \frac{e^{-\beta\varepsilon_j}}{\sum_{i=1}^{d} e^{-\beta\varepsilon_j}}.
$$

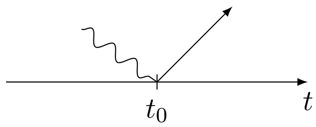
Conditions for positiveness A necessary and sufficient condition for populations to remain non-negative is simply that $W_{j\ell} \geq 0$ for all j and ℓ.

Proof. Necessary condition: suppose the initial condition is $\rho_{jk} = 0$ except for $j = k = j_0$ (for which $\rho_{j_0 j_0} = 1$). Then for $j \neq j_0$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{jj}\Big|_{t=0} = W_{j_0 j}\rho_{j_0 j_0} = W_{j_0 j}.$$

And since $\rho_{jj}(0) = 0$, this derivative has to be non-negative.
Sufficient condition: Let us suppose there exists t_0 and k_0 such that $\rho_{k_0 k_0}(t_0) = 0$. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{k_0 k_0}\Big|_{t=t_0} = \sum_{j \neq k_0} W_{j k_0}\rho_{jj}(t_0).$$



Either $t_0 = 0$ and this will persist until some time t_1 where for a j (for which $W_{jk_0} > 0$) $\rho_{jj}(t_1) > 0$ and then just after t_1, $\rho_{k_0 k_0}(t) > 0$.
Either $t_0 > 0$, and by the trace property there exist j_0 such that $\rho_{j_0 j_0}(t_0) > 0$. Suppose $W_{j_0 k_0} > 0$, then $\frac{\mathrm{d}}{\mathrm{d}t}\rho_{k_0 k_0}(t_0) > 0$, and $\frac{\mathrm{d}}{\mathrm{d}t}\rho_{k_0 k_0}$ cannot be continuous at time $t = t_0$ (and it should be by the Cauchy-Lipschitz theorem). This simply implies that $\rho_{k_0 k_0}(t_0)$ is impossible, and $\rho_{k_0 k_0}$ remains positive .
If $W_{j_0 k_0} = 0$, by continuity of the solutions of the equations with respect to the parameters, $\rho_{k_0 k_0}$ remains non-negative. □

A sub-property of positiveness is that $|\rho_{jk}(t)|^2 \leq \rho_{jj}(t)\rho_{kk}(t)$ (the sub-matrix corresponding to j and k indices has a positive determinant). A necessary and sufficient condition to ensure this is that $2\gamma_{jk} \geq \Gamma_j + \Gamma_k - \sqrt{W_{jk}W_{kj}}$.

Proof. Hint: study the derivative of $f(t) = \rho_{jj}(t)\rho_{kk}(t) - \rho_{jk}(t)\rho_{kj}(t)$. □

Let us suppose that the transverse relaxations read as

$$\gamma_{jk} = \frac{1}{2}(\Gamma_j + \Gamma_k) + \gamma_j + \gamma_k - A_j \cdot A_k$$

where $\gamma_j \in \mathbb{R}$ and $A_j \in \mathbb{R}^d$ (which does not allow to express the previous $\sqrt{W_{jk}W_{kj}}$) then a sufficient condition for ρ to be nonnegative is $\gamma_j \geq \frac{1}{2}\|A_j\|^2$.

Proof. Hint: study the derivative of $g(t) = X^*\rho(t)X$ for $X \in \mathbb{C}^d$. □

From Lindblad to relaxations What we want to be a relaxation term would stem from the $V_\alpha \rho V_\alpha^* - \frac{1}{2}\{V_\alpha^* V_\alpha, \rho\}$ term. Let us compute this for $V_\alpha = \alpha_{jk}|e_j\rangle\langle e_k|$.

$$\begin{aligned}
V_\alpha \rho V_\alpha^* &= \alpha_{jk}|e_j\rangle\langle e_k|\rho|e_k\rangle\langle e_j|\overline{\alpha_{jk}} = |\alpha_{jk}|^2\rho_{kk}|e_j\rangle\langle e_j|,\\
V_\alpha^* V_\alpha &= |e_k\rangle\langle e_j|\overline{\alpha_{jk}}\alpha_{jk}|e_j\rangle\langle e_k| = |\alpha_{jk}|^2|e_k\rangle\langle e_j \mid e_j\rangle\langle e_k| = |\alpha_{jk}|^2|e_k\rangle\langle e_k|,\\
V_\alpha^* V_\alpha \rho &= |\alpha_{jk}|^2|e_k\rangle\langle e_k|\rho = |\alpha_{jk}|^2|e_k\rangle\langle e_k|\sum_{\ell,m=1}^{d}\rho_{\ell m}|e_\ell\rangle\langle e_m| = |\alpha_{jk}|^2\sum_{\ell,m=1}^{d}\rho_{\ell m}|e_k\rangle\langle e_k \mid e_\ell\rangle\langle e_m|\\
&= |\alpha_{jk}|^2\sum_{\ell,m=1}^{d}\rho_{\ell m}|e_k\rangle\delta_{k\ell}\langle e_m| = |\alpha_{jk}|^2\sum_{\ell,m=1}^{d}\rho_{\ell m}\delta_{k\ell}|e_k\rangle\langle e_m| = |\alpha_{jk}|^2\sum_{m=1}^{d}\rho_{km}|e_k\rangle\langle e_m|,\\
\rho V_\alpha^* V_\alpha &= \rho|\alpha_{jk}|^2|e_k\rangle\langle e_k| = |\alpha_{jk}|^2\sum_{\ell,m=1}^{d}\rho_{\ell m}|e_\ell\rangle\langle e_m|\ |e_k\rangle\langle e_k| = |\alpha_{jk}|^2\sum_{\ell,m=1}^{d}\rho_{\ell m}|e_\ell\rangle\langle e_m \mid e_k\rangle\langle e_k|\\
&= |\alpha_{jk}|^2\sum_{\ell,m=1}^{d}\rho_{\ell m}|e_\ell\rangle\delta_{mk}\langle e_m| = |\alpha_{jk}|^2\sum_{\ell,m=1}^{d}\rho_{\ell m}\delta_{mk}|e_\ell\rangle\langle e_m| = |\alpha_{jk}|^2\sum_{\ell=1}^{d}\rho_{\ell k}|e_\ell\rangle\langle e_k|.
\end{aligned}$$

For a generic V_α, we have to sum up these contributions over j and k but we want to sum up only d^2-1 contributions. To to this in an elegant way, we can simply sum for all $j,k=1,\dots,d$ but suppose that one of the α_{jj} is zero, e.g. $\alpha_{11}=0$. For diagonal terms, we have

$$\begin{aligned}\sum_\alpha\left(V_\alpha\rho V_\alpha^*-\frac{1}{2}\{V_\alpha^*V_\alpha,\rho\}\right)_{nn}&=\sum_{k=1}^d|\alpha_{nk}|^2\rho_{kk}-\frac{1}{2}\sum_{j=1}^d|\alpha_{jn}|^2\rho_{nn}-\frac{1}{2}\sum_{j=1}^d|\alpha_{jn}|^2\rho_{nn}\\&=\sum_{j=1}^d\left(|\alpha_{nj}|^2\rho_{jj}-|\alpha_{jn}|^2\rho_{nn}\right)=\sum_{j\neq n}\left(|\alpha_{nj}|^2\rho_{jj}-|\alpha_{jn}|^2\rho_{nn}\right).\end{aligned}$$

where we selected the coefficients of $|e_n\rangle\langle e_n|$ in the previous contributions. Similarly, for the off-diagonal terms

$$\sum_\alpha\left(V_\alpha\rho V_\alpha^*-\frac{1}{2}\{V_\alpha^*V_\alpha,\rho\}\right)_{nm}=-\frac{1}{2}\sum_{j=1}^d|\alpha_{jn}|^2\rho_{nm}-\frac{1}{2}\sum_{j=1}^d|\alpha_{jm}|^2\rho_{nm}=-\frac{1}{2}\sum_{j=1}^d\left(|\alpha_{jn}|^2+|\alpha_{jm}|^2\right)\rho_{nm}.$$

We recover a model where populations are governed by a master equation with $W_{nj}=|\alpha_{jn}|^2$ for $n\neq j$ (we do have $\Gamma_n=\sum_{j\neq n}W_{nj}$) and $\gamma_{nm}=\frac{1}{2}(\Gamma_n+\Gamma_m)+\gamma_n+\gamma_m$ with $\gamma_n=|\alpha_{nn}|^2$.

