Numerical analysis of the conditional equation within the exact factorization of molecular time-dependent Schrödinger wavefunctions

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Abstract. In this paper, we are interested in the numerical analysis of the conditional equation within the Exact Factorization (EF) of wavefunctions to molecular time-dependent Schrödinger equations. After a mathematical analysis of toy-versions of the conditional equations, we provide a detailed mathematical analysis of elaborated numerical methods approximating this equation. Some illustrating numerical computations are provided along the paper.

Time-dependent Schrödinger equation; beyond Born-Oppenheimer; stability analysis;

1. Introduction

This paper is dedicated to a mathematical study of the Exact Factorization (EF) of the molecular time-dependent Schrödinger equation which was proposed in [3, 2, 4, 1], and which allows to construct efficient computational methods for molecular time-dependent Schrödinger equations beyond the Born-Oppenheimer approximation [11]. Some numerical computations and partial analysis was proposed in [6], illustrating in particular the nice features of the model, but also some difficult computational issues. In the latter reference, was raised numerous fundamental questions along the derivation of a computational method for solving the EF equation. In this paper, we propose a non-exhaustive mathematical analysis of i) the conditional equation within the EF model, and ii) of its numerical approximation. We exhibit some issues in the model from the well-posedness point of view, as well as some alternatives to fix these issues, along with stable and convergent numerical approximations. We are not specifically interested in providing full physical simulations, but rather avenues to derive relatively simple numerical schemes that would allow for accurate and robust physical simulations.

In summary, the proposed methodology is i) to mathematically analyze different simplified versions of the conditional equation, and ii) to derive efficient and stable computational
methods. Most of the proposed analysis relies on some well established mathematical tools and methods [12, 5] for studying and approximating partial differential equations [10, 8]. We will propose below a hierarchy of models approximating the conditional equation, from one-dimensional scalar linear equations to multidimensional nonlinear systems, in order to exhibit some mathematical issues related to this model.

1.1. Exact factorization of the molecular wavefunction

We recall below the basics of the exact factorization of the time-dependent molecular Schrödinger equation. The latter constitutes an exact reformulation of the quantum dynamics of interacting electronic and nuclear systems [3]. In this formalism, the overall molecular wavefunction $Ψ$ is factorized as follows:

$$Ψ(t, r, R) = φ_R(t, r)χ(t, R),$$

where $χ$ is the marginal wavefunction, and $φ_R$ the conditional one. Variable $R$ denotes the set of nuclear coordinates, and $r$ the electronic ones. The normalization condition reads, for any $t, R$, as

$$∥φ_R(t, ·)∥_2 = ∫|φ_R(t, r)|^2 dr = 1.$$

It is shown in [3, 2, 6], that $φ_R$ satisfies the conditional equation

$$i∂_t φ_R(t, r) = [\hat{H}_{BO} + \hat{V}_{ext}^e(t, r) + \hat{U}_{en} - ε(t, R)]φ_R(t, r), \quad (1)$$

and $χ$ satisfies the marginal equation

$$i∂_t χ(t, R) = \left[\left(-i\nabla_R + A(t, R)\right)^2 + V_{ext}^n(t, R) + ε(t, R)\right]χ(t, R), \quad (2)$$

where

$$\begin{cases}
ε(t, R) &= ∫ φ_R^\dagger(t, r) [\hat{H}_{BO} + \hat{V}_{ext}^e(t, r) + \hat{U}_{en} - i∂_t]φ_R(t, r) dr,
A(t, R) &= -i ∫ φ_R^\dagger(t, r)∇_R φ_R(t, r) dr,
\end{cases}$$

$$\hat{U}_{en}[φ, χ] = \frac{1}{M}\left[\frac{(-i∇_R - A)^2}{2} + \left(-i∇_R χ + A\right) · (-i∇_R - A)\right].$$

The operator $\hat{H}_{BO}$ is the standard Born-Oppenheimer hamiltonian with electronic kinetic energy, electron-electron, electron-nuclear, and nuclear-nuclear Coulomb potentials and $\hat{V}_{ext}^{e,n}$ denotes the exterior potentials. Finally, $ε$ is a time-dependent potential energy surface and $\hat{U}_{en}$ is a coupling operator. We do not detail further the model and rather refer to [3, 2, 4, 1] for details.
1.2. Model under consideration

Rather than an exhaustive study of (1), we rewrite $\phi_R(t, r)$ as proposed in [6], as follows

$$\phi_R(t, r) = \sum_j C_j(t, R)\phi^{j, \text{BO}}_R(r),$$

where $\tilde{H}_{BO}\phi^{j, \text{BO}}_R(r) = \varepsilon^j(R)\phi^{j, \text{BO}}_R(r)$. Thus, it can easily proven that $\{C_i\}_i$ satisfies, what we will hereafter referred as local conditional equation

$$\partial_t C_i(t, R) = (\varepsilon_i(R) - \varepsilon(t, R))C_i + U^i_{\text{en}}(t, R), \quad (3)$$

where the projection of $U_{\text{en}}$ on $\phi^i_R$ reads

$$U^i_{\text{en}} = \frac{1}{M_n} \left[ (\frac{1}{2} \nabla \cdot A - A^2 - \nabla^2) + \frac{\nabla \chi}{\chi} (iA - \nabla) \right] C_i - \sum_j \left( \frac{1}{2} d^2_{ij} + d_{ij} \nabla + \frac{\chi}{\chi} d_{ij} \right) C_j,$$

and where

$$d_{ij}(R) = \langle \phi^i_R | \nabla_R \phi^j_R \rangle, \quad d^2_{ij}(R) = \langle \phi^i_R | \nabla^2_R \phi^j_R \rangle,$$

and

$$A(t, R) = -i \left[ \sum_{i,j} C^*_i C_j d_{ij} + \sum_i C^*_i \nabla_R C_i \right] \varepsilon(t, R) = \sum_i (C^*_i U^i_{\text{en}} + |C_i|^2 \varepsilon_i) .$$

We will be then interested in pointing out some mathematical issues in (3), assuming that $\chi$ is given.

1.3. Organization of the paper

In Section 2, we propose a simple analysis of a linear version of the conditional equation (3), and then propose an analysis of simple computational methods for this linear model. Section 3 is then dedicated to the mathematical and numerical analysis of more general equations. In Subsection 3.4 some possible avenues for stable and accurate approximations of the full FE equation are proposed. We finally conclude in Section 4.

2. Scalar toy-models

An exhaustive analytical study of (1)-(3) would be very fastidious, so that we prefer to exhibit and to analyze some key-properties and issues of this model, thanks first to the analysis of toy-versions. Some numerical approximations of this simplified versions will then proposed and mathematically analyzed. We will then start with very elementary models then will complexify the equation.
2.1. About the well-posedness issue

We are interested in the stability of the solution with respect to the initial data; that is, any perturbation of the initial data, implies a small perturbation on the solution. We focus first on the \( \nabla \chi / \chi \)-term contribution in (3). In this goal, let us consider a first toy-model in \( \mathbb{R}_+ \times \mathbb{R} \):

\[
\partial_t \phi(t, x) + (\lambda + i \mu) \partial_x \phi(t, x) = 0, \quad \phi(0, x) = \phi_0(x) \in L^2(\mathbb{R}),
\]

where, \( \lambda, \mu \) are real. Basically \((\lambda + i \mu) \) ”models” \( i \nabla \chi / \chi \). Denoting, the Fourier transform of \( \phi \) with respect to \( x \) as \( \hat{\phi}(t, \xi) \), the solution to (15) in Fourier space reads:

\[
\hat{\phi}(t, \xi) = \exp \left( (\xi \mu - i \xi \lambda) t \right) \hat{\phi}_0(\xi).
\]

This leads to the following \( L^2 \)-norm (if it exists)

\[
\| \hat{\phi}(t, \cdot) \|_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \exp(2 \xi \mu t) |\hat{\phi}_0(\xi)|^2 d\xi.
\]

By Parseval \( \| \hat{\phi}(t, \cdot) \|_{L^2(\mathbb{R})} = \| \phi(t, \cdot) \|_{L^2(\mathbb{R})} \) and as a consequence the problem is ill-posed (unstable) whenever \( \mu \neq 0 \) (the \( L^2 \)-norm goes to infinity when \( t \) goes to infinity) for \( \mu \xi > 0 \). We can easily deduce that the corresponding numerical scheme will be unstable, as any small perturbation of the initial data (or approximate solution at a given time iteration \( n \)), will generate an unbounded perturbation growing to infinity when \( n \) goes to infinity. In the following, we will assume that the initial data are (only) \( L^2(\mathbb{R}) \), possibly \( BV(\mathbb{R}) \) or \( L^2(\mathbb{R}) \cap C^2(\mathbb{R}) \).