4.1.3 "Classical" methods do not preserve positiveness

The equation governing ρ is a classical ordinary differential equation (ODE) that also reads $\rho'(t)=f(t,\rho(t))$. One could *a priori* use any classical method to solve this ODE.

In the sequel we will consider a uniform discretization of time and consider discrete times $t_p=p\delta t$, where δt is the time step. A time varying matrix $A(t)$ will be approximated at time t_p by A^p. Half times will also be considered and $A^{p+1/2}$ will be an approximation of $A(t_{p+1/2})$ where $t_{p+1/2}=(t_p+t_{p+1})/2$.

The problems with classical methods do not stem from the relaxation operator, so we omit it here.

First attempt: Euler scheme The (forward) Euler scheme simply reads

$$\frac{\rho^{p+1}-\rho^p}{\delta t}=-i[H^p,\rho^p].$$

This preserves Hermicity:

$$\begin{aligned}(\rho^{p+1})^*&=(\rho^p-i\delta t(H^p\rho^p-\rho^pH^p))^*=(\rho^p)^*+i\delta t((\rho^p)^*(H^p)^*-(H^p)^*(\rho^p)^*)\\&=\rho^p-i\delta t(H^p\rho^p-\rho^pH^p)=\rho^{p+1}.\end{aligned}$$

Trace is also preserved, since $\mathrm{tr}([H^p,\rho^p])=0$.
If we write this in a basis where H^p is diagonal, and denote its eigenvalues by λ_j^p, this reads

$$\frac{\tilde\rho_{jk}^{p+1}-\tilde\rho_{jk}^p}{\delta t}=-i(\lambda_j^p\tilde\rho_{jk}^p-\tilde\rho_{jk}^p\lambda_k^p),$$

and therefore

$$\tilde\rho_{jk}^{p+1}=\left(1-i\delta t(\lambda_j^p-\lambda_k^p)\right)\tilde\rho_{jk}^p.$$

Let us consider the two-level case and suppose that $\tilde\rho_{jk}^p=a_j\overline{a_k}$ (a pure state), then

$$\begin{aligned}\det\tilde\rho^{p+1}&=\tilde\rho_{11}^{p+1}\tilde\rho_{22}^{p+1}-|\tilde\rho_{12}^{p+1}|^2=\tilde\rho_{11}^p\tilde\rho_{22}^p-|1-i\delta t(\lambda_1^p-\lambda_2^p)|^2|\tilde\rho_{12}^p|^2\\&=\left(1-|1-i\delta t(\lambda_1^p-\lambda_2^p)|^2\right)|a_1|^2|a_2|^2=-\delta t^2(\lambda_1^p-\lambda_2^p)^2|a_1|^2|a_2|^2<0.\end{aligned}$$

Hence matrix ρ^{p+1} is not positive, and the (forward) Euler scheme does no.

Backward Euler scheme The backward Euler scheme now reads

$$\frac{\rho^{p+1} - \rho^p}{\delta t} = -i[H^{p+1}, \rho^{p+1}].$$

Once more, in a basis where H^{p+1} is diagonal,

$$\tilde{\rho}_{jk}^{p+1} = \frac{1}{1 + i\delta t(\lambda_j^{p+1} - \lambda_k^{p+1})}\tilde{\rho}_{jk}^{p}.$$

The preservation of Hermicity can be seen on this form, hence the eigenvalues of $\tilde{\rho}^{p+1}$ are real. In the two level case, let us first suppose that $\tilde{\rho}^p$ is a pure state. Then (following the same lines as before)

$$\det \tilde{\rho}^{p+1} = \frac{\delta t^2(\lambda_1^{p+1} - \lambda_2^{p+1})^2}{1 + \delta t^2(\lambda_1^{p+1} - \lambda_2^{p+1})^2}|a_1|^2|a_2|^2 > 0.$$

The trace and the determinant of $\tilde{\rho}^{p+1}$ are both non negative, the eigenvalues are non negative and $\tilde{\rho}^{p+1} \geq 0$.
In fact, since $\tilde{\rho}^p$ is a density matrix, it can be expressed as a mixture of states. By linearity each pure component of the mixture is transformed by the Euler scheme in a non negative matrix, and the sum is non negative.

$$\tilde{\rho}^p = \sum_{j=1}^N p_j \tilde{\rho}_j^p \longrightarrow \sum_{j=1}^N p_j \underbrace{\tilde{\rho}_j^{p+1}}_{\geq 0} = \tilde{\rho}^{p+1} \geq 0.$$

This does not say anything for a larger number of levels. However, we will see in the practical session that this scheme has flaws...

Second attempt: Crank-Nicolson scheme Historically, because it is second order, and was coupled to second order schemes for Maxwell equations, the Bloch equations have been discretized by the Crank-Nicolson scheme.

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

Once more we can write this in a basis where $H^{p+1/2}$ is diagonal and

$$\tilde{\rho}_{jk}^{p+1} = \frac{1 - \frac{i\delta t}{2}(\lambda_j^{p+1/2} - \lambda_k^{p+1/2})}{1 + \frac{i\delta t}{2}(\lambda_j^{p+1/2} - \lambda_k^{p+1/2})}\tilde{\rho}_{jk}^{p}.$$

It clearly still preserves Hermicity and trace. For the previous two-level case, it gives $\det \tilde{\rho}^{p+1} = 0$ (thus it preserves Hermicity and positiveness). This time you have to consider a three-level case to obtain a counter-example to positiveness.

What structure is not preserved? The solution to $i\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [H(t), \rho(t)]$ is

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

Exponentials can be hard and costly to compute. A scheme that would preserve this structure is a scheme where the exponentials are discretized in a coherent way. For example

$$\rho^{p+1} = \left(\mathbb{1} - \frac{1}{2}i\delta t H^p\right)\left(\mathbb{1} + \frac{1}{2}i\delta t H^p\right)^{-1}\rho^p\left(\mathbb{1} + \frac{1}{2}i\delta t H^p\right)\left(\mathbb{1} - \frac{1}{2}i\delta t H^p\right)^{-1}.$$

This works, but now you have inverses of matrices to compute.

4.1.4 Splitting methods

General principle The principle of splitting methods is to split the operator of the time evolution in pieces that you solve separately. There are many reasons to this

- simplify each step of the solution. This is the case for direction splitting often used to split the computation of a Laplacian in the successive computation in each direction;
- use different methods for each part of the equation. For example you may want to solve differential operators in the frequency domain and nonlinear operators in the time domain;
- here, preserve exactly the physical properties for each part of the equation, while it is difficult to do on the whole equation.

Let us consider an equation reads $\frac{\mathrm{d}}{\mathrm{d}t}x(t) = Ax(t) + Bx(t)$, and we denote $S_A(t)$ the *evolution semi-group*[1] for equation $\frac{\mathrm{d}}{\mathrm{d}t}y(t) = Ay(t)$ and $S_B(t)$ the evolution semi-group for equation $\frac{\mathrm{d}}{\mathrm{d}t}z(t) = Bz(t)$, i.e. $y(t) = S_A(t)y(0)$ and $z(t) = S_B(t)z(0)$.

Lie splitting consists in writing

$$x^{p+1} = S_B(\delta t)S_A(\delta t)x^p.$$

Strang splitting consists in writing

$$x^{p+1} = S_A(\delta t/2)S_B(\delta t)S_A(\delta t/2)x^p.$$

Provided there are no stiffness issues, Lie splitting is a first order scheme and Strang splitting is a second order scheme. This splitting error adds to the possible errors for the separate numerical solution of $S_A(\delta t)$ and $S_B(\delta t)$. Higher order methods are possible if one of the operator is also well defined for negative times. (This is a complex matter quite out of the scope of this course).

Case of the Bloch equation For this we anew consider relaxation terms. We have to solve $\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i[H(t), \rho(t)] + Q(\rho(t))$ where $H(t) = H_0 + V(t)$. Each of the three parts of the equation can be solved easily preserving positiveness properties. It is also convenient to solve only two parts taking H_0 into account either with the relaxation Q or with the potential $V(t)$.

The Hamiltonian part should be solved as already seen with a suitable discretization of the exponentials in

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

The relaxation part can be solved exactly. Off-diagonal terms read $\frac{\mathrm{d}}{\mathrm{d}t}\rho_{jk}(t) = -\gamma_{jk}\rho_{jk}(t)$ if relaxation alone is considered and $\frac{\mathrm{d}}{\mathrm{d}t}\rho_{jk}(t) = -(\gamma_{jk} + i(\varepsilon_j - \varepsilon_k))\rho_{jk}(t)$ if H_0 is also considered. In any case the exact solution is $\rho_{jk}^{p+1} = \exp(-\gamma_{jk}\delta t)\rho_{jk}^p$ or $\rho_{jk}^{p+1} = \exp(-(\gamma_{jk} + i(\varepsilon_j - \varepsilon_k))\delta t)\rho_{jk}^p$.
For the diagonal part, we can gather all the populations in one single vector $N(t)$ (which is the diagonal of the density matrix). Then setting

$$\tilde{W} = \begin{pmatrix} -\sum_{j=1}^d W_{1j} & W_{21} & \dots & W_{d1} \\ W_{12} & -\sum_{j=1}^d W_{2j} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ W_{1d} & \dots & \dots & -\sum_{j=1}^d W_{dj} \end{pmatrix},$$

[1] An evolution semi-group is a time-dependent family of operators $S(t)$ defined for $t \geq 0$ such that $S(0) = \mathbb{1}$; for all $t, s \geq 0$, $S(t+s) = S(t)S(s)$ (composition of operators); $\lim_{t\to 0^+} S(t) = \mathbb{1}$. We define the infinitesimal generator $(A, D(A))$ of this semi-group by

$$D(A) = \left\{x \in \mathcal{H},\ \lim_{t\to 0^+}\frac{S(t)x - x}{t} \text{ exists}\right\} \text{ and } \forall x \in D(A),\ Ax = \lim_{t\to 0^+}\frac{S(t)x - x}{t}.$$

the solution to the master equation is $N(t) = e^{t\tilde{W}}N(0)$. On a time step, you always use $e^{\delta t\tilde{W}}$, which can be hard to compute, but that you only have to compute once.

4.2 Interaction with an external classical electromagnetic field

4.2.1 Maxwell equations

An electromagnetic phenomenon can be described by four vector-valued functions depending on the space $\mathbf{x}$ and the time t: the electric field $\mathbf{E}(\mathbf{x},t)$, the magnetic field $\mathbf{B}(\mathbf{x},t)$, the displacement field $\mathbf{D}(\mathbf{x},t)$ and the magnetizing field $\mathbf{H}(\mathbf{x},t)$.

Under some assumptions, these quantities are linked by constitutive relations that describe the material in which the electromagnetic field evolves. We restrict the presentation to perfect media (local relation in time and space) with a linear and isotropic (independent of the direction) law without additional magnetization. It gives the constitutive relations

$$\mathbf{D}(\mathbf{x},t) = \varepsilon(\mathbf{x})\mathbf{E}(\mathbf{x},t), \qquad \mathbf{H}(\mathbf{x},t) = \frac{1}{\mu(\mathbf{x})}\mathbf{B}(\mathbf{x},t),$$

where ε is the permittivity of the material (that measures the response of the material to an applied electric field) and μ its permeability (that measures its response to an applied magnetic field). For homogeneous materials, ε and μ are constant throughout the material. Generally, materials are dispersive and ε and μ depend on the frequency of the incident electromagnetic wave. The permittivity and the permeability are often represented by a relative permittivity ε_r and a relative permeability μ_r (dimensionless quantities) via the expressions $\varepsilon = \varepsilon_r\varepsilon_0$ and $\mu = \mu_r\mu_0$ where ε_0 is the vacuum permittivity and μ_0 the vacuum permeability, both being linked to the speed of light c by the relation $c^2\varepsilon_0\mu_0 = 1$. In the same way, the permittivity ε and the permeability μ of the material determine the velocity v of the electromagnetic waves through the medium via the relation $v^2\varepsilon\mu = 0$.

Finally, we can also consider a perturbation in the electrical constitutive law

$$\mathbf{D}(\mathbf{x},t) = \varepsilon(\mathbf{x})\mathbf{E}(\mathbf{x},t) + \mathbf{P}(\mathbf{x},t)$$

by introducing a polarization $\mathbf{P}$. For instance, it can describe the electric dipole moments (measures of the separation of positive and negative electrical charges) in a dielectric material, an electrical insulator that can be polarized by an applied electric field due to the displacement (in a microscopic volume) of bound charges. These charges are called bound charges because they are associated to an atom or a molecule (by opposition to free charges that move within the material). In that case, the polarization $\mathbf{P}$ is linked to the bound charge density ρ_{bound} by the relation $-\operatorname{div}\mathbf{P} = \rho_{\text{bound}}$ and it creates a polarization current $\mathbf{J}_P = \partial_t\mathbf{P}$. For us, as we will see later, the dipole approximation will be used to express the influence of quantum objects on the electromagnetic field.

In a material with an electric (free) charge density $\rho(\mathbf{x},t)$ and an electric (free) current density $\mathbf{J}(\mathbf{x},t)$, Maxwell's equations are the following set of partial differential equations:

Gauss's equation that says the divergence of the electric field is proportional to the electric charge distribution

$$\operatorname{div}(\varepsilon\mathbf{E}) = \rho + \rho_{\text{bound}},$$

Gauss's equation for magnetism that states there are no magnetic monopoles (only magnetic dipoles) and thus the magnetic flux through a surface is zero

$$\operatorname{div}(\mathbf{B}) = 0,$$

Faraday's equation that says a time variation of a magnetic field induces an electric field

$$\operatorname{curl}(\mathbf{E}) = -\partial_t \mathbf{B},$$

Ampère's equation that says a magnetic field can be generated either by a time variation of an electric field or an electrical current

$$\operatorname{curl}\Big(\frac{1}{\mu}\mathbf{B}\Big) = \varepsilon \partial_t \mathbf{E} + \big(\mathbf{J} + \mathbf{J}_P\big).$$

Charge conservation A (macroscopic) charge conservation can be derived from Maxwell's equation. Indeed, the left-hand side of the Ampère's equation has a zero divergence by the div–curl identity. Interchanging the divergence and the time derivative, it gives

$$0 = \partial_t \operatorname{div}(\varepsilon \mathbf{E}) + \operatorname{div}\big(\mathbf{J} + \mathbf{J}_P\big) = \partial_t \operatorname{div}(\varepsilon \mathbf{E} + P) + \operatorname{div} \mathbf{J}.$$

Finally, applying the Gauss's equation, we obtain the charge conservation equation

$$\partial_t \rho + \operatorname{div} \mathbf{J} = 0.$$

4.2.2 Propagation equations

In the sequel, we consider dimensionless Maxwell's equations in a homogeneous material without source terms. It reads

$$\left|\begin{array}{l} \operatorname{div}(\mathbf{B}) = 0, \\ \operatorname{div}(\mathbf{E}) = 0, \end{array}\right. \qquad \left|\begin{array}{l} \operatorname{curl}(\mathbf{E}) = -\partial_t \mathbf{B}, \\ \operatorname{curl}(\mathbf{B}) = \dfrac{1}{v^2}\partial_t \mathbf{E}. \end{array}\right.$$

These simplified equations allow to better understand why Maxwell's equations describe wave propagation phenomena.