This remark can be extended to space dependent coefficients by using Gronwall’s inequality.

**Proposition 2.1** The following toy-model

\[
\partial_t \phi(t, x) + (\lambda(x) + i \mu(x)) \partial_x \phi(t, x) = 0, \quad \phi(0, x) = \phi_0(x) \in L^2(\mathbb{R})
\]

where, \( \lambda, \mu \) are two bounded, non-null, real functions, is such that the unique solution is unstable with respect to the initial data.

**Proof.** According to the above remark, for \( \tilde{\lambda}, \tilde{\mu} \) constant, the following equation is ill-posed:

\[
\partial_t \tilde{\phi}(t, x) + (\tilde{\lambda} + i \tilde{\mu}) \partial_x \tilde{\phi}(t, x) = 0, \quad \tilde{\phi}(0, x) = \phi_0(x).
\]

Let us assume that \( \lambda \) (resp. \( \mu \)) is close enough to \( \tilde{\lambda} \) (resp. \( \tilde{\mu} \)). We set \( \varepsilon_\lambda := \lambda - \tilde{\lambda} \) and \( \varepsilon_\mu := \mu - \tilde{\mu} \), such that

\[
\| \varepsilon_\lambda \|_\infty < \varepsilon, \quad \| \varepsilon_\mu \|_\infty < \varepsilon,
\]

where \( \varepsilon \) is as small as wanted. Then setting \( \Psi := \phi - \tilde{\phi} \), with \( \Psi(0, x) = 0 \), we have

\[
\partial_t \Psi + (\tilde{\lambda} + i \tilde{\mu}) \partial_x \Psi(t, x) = -(\varepsilon_\lambda(x) + i \varepsilon_\mu(x)) \partial_x \phi(t, x).
\]

We multiply by \( \Psi^\dagger \) and take the real part:

\[
\partial_t |\Psi|^2 + \tilde{\lambda} \partial_x |\Psi|^2 = -2 \text{Re} \left( (\varepsilon_\lambda(x) + i \varepsilon_\mu(x)) \Psi^\dagger \partial_t \phi \right) \leq \varepsilon \sqrt{2} \left( |\Psi|^2 + |\partial_x \phi|^2 \right).
\]

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Assume that for any \((t, x) \in \mathbb{R}_+ \times \mathbb{R}, |\partial_x \phi|^2\) is bounded by a constant \(C > 0\)

\[
\partial_t |\Psi|^2 + \tilde{\lambda} \partial_x |\Psi|^2 \leq \varepsilon \sqrt{2}(C + |\Psi|^2).
\]

Along the characteristic curves \(X(t): \{(t, x_0 - \tilde{\lambda} t) : t > 0, x_0 \in \mathbb{R}\}\), we set \(V(t) := |\Psi(t, X(t))|^2\), so that

\[
V'(t) \leq \varepsilon \sqrt{2}(C + V(t)).
\]

Then for \(t \geq 0\), by Gronwall’s inequality we get

\[
V(t) \leq V_0 \exp(\varepsilon \sqrt{2}t) + \sqrt{2}C \varepsilon t,
\]

as \(V_0 = 0\). Then, there exists \(C > 0\) such that

\[
|\phi(t, X(t)) - \tilde{\phi}(t, X(t))| \leq C \varepsilon t.
\]

As the solution (6) is exponentially unstable with respect to initial data \(\phi_0\), \(\phi\) can not be bounded. On the other hand, if \(|\partial_x \phi|\) is unbounded by integrating in time (5), we again deduce the instability with respect to \(\phi_0\).

How to (partially) deal with this issue? A possibility is to add some artificial diffusion. In fact, usual stable numerical schemes produce some artificial (then called numerical) diffusion which modifies the equation which is genuinely solved (the equivalent equation). That is the scheme approximates the following equation (including as well a Schrödinger operator):

\[
\partial_t \phi(t, x) + (\lambda + i \mu) \partial_x \phi(t, x) = (\varepsilon + i \alpha) \partial^2_x \phi(t, x), \quad \phi(0, x) = \phi_0(x), \quad (7)
\]

for some \(\varepsilon > 0\). The same calculation as for (15), leads this time to

\[
\|\hat{\phi}(t, \cdot)\|_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \exp(2t(\xi \mu - \varepsilon \xi^2))|\hat{\phi}_0(\xi)|^2 d\xi.
\]