Wave equations

From Faraday's equation, we immediately have

$$\operatorname{curl}(\operatorname{curl}(\mathbf{E})) = -\partial_t(\operatorname{curl}(\mathbf{B})) = -\frac{1}{v^2}\partial_t^2 \mathbf{E}.$$

Since $\operatorname{curl}\operatorname{curl} = \nabla \operatorname{div} - \Delta$ and $\operatorname{div}(\mathbf{E}) = 0$, we obtain

$$\partial_t^2 \mathbf{E} - v^2 \Delta \mathbf{E} = 0.$$

Thus, the electric field is governed by a wave equation. By symmetry, we also obtain that the magnetic field is governed by the wave equation

$$\partial_t^2 \mathbf{B} - v^2 \Delta \mathbf{B} = 0.$$

Consequently, the electromagnetic field has properties specific to the solution of a hyperbolic partial differential equation (finite propagation speed, propagation of singularities, energy conservation. . .).

For instance, if we multiply (dot product) the wave equation by $\partial_t \mathbf{E}$ and integrate in space (assuming that the behavior of the solution at infinity is such that all integrals are well defined), we have

$$\int_{\mathbb{R}^3} \partial_t^2 \mathbf{E} \cdot \partial_t \mathbf{E} \, \mathrm{d}\mathbf{x} - v^2 \int_{\mathbb{R}^3} \Delta \mathbf{E} \cdot \partial_t \mathbf{E} \, \mathrm{d}\mathbf{x} = 0.$$

Then,

$$\int_{\mathbb{R}^3} \partial_t^2 \mathbf{E} \cdot \partial_t \mathbf{E} \, \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \frac{1}{2} \partial_t |\partial_t \mathbf{E}|^2 \mathrm{d}\mathbf{x} = \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^3} |\partial_t \mathbf{E}|^2 \mathrm{d}\mathbf{x},$$

$$\int_{\mathbb{R}^3} \Delta \mathbf{E} \cdot \partial_t \mathbf{E} \, \mathrm{d}\mathbf{x} = -\int_{\mathbb{R}^3} \nabla \mathbf{E} \cdot \nabla \partial_t \mathbf{E} \, \mathrm{d}\mathbf{x} = -\int_{\mathbb{R}^3} \frac{1}{2} \partial_t |\nabla \mathbf{E}|^2 \mathrm{d}\mathbf{x} = -\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^3} |\nabla \mathbf{E}|^2 \mathrm{d}\mathbf{x}.$$

Thus, taking $\widetilde{\mathcal{E}}(t) = \frac{1}{2} \int_{\mathbb{R}^3} (|\partial_t \mathbf{E}|^2 + v^2 |\nabla \mathbf{E}|^2) \mathrm{d}\mathbf{x}$, we obtain $\frac{\mathrm{d}\widetilde{\mathcal{E}}(t)}{\mathrm{d}t} = 0$ which means that $\widetilde{\mathcal{E}}(t)$ is constant in time.

Similarly, starting from Maxwell's equations, we multiply (dot product) Faraday's equation by $\mathbf{B}$, Ampère's equation by $\mathbf{E}$ and sum the two expressions. It gives

$$\frac{1}{2} \partial_t |\mathbf{B}|^2 + \frac{1}{2v^2} \partial_t |\mathbf{E}|^2 = -\operatorname{curl}(\mathbf{E}) \cdot \mathbf{B} + \operatorname{curl}(\mathbf{B}) \cdot \mathbf{E}.$$

Integrating in space, the second member disappears. Thus, the energy defined by

$$\mathcal{E}(t) = \frac{1}{2} \int_{\mathbb{R}^3} (|\mathbf{B}|^2 + \frac{1}{v^2} |\mathbf{E}|^2) \mathrm{d}\mathbf{x}$$

is constant in time.

Schrödinger equation

In plenty of devices, the electromagnetic wave propagates in a given direction z (paraxial approximation) and is closed to be monochromatic. That is why it is interesting to write the electric field $\mathbf{E}$ in the form

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) \exp(i(kz - \omega t)).$$

We first notice that the wave propagates only when the wavevector k verifies the dispersion relation

$$\omega^2 = v^2 k^2.$$

Then, inserting the expression of $\mathbf{E}(\mathbf{x}, t)$ into the wave equation, we obtain that the function A is governed by the equation

$$\left(\partial_t^2 \mathbf{A} - 2i\omega \partial_t \mathbf{A} - \omega^2 \mathbf{A}\right) - v^2 \left(\Delta \mathbf{A} + 2ik \partial_z \mathbf{A} - k^2 \mathbf{A}\right) = 0.$$

The function A is called envelope function of the field since the aim of the ansatz is to decompose the wave into a fast oscillating part and a slow varying part. Consequently, we make the following assumptions on the envelope function

$$\partial_t^2 \mathbf{A} \ll \omega \partial_t \mathbf{A} \ll \omega^2 \mathbf{A} \quad \text{and} \quad \partial_z^2 \mathbf{A} \ll k \partial_z \mathbf{A} \ll k^2 \mathbf{A}.$$

We obtain

$$-2i\omega \partial_t \mathbf{A} - v^2 \left(\Delta_\perp \mathbf{A} + 2ik \partial_z \mathbf{A}\right) = 0,$$

that can be written as the Schrödinger type equation

$$(\partial_z + \frac{1}{v} \partial_t - \frac{i}{2k} \Delta_\perp) \mathbf{A} = 0.$$

Helmholtz equation

Another usual approximation consists in fixing a frequency, making the ansatz

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) \exp(-i\omega t).$$

This time we obtain

$$\left(\partial_t^2 \mathbf{A} - 2i\omega \partial_t \mathbf{A} - \omega^2 \mathbf{A}\right) - v^2 \Delta \mathbf{A} = 0.$$

Neglecting the time derivatives, we obtain the Helmholtz equation

$$\Delta \mathbf{A} = -k^2 \mathbf{A}.$$

4.2.3 Coupling Maxwell and Bloch equations

We now consider a classical electromagnetic field $(\mathbf{E}, \mathbf{B})$ solution to the dimensionless Maxwell's equations in a homogeneous material with a polarization current $\mathbf{J}_P$ that describes the influence of a quantum object (or a collection of quantum objects) on the electromagnetic field using the dipole approximation. It gives

$$\partial_t \mathbf{B}(\mathbf{x}, t) = -\operatorname{curl} \mathbf{E}(\mathbf{x}, t),$$
$$\partial_t \mathbf{E}(\mathbf{x}, t) = v^2 \operatorname{curl} \mathbf{B}(\mathbf{x}, t) - \mathbf{J}_P(\mathbf{x}, t),$$

where $\mathbf{J}_P$ is expressed via the time derivative of the polarization

$$\mathbf{J}_P(\mathbf{x}, t) = \zeta g(\mathbf{x}) \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{P}(t)$$

with ζ a scaling parameter that says how strong is the interaction, g a given function that indicates the localization of the quantum object and $\mathbf{P}$ the polarization defined by the expectation value of the polarizability $\mathbf{p}$

$$\mathbf{P}(t) = \langle \mathbf{p} \rangle_{\rho(t)} = \operatorname{tr}(\rho(t)\mathbf{p}),$$

the density matrix ρ being the solution to the Bloch equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \rho(t) = -i[H_0 + \mathbf{p} \cdot \mathbf{E}(t), \rho(t)] + Q(\rho(t)).$$

On the one hand, the electric field acts on the quantum object, in particular on the time evolution of populations. With such a model, we can for instance make simulations of self-induced transparency phenomena (illustrated during the practical). On the other hand, there is a feedback of the quantum system to the electromagnetic field via the polarization current $\mathbf{J}_P$. For instance, it has an effect on the energy conservation. Indeed, performing the same computation as in the previous section, we obtain

$$\frac{\mathrm{d}\mathcal{E}(t)}{\mathrm{d}t} = -\frac{1}{v^2} \int_{\mathbb{R}^3} \mathbf{J}_P \cdot \mathbf{E} \; \mathrm{d}\mathbf{x}.$$

An estimate of the term $\int_{\mathbb{R}^3} \mathbf{J}_P \cdot \mathbf{E} \; \mathrm{d}\mathbf{x}$ is needed, eventually with an adaptation of the energy definition.