Now, the solution to (7) reads

\[
\phi(t, x) = G_\varepsilon(t, \cdot) *_x \phi_0(x),
\]

where \(*_x\) denotes the convolution product with respect to \(x\), and \(G_\varepsilon\) is the inverse Fourier transform \(\hat{G}_\varepsilon(t, \xi) = \exp(t(\mu \xi - i \lambda \xi - \varepsilon \xi^2 - i \alpha \xi^2))\). The inverse Fourier transform exists and can be calculated as \(\hat{G}_\varepsilon(t, \cdot)\) is in \(L^2(\mathbb{R})\). Indeed

\[
\|G_\varepsilon(t, \cdot)\|^2_{L^2(\mathbb{R})} = \|\hat{G}_\varepsilon(t, \cdot)\|^2_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \exp\left(2t(\mu \xi - \varepsilon \xi^2)\right) d\xi = \int_{\mathbb{R}} \exp\left(-2\varepsilon t(\xi - \mu/2\varepsilon)^2 + t \mu^2 / 2\varepsilon\right) d\xi = \exp\left(t \mu^2 / 2\varepsilon\right) \sqrt{\pi / 2\varepsilon t}.
\]

However, this term still diverges whenever \(t\) goes to infinity, but for \(\mu^2 / 2\varepsilon\) (that corresponds to \(\text{Re} \nabla \chi / \chi\) in (1)) small enough, the growth is “moderate”. Notice as well that the discussion above remains valid for diagonal systems. Now, other terms in the equation could potentially counter-balance this effect. Notice that above arguments mainly remain valid in 3-d.
2.2. About the stability of finite difference numerical scheme

First recall that for (well-posed) equations of the form:

\[ \partial_t \phi(t, x) + \lambda(x) \partial_x \phi(t, x) = 0, \quad \phi(0, x) = \phi_0(x), \] (8)

with \( \lambda(x) \in \mathbb{R} \\setminus \{0\} \) smooth and bounded, stable explicit scheme must usually be upwinded.

That is denoting \( \phi_j^n \approx \phi(t_n, x_j) \) and \( \lambda_j = \lambda(x_j) \), we consider

\[ \phi_j^{n+1} = \phi_j^n - |\lambda_j| \Delta t \Delta x \left( \frac{\text{sign}(\lambda_j) + 1}{2} (\phi_j^n - \phi_{j-1}^n) + \frac{1 - \text{sign}(\lambda_j)}{2} (\phi_{j+1}^n - \phi_j^n) \right) \]

where sign is the sign function. This scheme is first order accurate and is stable under a CFL condition \( \sup_j |\lambda_j| \Delta t / \Delta x \leq 1 \). Now, an implicit scheme does not (often) require upwinding.

In particular

\[ \phi_j^{n+1} = \phi_j^n - \lambda_j \frac{\Delta t}{2 \Delta x} (\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}) \] (9)

is unconditionally stable. We next consider the equation:

\[ \partial_t \phi(t, x) + (\lambda + i \mu) \partial_x \phi(t, x) = 0, \quad \phi(0, x) = \phi_0(x), \] (10)

where we assume that \( \lambda, \mu \) are real constant (to simplify the analysis for now on). Without loss of generality, let us assume that \( \mu > 0 \). We consider the following implicit centered scheme, which extends (9)

\[ \phi_j^{n+1} = \phi_j^n - (\lambda + i \mu) \frac{\Delta t}{2 \Delta x} (\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}). \] (11)

We denote \( \hat{\phi}^n := \{ \hat{\phi}_k^n \}_{k \in \mathbb{Z}} \) the discrete Fourier transform of \( \{ \phi_j^n \}_{j \in \mathbb{Z}} \)

\[ \hat{\phi}_k^n = \sum_{j \in \mathbb{Z}} e^{ikj\Delta x} \phi_j^n. \]

**Proposition 2.2** The implicit scheme (11) approximating (10) is \( \ell^2 \)-stable under the condition

\[ \Delta t \geq \frac{2|\mu| \Delta x}{(\lambda^2 + \mu^2) \sin(\theta)}, \] (12)

for any \( \theta \in (-\pi, \pi) \setminus \{0\} \).

**Proof.** We first notice that

\[ |\hat{\phi}_k^{n+1}|^2 = \left| 1 + \frac{\Delta t (\mu - i \lambda)}{\Delta x \sin(\theta)} \right|^{-2} |\hat{\phi}_k^n|^2, \]

where \( \theta := \Delta x \xi \in (-\pi, \pi) \). The linear stability of the scheme reads for some \( C > 0 \)

\[ \|\hat{\phi}^n\|_{L^2(-\pi/\Delta x, \pi/\Delta x)} = \|\phi^n\|_{\ell^2(\Delta x \mathbb{Z})} = \sqrt{\Delta x} \left( \sum_{j \in \mathbb{Z}} |\phi_j^n|^2 \right)^{1/2} \leq C \|\phi_0\|_{\ell^2(\Delta x \mathbb{Z})}. \]
We set the contraction factor (see [10])
\[ g(\theta) := \frac{1}{1 + \frac{\Delta t(\mu - i\lambda)}{\Delta x} \sin(\theta)}. \]

The linear stability requires that for any frequency \( \theta \in (-\pi, \pi) \):
\[ |g^{-1}(\theta)| = \left| 1 - \frac{\Delta t(\mu - i\lambda)}{\Delta x} \sin(\theta) \right| \geq 1. \]

Now
\[ |g^{-1}(\theta)|^2 = \left| 1 - \frac{\Delta t \mu}{\Delta x} \sin(\theta) \right|^2 + \frac{\Delta t^2 \lambda^2}{\Delta x^2} \sin^2(\theta) \]
\[ = \left( 1 + \frac{\Delta t^2(\lambda^2 + \mu^2)}{\Delta x^2} \sin^2(\theta) - 2 \frac{\Delta t \mu}{\Delta x} \sin(\theta) \right)^2, \]
so that \( |g^{-1}(\theta)| \geq 1 \) for all \( \theta \in (-\pi, \pi) \) is equivalent to
\[ \Delta t \left( \frac{\lambda^2 + \mu^2}{\Delta x} \sin^2(\theta) + 2\mu \sin(\theta) \right) \geq 0. \]

For \( \theta \in \pi \mathbb{Z} \), the inequality is satisfied. If \( \sin(\theta) \neq 0 \), then stability requires
\[ \Delta t \geq \frac{2\mu \Delta x}{\lambda^2 + \mu^2 \sin(\theta)}, \tag{13} \]
which is automatically satisfied if \( \sin(\theta) < 0 \), while for \( \sin(\theta) > 0 \), it imposes a condition which can be very restrictive if \( \sin(\theta) \) is very small (and positive). Notice that if \( \mu < 0 \), the same argument would still be valid by inverting the sign of \( \sin(\theta) \). However, if \( \mu \) is small and \( \lambda \) large, we can expect a not too-restrictive condition. □

Basically, this result can be explained by the generation of artificial diffusion by the scheme when using larger time steps.

**Proposition 2.3** The Crank-Nicolson scheme
\[ \phi_j^{n+1} = \phi_j^n - (\lambda + i\mu) \frac{\Delta t}{4\Delta x} (\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}) - (\lambda + i\mu) \frac{\Delta t}{4\Delta x} (\phi_{j+1}^n - \phi_{j-1}^n) \]
approximating (10) is unconditionally unstable.

**Proof.** We easily show that the contraction factor reads:
\[ g(\theta) := \frac{1}{1 + \frac{\Delta t(\mu - i\lambda)}{2\Delta x} \sin(\theta)} \]
for $\theta \in (-\pi, \pi)$. The linear $\ell^2$-stability requires $|g(\theta)| \leq 1$ for all $\theta \in (-\pi, \pi)$, that is

$$|g(\theta)|^2 = \frac{1 + \Delta t^2(\lambda^2 + \mu^2)}{1 + \Delta t^2(\lambda^2 + \mu^2)} \sin^2(\theta) + \frac{\Delta t \mu}{\Delta x} \sin(\theta) \leq 1.$$ 

If $1 + \frac{\Delta t^2(\lambda^2 + \mu^2)}{4\Delta x^2} \sin^2(\theta) - \frac{\Delta t \mu}{\Delta x} \sin(\theta) > 0$

$$|g(\theta)|^2 \leq 1 \iff \frac{\Delta t \mu}{\Delta x} \sin(\theta) \leq 0,$$

which can not be satisfied for all $\theta \in (-\pi, \pi)$. If $1 + \frac{\Delta t^2(\lambda^2 + \mu^2)}{4\Delta x^2} \sin^2(\theta) + \frac{\Delta t \mu}{\Delta x} \sin(\theta) < 0,$

$$|g(\theta)|^2 \leq 1 \iff \frac{\Delta t \mu}{\Delta x} \sin(\theta) \geq 0.$$ 

The same conclusion holds. We conclude that the Crank-Nicolson version of the scheme is unconditionally unstable. □