4.2.4 One dimensional problem

In the sequel, we will restrict our study to one dimensional equations. We assume that the unknowns depend only on the space variable z. We can separate the equations into two independent systems for the x- and y-components:

$$\begin{cases} \partial_t B_x = \partial_z E_y, \\ \partial_t E_y = v^2 \partial_z B_x - J_y, \end{cases} \qquad \begin{cases} \partial_t B_y = -\partial_z E_x, \\ \partial_t E_x = -v^2 \partial_z B_y - J_x. \end{cases}$$

The other equations do not require further attention (for instance, we have $\partial_t B_z = 0$, $\partial_z B_z = 0$).

Assuming furthermore $\mathbf{p} = (p_x, 0, 0)$ (and thus $\mathbf{J} = (J_x, 0, 0)$) allows us to consider only the right system of the above systems. We can therefore simplify the notations setting $E = E_x$, $B = B_y$ $p = p_x$, $P = P_x$ and $J = J_x$. Notice that $\operatorname{tr}([p, \cdot]p) = 0$ and thus, in 1D,

$$\frac{\mathrm{d}}{\mathrm{d}t} P(t) = \operatorname{tr}\Big(\frac{\mathrm{d}}{\mathrm{d}t}\rho(t)p\Big) = \operatorname{tr}\Big(\big(-i[H_0 + pE(t), \rho(t)] + Q(\rho(t))\big)p\Big) = \operatorname{tr}\big(\operatorname{Rn}(\rho)p\big),$$

where we introduced the relaxation–nutation operator defined by

$$\operatorname{Rn}(\rho)_{jk} = \big(-i[H_0, \rho(t)] + Q(\rho(t))\big)_{jk} = -i(\varepsilon_j - \varepsilon_k)\rho_{jk} + Q(\rho)_{jk}.$$

The Maxwell–Bloch coupling finally reads

$$\begin{cases} \partial_t B = -\partial_z E, \\ \partial_t E = -v^2 \partial_z B - J, \quad \text{with} \quad J = \zeta g(z)\,\mathrm{tr}\left(\mathrm{Rn}(\rho)p\right), \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\rho = \mathrm{Rn}(\rho) - iE[p,\rho]. \end{cases} \tag{4.1}$$

4.3 Numerics for Maxwell–Bloch equations

4.3.1 Yee's scheme for Maxwell's equations

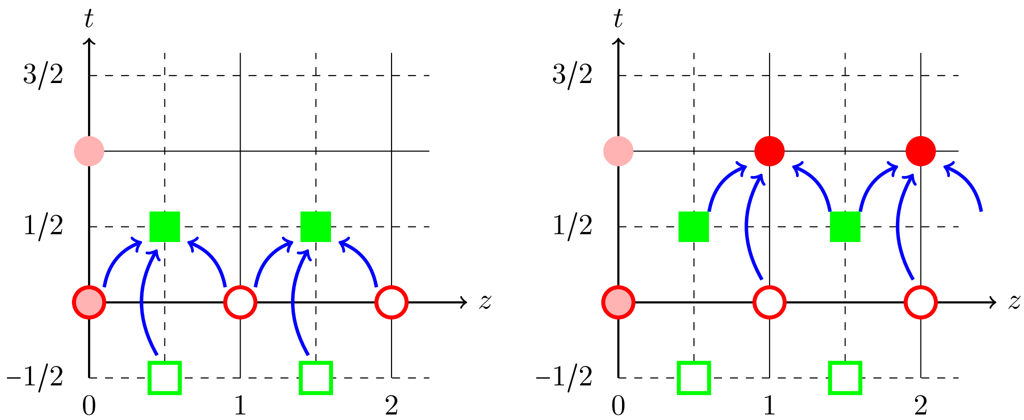
Scheme presentation We consider the (popular) Yee's scheme. It is a finite difference discretization defined on staggered grids in space and time. Localization of variables are chosen in order to have an explicit, simple to implement, scheme since Maxwell's equations are solved one after the other while preserving properties of the continuous system.

More precisely, for the one dimensional problem, we define $t_p = p\delta t$ for $p = 0, \ldots, N_t - 1$ where $\delta t = \frac{T}{N_t - 1}$ (T being the final time) and $z_j = j\delta z$ for $j = 0, \ldots, N_z - 1$ where $\delta z = \frac{L}{N_z - 1}$ (L being the length of the device). The electric field E is computed at the integer discretization points, the magnetic field B, instead, is computed at half grid points. Thus, we successively compute $B_{j+1/2}^{p+1/2}$ and E_j^{p+1} that are respectively approximations of $B((t_p + t_{p+1})/2, (z_j + z_{j+1})/2)$ and $E(t_{p+1}, z_j)$. It gives, for all $p = 0, \ldots, N_t - 2$,

$$\frac{B_{j+1/2}^{p+1/2} - B_{j+1/2}^{p-1/2}}{\delta t} + \frac{E_{j+1}^{p} - E_j^{p}}{\delta z} = 0, \quad \forall j = 0, \ldots, N_z - 2,$$

$$\frac{E_j^{p+1} - E_j^{p}}{\delta t} + v^2 \frac{B_{j+1/2}^{p+1/2} - B_{j-1/2}^{p+1/2}}{\delta z} = 0, \quad \forall j = 1, \ldots, N_z - 2,$$

completed with a discretization of the initial conditions (to compute $B^{-1/2}$ and E^0) and the boundary conditions (to compute E_0 and E_{N_z-1}).



Convergence For linear equations, a finite difference method leads to the resolution of a linear system $A_h U_h = F$, while the exact equation can be seen as $A_h U = F + E_h$. We remind that the scheme is said to be consistent when $E_h \to 0$ as $h \to 0$. The error of the numerical approximation is $\|U_h - U\| = \|A_h^{-1} E_h\| \le \|A_h^{-1}\| \|E_h\|$. The scheme is said to be stable when $\|A_h^{-1}\|$ is bounded independently of h. We can prove the Lax principle that says that a stable and consistent scheme is convergent, i.e. $U_h \to U$ as $h \to 0$.

Proposition 5. *Assuming enough regularity on (E, B), the Yee's scheme is a consistent scheme of order 2 for Maxwell's equations.*

Proof. We assume that E and B of class at least $\mathcal{C}^5$ both in time and space and we compute Taylor expansions. For instance,

$$\frac{B(t_{p+1/2}, z) - B(t_{p-1/2}, z)}{\delta t} = \partial_t B(t_p, z) + \frac{\delta t^2}{24} \partial_t^3 B(t_p, z) + o(\delta t^3).$$

After computations, we obtain

$$\Big(\frac{B(t_{p+1/2}, z_{j+1/2}) - B(t_{p-1/2}, z_{j+1/2})}{\delta t} + \frac{E(t_p, z_{j+1}) - E(t_p, z_j)}{\delta z} \Big) - \Big(\partial_t B(t_p, z_{j+1/2}) + \partial_z E(t_p, z_{j+1/2}) \Big)$$
$$= \frac{1}{24} \partial_z^3 E(t_p, z_{j+1/2})(-v^2 \delta t^2 + \delta z^2) + o(\delta t^3 + \delta z^3),$$

$$\Big(\frac{E(t_{p+1}, z_j) - E(t_p, z_j)}{\delta t} + v^2 \frac{B(t_{p+1/2}, z_{j+1/2}) - B(t_{p+1/2}, z_{j-1/2})}{\delta z} \Big) - \Big(\partial_t E(t_{p+1/2}, z_j) + v^2 \partial_z B(t_{p+1/2}, z_j) \Big)$$
$$= \frac{v^2}{24} \partial_z^3 B(t_{p+1/2}, z_j)(-v^2 \delta t^2 + \delta z^2) + o(\delta t^3 + \delta z^3).$$

□

Remark. The equivalent equations associated to this scheme are

$$\partial_t B + \partial_z E + \frac{\delta z^2}{24}(1 - \lambda^2)\partial_z^3 E = 0,$$
$$\partial_t E + v^2 \partial_z B + \frac{v^2 \delta z^2}{24}(1 - \lambda^2)\partial_z^3 B = 0,$$

defining $\lambda = \frac{v\delta t}{\delta z}$. It means that it is a dispersive scheme. Also, taking the time derivative of this second equivalent equation, we obtain the following equivalent equation (for the wave equation)

$$\partial_t^2 E - v^2 \partial_z^2 E - \frac{v^2 \delta z^2}{12}(1 - \lambda^2)\partial_z^4 E = 0.$$

It gives a diffusive dominant error term with a factor $(1 - \lambda^2)$. Consequently, if λ is not chosen close to 1, the numerical diffusion associated to the scheme could be perceptible.

Proposition 6. *A necessary condition for the L^2 stability of the Yee's scheme is given by the CFL condition*

$$\lambda := \frac{v\delta t}{\delta z} \leq 1.$$

Proof. To investigate the L^2 stability, we consider periodic boundary conditions and use the Von Neumann's method that consists in saying that the scheme is stable if and only if it is stable for any individual Fourier mode. We set

$$B_{j+1/2}^{p-1/2} = \alpha_p e^{i\xi(j+1/2)\delta z} \quad \text{and} \quad E_j^p = \beta_p e^{i\xi j \delta z}.$$

Injecting these expressions into the discretized equations, we obtain

$$\begin{pmatrix} \alpha_{p+1} \\ \beta_{p+1}/v \end{pmatrix} = \begin{pmatrix} 1 & -ia(\xi) \\ -ia(\xi) & 1 - a(\xi)^2 \end{pmatrix} \begin{pmatrix} \alpha_p \\ \beta_p / v \end{pmatrix},$$

where $a(\xi) = 2\lambda \sin(\xi\delta z/2)$. We denote this amplification matrix $A(\xi)$. A necessary condition for the L^2 stability is that $\rho(A(\xi)) \le 1$ for all ξ. Indeed, for any matrix A and any matrix norm $\|\cdot\|$, $\rho(A) \le \|A\|$ and thus $\rho(A)^p \le \|A^p\| \le \|A\|^p$. We have $\mathrm{tr}(A(\xi)) = 2 - a(\xi)^2$ and $\det(A(\xi)) = 1$. The critical ξ are given for $\sin(\xi\delta z/2) = 1$. In that case, the discriminant of the characteristic polynomial is given by $\Delta = 16\lambda^2(\lambda^2 - 1)$. It means that eigenvalues are real and of product 1 if $\lambda > 1$, equal to -1 if $\lambda = 1$ and complex and of modulus 1 if $\lambda < 1$. Thus, $\rho(A(\xi)) \le 1$ for all ξ if and only if $\lambda < 1$. □

This computation gives only a necessary condition because the amplification matrix is not normal[2]. Nevertheless, we have the following result.

Proposition 7. *The condition $\lambda < 1$ is a sufficient condition for the L^2 stability of the Yee's scheme.*

Proof. If $\lambda < 1$ and $\sin(\xi\delta z/2) \ne 0$ (stable if $\sin(\xi\delta z/2)$ since $A = I_2$), the two eigenvalues $\mu_\pm$ of A

$$\mu_\pm = 1 - \frac{a(\xi)^2}{2} \pm i\frac{a(\xi)}{2}\sqrt{4 - a(\xi)^2}$$

are distinct and of multiplicity 1. We can diagonalize A and then write $A^p = PD^pP^{-1}$ with

$$D = \begin{pmatrix} \mu_+ & 0 \\ 0 & \mu_- \end{pmatrix} \quad \text{and} \quad P = \begin{pmatrix} \frac{ia(\xi)}{1-\mu_+} & \frac{ia(\xi)}{1-\mu_-} \\ 1 & 1 \end{pmatrix}.$$

We have

$$\|A^p\| \le \|P\|\|D^p\|\|P^{-1}\| < \infty$$

since $\|D^p\|_\infty = 1$, $\|P\|_\infty = 2$ (because $|1 - \mu_\pm| = |a(\xi)|$) and $\|P^{-1}\|_\infty = \frac{2}{\sqrt{4-a(\xi)^2}}$. Thus the scheme is stable for $\lambda < 1$.

If $\lambda = 1$, -1 is an eigenvalue of A with multiplicity 2 and A is not diagonalizable. By Jordan decomposition, we can write $A^p = PJ^pP^{-1}$ with

$$J = \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad P = \begin{pmatrix} \frac{ia(\xi)}{2} & \frac{ia(\xi)}{4} \\ 1 & 0 \end{pmatrix}.$$

Since $J^p = (-1)^p \begin{pmatrix} 1 & p \\ 0 & 1 \end{pmatrix}$, its norm is not bounded uniformly in p and it leads to instabilities. □

Discrete energy conservation Recall we had for the continuous equation that the energy defined by

$$\mathcal{E}(t) = \frac{1}{2}\int_{\mathbb{R}} (B^2 + \frac{1}{v^2}E^2)\mathrm{d}x$$

is constant in time. The goal is to obtain a similar result for the discrete equations.

Proposition 8. *Imposing periodic boundary conditions, the discrete energy*

$$\mathcal{E}^{p-1/2} = \frac{1}{2}\sum_{j=0}^{N_z-2}\left((B_{j+1/2}^{p-1/2})^2 + \frac{1}{v^2}(E_j^{p-1/2})^2 - \frac{\lambda^2}{4}(B_{j+1/2}^{p-1/2} - B_{j-1/2}^{p-1/2})^2\right)$$

with $E_j^{p-1/2} = \frac{E_j^p + E_j^{p-1}}{2}$ (defining E_j^{-1} by $E_j^0 + v\lambda(B_{j+1/2}^{-1/2} - B_{j-1/2}^{-1/2})$), is preserved for all p.

Remark. For simplicity, we impose here periodic boundary conditions to avoid technical difficulties due to boundaries. Assuming $E_0 = E_{N_z-1}$ and $B_{-1/2} = B_{(N_z-1)-1/2}$, we have

$$\sum_{j=0}^{N_z-2} E_j = \sum_{j=0}^{N_z-2} E_{j+1} \quad \text{and} \quad \sum_{j=0}^{N_z-2} B_{j-1/2} = \sum_{j=0}^{N_z-2} B_{j+1/2}.$$

[2] A matrix A is normal when $A^*A = AA^*$. If A is a normal matrix then $\|A\|_2 = \rho(A)$.

Proof. We multiply the discretization of Faraday's equation by $\frac{B^{p+1/2}_{j+1/2}+B^{p-1/2}_{j+1/2}}{2}$ and the discretization of Ampère's equation by $\frac{1}{v^2}\frac{E^{p+1}_j+E^p_j}{2}$:

$$\frac{(B^{p+1/2}_{j+1/2})^2-(B^{p-1/2}_{j+1/2})^2}{2}+\frac{\lambda}{2v}(E^p_{j+1}-E^p_j)(B^{p+1/2}_{j+1/2}+B^{p-1/2}_{j+1/2})=0, \tag{4.2}$$

$$\frac{(E^{p+1}_j)^2-(E^p_j)^2}{2v^2}+\frac{\lambda}{2v}(B^{p+1/2}_{j+1/2}-B^{p+1/2}_{j-1/2})(E^{p+1}_j+E^p_j)=0.$$

At the previous time iteration, the last equation reads

$$\frac{(E^p_j)^2-(E^{p-1}_j)^2}{2v^2}+\frac{\lambda}{2v}(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2})(E^p_j+E^{p-1}_j)=0.$$

Writing the average of the two equations, we obtain

$$\frac{(E^{p+1}_j)^2+(E^p_j)^2}{4v^2}-\frac{(E^p_j)^2+(E^{p-1}_j)^2}{4v^2}+\frac{\lambda}{2v}(B^{p+1/2}_{j+1/2}-B^{p+1/2}_{j-1/2})E^{p+1/2}_j+\frac{\lambda}{2v}(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2})E^{p-1/2}_j=0. \tag{4.3}$$