How to stabilize even more the scheme (11)? Basically, we need to include an additional term in the equation in order to ensure stability:

$$\partial_t \phi(t, x) + (\lambda + i \mu) \partial_x \phi(t, x) = \varepsilon \partial_x^2 \phi(t, x), \quad \phi(0, x) = \phi_0(x),$$

where we assume that $\lambda, \mu$ are real constant and $\varepsilon > 0$. We consider the following implicit centered scheme with diffusion

$$\phi^{n+1}_j = \phi^n_j - (\lambda + i \mu) \frac{\Delta t}{2\Delta x} (\phi^{n+1}_{j+1} - \phi^{n+1}_{j-1}) + \varepsilon \frac{\Delta t}{\Delta x^2} (\phi^{n+1}_{j+1} - 2\phi^{n+1}_j + \phi^{n+1}_{j-1}).$$

Then, we easily show that

$$|\hat{\phi}^{n+1}_k|^2 = \left|1 - \frac{\Delta t(\mu - 1 \lambda)}{\Delta x} \sin(\theta) + 2\varepsilon \frac{\Delta t}{\Delta x^2} (1 - \cos(\theta)) \right|^2 |\hat{\phi}^n_k|^2,$$

where $\theta = \Delta x \xi$. As $1 - \cos(\theta) = 2 \sin^2(\theta/2)$, we set

$$g(\theta) := \frac{1}{1 - \frac{\Delta t(\mu - 1 \lambda)}{\Delta x} \sin(\theta) + 4\varepsilon \frac{\Delta t}{\Delta x^2} \sin^2(\theta/2)}.$$

Then as $\sin(\theta) = 2 \cos(\theta/2) \sin(\theta/2)$,

$$|g^{-1}(\theta)|^2 = \left(1 + 4\varepsilon \frac{\Delta t}{\Delta x^2} \sin^2(\theta/2) - \frac{\Delta t \mu}{\Delta x} \sin(\theta)\right)^2 + \frac{\Delta t^2 \lambda^2}{\Delta x^2} \sin^2(\theta).$$
The additional diffusion term has indeed a stabilization effect. More specifically, it was noted that the stability condition (13) could become restrictive for small $\theta$ positive. In the latter case, we have

$$|g^{-1}(\theta)|^2 \approx \left(1 + \frac{\theta \Delta t}{\Delta x} \left(\varepsilon - \frac{\theta}{\Delta x} - \mu\right)\right)^2 + \frac{\Delta t^2 \lambda^2}{\Delta x^2} \theta^2.$$  

Then

$$|g(\theta)|^2 \leq 1 \iff \frac{\theta \Delta t}{\Delta x} \left(\varepsilon \frac{\theta}{\Delta x} - \mu\right) \left(\frac{\theta \Delta t}{\Delta x} \left(\varepsilon \frac{\theta}{\Delta x} - \mu\right) + 2\right) + \frac{\Delta t^2 \lambda^2}{\Delta x^2} \theta^2 \geq 0.$$  

As $\mu > 0$ (by assumption), by taking $\varepsilon \geq \mu \Delta x/\theta$, we ensure that $|g(\theta)| \leq 1$. From a computational point of view, the spatial wavenumber $\theta_{\Delta}$ will vary from $(\pi/L, \pi/\Delta x)$ where $L$ is the overall computational spatial domain, so that roughly speaking by taking $\varepsilon \geq L \mu \Delta x/\pi$, we can expect unconditional stability of the scheme. This may still be required $\Delta x$ small enough.

**At first sight.** The Crank-Nicolson scheme should be avoided for discretizing the contribution $Re \nabla \chi/\chi$, and fully implicit is “more” stable; while adding some artificial implicit diffusion should help as well.