Then, we perform a discrete integration by parts using periodic boundary conditions

$$\begin{aligned}\sum_{j=0}^{N_z-2}(E^p_{j+1}-E^p_j)(B^{p+1/2}_{j+1/2}+B^{p-1/2}_{j+1/2}) &= \sum_{j=0}^{N_z-2}E^p_{j+1}(B^{p+1/2}_{j+1/2}+B^{p-1/2}_{j+1/2})-\sum_{j=0}^{N_z-2}E^p_j(B^{p+1/2}_{j+1/2}+B^{p-1/2}_{j+1/2})\\ &=\sum_{j=0}^{N_z-2}E^p_j(B^{p+1/2}_{j-1/2}+B^{p-1/2}_{j-1/2})-\sum_{j=0}^{N_z-2}E^p_j(B^{p+1/2}_{j+1/2}+B^{p-1/2}_{j+1/2})\\ &=-\sum_{j=0}^{N_z-2}E^p_j(B^{p+1/2}_{j+1/2}-B^{p+1/2}_{j-1/2})-\sum_{j=0}^{N_z-2}E^p_j(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2}).\end{aligned}$$

Thus, adding (4.2) and (4.3) and summing on j, we obtain $\mathcal{E}^{p+1/2}=\mathcal{E}^{p-1/2}$ with

$$\mathcal{E}^{p-1/2}=\frac{1}{2}\sum_{j=0}^{N_z-2}\Big((B^{p-1/2}_{j+1/2})^2+\frac{1}{v^2}\frac{(E^p_j)^2+(E^{p-1}_j)^2}{2}+\frac{\lambda}{v}\frac{E^p_j-E^{p-1}_j}{2}(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2})\Big).$$

Since $(E^p_j)^2+(E^{p-1}_j)^2=\frac{(E^p_j+E^{p-1}_j)^2+(E^p_j-E^{p-1}_j)^2}{2}$, $\mathcal{E}^{p-1/2}$ reads

$$\mathcal{E}^{p-1/2}=\frac{1}{2}\sum_{j=0}^{N_z-2}\Big[(B^{p-1/2}_{j+1/2})^2+\frac{1}{v^2}(E^{p-1/2}_j)^2+\Big(\frac{E^p_j-E^{p-1}_j}{2v}\Big)\Big(\frac{E^p_j-E^{p-1}_j}{2v}+\lambda(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2})\Big)\Big].$$

By Ampère's equation,

$$\frac{E^p_j-E^{p-1}_j}{2v}=-\frac{\lambda}{2}(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2}).$$

Consequently,

$$\mathcal{E}^{p-1/2}=\frac{1}{2}\sum_{j=0}^{N_z-2}\Big((B^{p-1/2}_{j+1/2})^2+\frac{1}{v^2}(E^{p-1/2}_j)^2-\frac{\lambda^2}{4}(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2})^2\Big).$$

□

Notice that we have

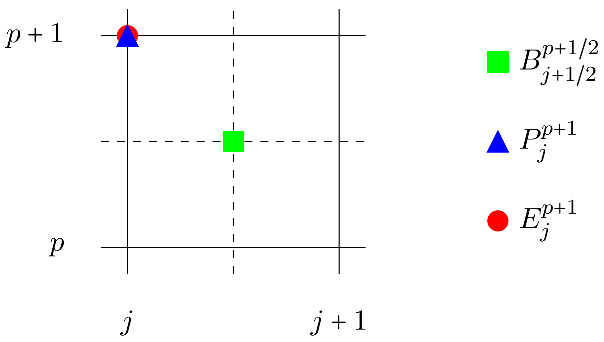
$$\sum_{j=0}^{N_z-2}(B^{p-1/2}_{j+1/2}-B^{p-1/2}_{j-1/2})^2\le 2\sum_{j=0}^{N_z-2}\Big((B^{p-1/2}_{j+1/2})^2+(B^{p-1/2}_{j-1/2})^2\Big)=4\sum_{j=0}^{N_z-2}(B^{p-1/2}_{j+1/2})^2.$$

Thus $\mathcal{E}^{p-1/2}$ is positive under the CFL condition $\lambda<1$.

4.3.2 Maxwell–Bloch coupling

The goal is to build a scheme for the Maxwell–Bloch coupling (4.1) that allows to decouple the different equations and to preserve physical properties of interest.

Historically, the location of the variables was the following



The Crank-Nicolson scheme was used for the Bloch equation, so we had

$$\frac{B_{j+1/2}^{p+1/2} - B_{j+1/2}^{p-1/2}}{\delta t} + \frac{E_{j+1}^p - E_j^p}{\delta z} = 0,$$

$$\frac{E_j^{p+1} - E_j^p}{\delta t} + v^2 \frac{B_{j+1/2}^{p+1/2} - B_{j-1/2}^{p+1/2}}{\delta z} = -\frac{P_j^{p+1} - P_j^p}{\delta t}, \quad \text{with} \quad P_j^{p+1} = \zeta g(x_j) \operatorname{tr}\left(p\rho_j^{p+1}\right),$$

$$\frac{\rho_j^{p+1} - \rho_j^p}{\delta t} = \mathrm{Rn}\left(\frac{\rho_j^{p+1} + \rho_j^p}{2}\right) - i\left[p\frac{E_j^{p+1} + E_j^p}{2}, \frac{\rho_j^{p+1} + \rho_j^p}{2}\right].$$

It is very natural to keep the space location for ρ, P or J at integer grid points j. But for the time location: Do we use ρ_j^p or $\rho_j^{p+1/2}$? Do we use P or J? Where do we locate them? Do we consider P_j^p, $P_j^{p+1/2}$, J_j^p, $J_j^{p+1/2}$? For the right-hand side of the Ampère equation, we may have

$$-\frac{P_j^{p+1} - P_j^p}{\delta t}, \quad -J_j^{p+1/2}, \quad -\frac{J_j^{p+1} + J_j^p}{2}.$$

Also, the links with ρ may be the following (not exhaustive):

$$P_j^p = \zeta g(x_j) \operatorname{tr}(p\rho_j^p), \quad J_j^{p+1/2} = \zeta g(x_j) \operatorname{tr}\left(p\frac{\rho_j^{p+1} - \rho_j^p}{\delta t}\right).$$

In 1D, there are simplifications (due to the fact that $\operatorname{tr}(p[p,\rho]) = 0$) and we can use

$$J_j^p = \zeta g(x_j) \operatorname{tr}\left(p\,\mathrm{Rn}(\rho_j^p)\right) \text{ or } J_j^{p+1/2} = \zeta g(x_j) \operatorname{tr}\left(p\,\mathrm{Rn}(\rho_j^{p+1/2})\right).$$

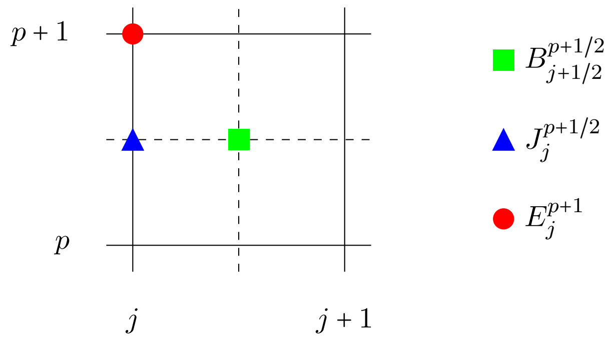
Concerning the discretization of the Bloch equation, we know we want to use a splitting (to preserve properties of ρ) of order 2 (as Yee's scheme). A possible one is

$$\rho_j^{p+1/2} = S_{\mathrm{Rn}}(\frac{\delta t}{2}) S_E(\delta t, E_j^p) S_{\mathrm{Rn}}(\frac{\delta t}{2}) \rho_j^{p-1/2}$$

where S_{Rn} and S_E are the two semi-groups associated respectively to the relaxation nutation part and to the interaction with the field part, but another choice could be

$$\rho_j^{p+1} = S_{\mathrm{Rn}}(\delta t) S_E(2\delta t, E_j^p) S_{\mathrm{Rn}}(\delta t) \rho_j^{p-1}.$$