Let us add that for $\mu = 0$, we have

**Proposition 2.4** Consider the equation

$$\partial_t \phi + \lambda \partial_x \phi = \varepsilon \partial_x^2 \phi + i \eta \partial_x^2 \phi, \quad (t, x) \in [0, T] \times \mathbb{R}, \quad \phi(0, x) \in L^2(\mathbb{R}) \cap BV(\mathbb{R}),$$

where $\eta$, $\lambda$, and $\varepsilon$ are real numbers. Denoting $\{\phi_j^n\}$ the approximate solution to the centered implicit scheme is such that there exists $C(T) > 0$, with

$$\max_{0 \leq |j| \leq J} |\phi(t_n, x_j) - \phi_j^n| \leq C(T) (\Delta t + \Delta x^2).$$

We next propose some numerical experiments in order to illustrate the analysis providing above.

**2.3. Numerical Experiments.**

(i) A simple numerical illustration: we consider the equation

$$\partial_t \phi + (\lambda + i \mu) \partial_x \phi = \varepsilon \partial_x^2 \phi, \quad \phi(0, x) = \phi_0(x) = \exp(-50x^2/2)/\mathcal{N},$$

with $\lambda = 1$ and $\mu = 1$ and $\mathcal{N}$ is such that $\|\phi_0\|_{L^2(D)} = 1$. We report the $\ell^2-$norm of the solution obtained with a fully implicit scheme with different values of $\varepsilon \geq 0$, at time $T = 0.32$. The diffusion term is also implicit in order to avoid stability issues. The domain is $D = [-2, 2]$, we take $\Delta t = \Delta x$ and $N = 1001$ grid points, that is $\Delta x = 1/250$. We respectively take $\varepsilon = 0, 10^{-2}, 5 \times 10^{-2}, 10^{-1}, 5 \times 10^{-1}$, and compare in semilogscale in Fig. 1 the $\ell^2$-norm of $\{\phi_j^n\}_j$ as a function of time, that is

$$\left\{ (t_n, (\Delta x \sum_j |\phi_j^n|^2)^{1/2}) : t_n \in [0, T] \right\}.$$

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We observe that a strong enough artificial diffusion allows to stabilize the scheme, at least for short times.

(ii) A second experiment is proposed to illustrate the stability of the implicit scheme for different values of $\mu$. We consider

$$\partial_t \phi + (\lambda + i \mu) \partial_x \phi = \varepsilon \partial_x^2 \phi, \quad \phi(0, x) = \exp(-50x^2/2)/N.$$  

We take $\lambda = 1$, $\varepsilon = 10^{-2}$, and we take $N = 1001$ grid points, and the domain is $D = [-2, 2]$. We compare in Fig. 2, the semilogscale of the $\ell^2$-norm for different values of $\mu$: $\mu = \pm 1, 10^{-1}, 5, 10$. The stability is shown to be strongly dependent on $\mu$, as analytically observed above.

(iii) A third experiment is proposed to illustrate the stability of the implicit scheme for different values of $\Delta t$. We consider

$$\partial_t \phi + (\lambda + i \mu) \partial_x \phi = 0, \quad \phi(0, x) = \exp(-50x^2/2)/N.$$  

As it was shown above the implicit scheme is in principle stable for $\Delta t \geq 2\mu \Delta x/(\lambda^2 + \mu^2) \sin(\theta_{\Delta}) = \Delta x/\sin(\theta_{\Delta})$ where $\theta_{\Delta} = \Delta x \xi_{\Delta x}$. We take $\mu = \lambda = 1$ and we choose $N = 1001$ grid points, and the domain is $D = [-2, 2]$. We compare in Fig. 3, the
semilogscale of the $\ell^2$-norm for different values of $\Delta t$: $\Delta t = 10\Delta x, 5\Delta x, \Delta x, \Delta x/2, \Delta x/5$. As expected a larger time-step stabilizes the schemes, thanks to the generation of artificial diffusion mimicking the stabilization effect of $\varepsilon \partial_x^2 \phi$.

(iv) In the next experiment, we consider the following equation (including kinetic operator and real and complex transport)

$$\partial_t \phi + (\lambda + i\mu) \partial_x \phi = i\eta \partial_x^2 \phi, \quad \phi(0, x) = \exp(-50x^2/2)/N.$$ 

We take $\mu = \lambda = \eta = 1$ and we take $N = 4001$ grid points, and the domain is $D = [-2, 2]$. We again compare in Fig. 4 the semilogscale of the $\ell^2$-norm for different values of $\Delta t$ this time: $\Delta t = 50\Delta x, 10\Delta x, 5\Delta x, \Delta x, \Delta x/2$. Again, it is shown that larger time steps allow for a stabilization of the overall numerical scheme, by generation of numerical diffusion.