Among all these choices, our preference in 1D is to choose the grid



and the following discretization

$$\rho_j^{p+1/2} = S_{\mathrm{Rn}}(\frac{\delta t}{2}) S_E(\delta t, E_j^p) S_{\mathrm{Rn}}(\frac{\delta t}{2}) \rho_j^{p-1/2},$$

$$\frac{B^{p+1/2}_{j+1/2} - B^{p-1/2}_{j+1/2}}{\delta t} + \frac{E^p_{j+1} - E^p_j}{\delta z} = 0,$$
$$\frac{E^{p+1}_j - E^p_j}{\delta t} + v^2 \frac{B^{p+1/2}_{j+1/2} - B^{p+1/2}_{j-1/2}}{\delta z} = -J_j^{p+1/2},$$

with

$$J_j^{p+1/2} = \zeta g(x_j) \operatorname{tr}\left(p \operatorname{Rn}(\rho_j^{p+1/2})\right).$$

This weak coupling preserves the properties of ρ (trace, Hermicity, positiveness) thanks to the use of the splitting. Also, the following proposition states it is nonlinearly stable under suitable CFL conditions. To prove it, we study a discrete energy estimate (to compare with the one of the continuous model: $\frac{\mathrm{d}\mathcal{E}(t)}{\mathrm{d}t} = -\frac{1}{v^2}\int_{\mathbb{R}} JE \, \mathrm{d}x$).

Proposition 9. *Assuming that $g(x_j) = \delta_{jj_D}$ (j_D representing the index where the quantum object is located) and imposing periodic boundary conditions, this weak coupling is nonlinearly L^2-stable for $\lambda < 1$ and $\delta t < \delta t_0$ where δt_0 depends only on the coefficients of the equations.*

Proof. Making the same computation as in the previous section, we obtain

$$\mathcal{E}^{p+1/2} - \mathcal{E}^{p-1/2} = -\frac{\delta t}{2v^2} \sum_{j=0}^{N_z-2} \left(J_j^{p+1/2} E_j^{p+1/2} + J_j^{p-1/2} E_j^{p-1/2} \right)$$

where

$$\mathcal{E}^{p-1/2} = \frac{1}{2} \sum_{j=0}^{N_z-2} \Big[(B^{p-1/2}_{j+1/2})^2 + \frac{1}{v^2} (E_j^{p-1/2})^2 + \Big(\frac{E^p_j - E^{p-1}_j}{2v} \Big) \Big(\frac{E^p_j - E^{p-1}_j}{2v} + \lambda (B^{p-1/2}_{j+1/2} - B^{p-1/2}_{j-1/2}) \Big) \Big].$$

This time, by Ampère's equation,

$$\frac{E^p_j - E^{p-1}_j}{2v} = -\frac{\lambda}{2} (B^{p-1/2}_{j+1/2} - B^{p-1/2}_{j-1/2}) - \frac{\delta t}{2v} J_j^{p-1/2}.$$

Consequently, $\mathcal{E}^{p-1/2}$ reads

$$\mathcal{E}^{p-1/2} = \frac{1}{2} \sum_{j=0}^{N_z-2} \Big((B^{p-1/2}_{j+1/2})^2 + \frac{1}{v^2} (E_j^{p-1/2})^2 + \frac{\delta t^2}{4v^2} (J_j^{p-1/2})^2 - \frac{\lambda^2}{4} (B^{p-1/2}_{j+1/2} - B^{p-1/2}_{j-1/2})^2 \Big).$$

Next, for the polarization current of the Maxwell-Bloch coupling, we have

$$
\begin{aligned}
\mathcal{E}^{p+1/2} - \mathcal{E}^{p-1/2} &= -\frac{\zeta\delta t}{2v^2}\Big(\operatorname{tr}(\mathrm{Rn}(\rho^{p+1/2})p)E_{j_D}^{p+1/2} + \operatorname{tr}(\mathrm{Rn}(\rho^{p-1/2})p)E_{j_D}^{p-1/2}\Big)\\
&\leq \frac{\zeta\delta t}{4v}\Big(\operatorname{tr}(\mathrm{Rn}(\rho^{p+1/2})p)^2 + \operatorname{tr}(\mathrm{Rn}(\rho^{p-1/2})p)^2 + \frac{1}{v^2}(E_{j_D}^{p+1/2})^2 + \frac{1}{v^2}(E_{j_D}^{p-1/2})^2\Big)\\
&\leq \frac{\zeta\delta t}{4v}\Big(\alpha\|\rho^{p+1/2}\|^2 + \alpha\|\rho^{p-1/2}\|^2 + \frac{1}{v^2}(E_{j_D}^{p+1/2})^2 + \frac{1}{v^2}(E_{j_D}^{p-1/2})^2\Big),
\end{aligned}
$$

where α is a constant depending on p and W.

For the splitting scheme, we analyze separately the two parts. One part requires the computing of $S_{\mathrm{Rn}}(\delta t)\rho$ which is solution to $\frac{\mathrm{d}}{\mathrm{d}t}\rho = \mathrm{Rn}(\rho)$. From Gronwall lemma, we find that there exists C_R (depending on W) such that

$$\|S_{\mathrm{Rn}}(\delta t)\rho(t)\|^2 \leq e^{C_R\delta t}\|\rho(t)\|^2.$$

The other part is the computation of $S_E(\delta t, E)\rho$ which is solution to $\frac{\mathrm{d}}{\mathrm{d}t}\rho = -iE[p,\rho]$. Choosing the norm $\|\cdot\|_2$ (defined by $\|\rho\|_2^2 = \operatorname{tr}(\rho^*\rho)$), we have

$$\|S_E(\delta t, E)\rho(t)\|_2^2 = \|\rho(t)\|_2^2.$$

Applying it to the second-order splitting scheme, we obtain

$$\|\rho^{p+1/2}\|_2^2 \leq e^{C_R\delta t}\|\rho^{p-1/2}\|_2^2.$$

Consequently, introducing $\widetilde{\mathcal{E}}^{p-1/2} = \mathcal{E}^{p-1/2} + \|\rho^{p-1/2}\|_2^2$, we obtain

$$
\begin{aligned}
\widetilde{\mathcal{E}}^{p+1/2} &\leq \widetilde{\mathcal{E}}^{p-1/2} + (e^{C_R\delta t}-1)\|\rho^{p-1/2}\|^2 + \frac{\zeta\delta t}{4v}\Big(\alpha\|\rho^{p+1/2}\|^2 + \alpha\|\rho^{p-1/2}\|^2 + \frac{1}{v^2}(E_{j_D}^{p+1/2})^2 + \frac{1}{v^2}(E_{j_D}^{p-1/2})^2\Big)\\
&\leq (e^{C_R\delta t} + C_2\delta t)\widetilde{\mathcal{E}}^{p-1/2} + C_2\delta t\widetilde{\mathcal{E}}^{p+1/2}
\end{aligned}
$$

where $C_2 = \frac{\zeta}{4v}\max\{\alpha, 1\}$. Thus, provided that $\delta t < \frac{1}{C_2}$ (in order that $1 - C_2\delta t > 0$), there exists C such that

$$\widetilde{\mathcal{E}}^{p+1/2} \leq \frac{1 + C\delta t}{1 - C\delta t}\widetilde{\mathcal{E}}^{p-1/2}.$$

This ensures the nonlinear stability under the previous CFL condition $\lambda < 1$ and for $\delta t < \frac{1}{C_2} := \delta t_0$. □

4.4 Practical sessions

In complement, two Python notebooks are proposed to study the numerical resolution of the von Neumann equation and of the Maxwell-Bloch coupling. They are available at the url: `https://membres-ljk.imag.fr/Brigitte.Bidegaray/teaching/courses/`