2.4. Variable artificial diffusion

In this part, we propose to study the effect of a space-dependent artificial diffusion added to the model. More specifically, we consider the equation

$$\partial_t \phi(t, x) + (\lambda(t, x) + i\mu(t, x)) \partial_x \phi(t, x) = \varepsilon(t) \partial_x^2 \phi(t, x), \quad \phi(0, x) = \phi_0(x) \in L^2(D).$$
where, $\lambda, \mu, \varepsilon$ are real functions. In the above equation $\varepsilon$ is introduced to stabilize (with respect to the initial data). The latter is chosen such that

$$
\varepsilon(t) = \varepsilon_\infty \|\mu(t, \cdot)\|_\infty .
$$

In the following example, we take $\mu(t, x) = \exp \left( - (t - T/2)^2 \right) \left( (1 + \cos(2x)) + i (0.5 \sin^2(x) + 1) \right)$ (see graph of $|\mu|$, Fig. 5 (Left)), and $\varepsilon(t) = \varepsilon_\infty \|\mu(t, \cdot)\|_\infty$. Moreover, we take $N = 2001$ on $\mathcal{D} = [-2, 2]$, and $\varepsilon_\infty$ respectively equal to $0$, $10^{-1}$, $2 \times 10^{-1}$, $5 \times 10^{-1}$, $1$. The time steps are computed $\Delta t = \Delta x / \|\mu(t, \cdot)\|_\infty$. We compare in semilogscale the $\ell^2$-norm as a function of time, Fig. 6. This example illustrates the fact that the non-trivial effect of space-dependent diffusion on the solution to the simplified conditional equation.

The simple analysis and experiments presented in the section allow for a better understanding of the general behavior of the solution to the conditional equation. We then consider below more elaborated versions of the conditional equation.

### 3. More general model systems/equations

We now consider more realistic models closer to the conditional equation (3) in the EF model. We more specifically focus on the analysis of combined spectral and finite difference
Figure 4. Experiment 4. Comparison of the $\ell^2$-norm of the numerical solution as function of time, for different values of $\Delta t$.

Figure 5. Experiment 5. (Left) Graph of $|\mu|: \{(t, x, |\mu(t, x)|)\}$. (Right) Time steps.

Approximations. The method of separation of variables is applied on $\phi_R$, so that

$$\phi_R(t, r) = \sum_j C_j(t, R) \phi_{R_j}^{BO}(r)$$
and, we denote $\mathbf{C} = (C_1, \cdots, C_N)^T$ which satisfies, with $\mathbf{C}^{(0)} = \mathbf{C}(0, \cdot)$

\begin{equation}
    i\partial_t \mathbf{C} = (\mathbf{e}(t, R) - \varepsilon(t, R) I) \mathbf{C} + \frac{1}{M_{\alpha}} \left( \mathbf{f}(\mathbf{C}, t, R) - \frac{\nabla_R \chi}{\chi} \nabla_R - \frac{1}{2} \nabla^2_R \right) \mathbf{C} \tag{16}
\end{equation}

\begin{equation}
    + \mathbf{D}(\mathbf{C}, t, R) \nabla_R \mathbf{C} + \mathbf{M}(\mathbf{C}, t, R) \mathbf{C}, \tag{17}
\end{equation}

where

\begin{equation*}
    \mathbf{f}(\mathbf{C}, t, R) = \frac{\nabla_R A(C, t, R) - A^2(C, t, R)}{2} I + i A(C, t, R) \frac{\nabla_R \chi}{\chi},
\end{equation*}

and $A$ is defined in (23). Moreover $\mathbf{e}(t, R) = \text{diag}(\varepsilon_1(t, R), \cdots, \varepsilon_N(t, R))$, $\mathbf{D}(\mathbf{C}, t, R) = \{d_{ij}(\mathbf{C}, t, R)\}_{1 \leq i, j \leq N}$ and $\mathbf{M}(\mathbf{C}, t, R) = \{d_{ij}^2/2 + d_{ij} \nabla_R \chi/\chi\}_{1 \leq i, j \leq N}$ where $d_{ij}(\mathbf{C}, t, R)$ is defined in (22).

As the analysis below is one-dimensional, we then have $\nabla_R = \partial_R$ and $\Delta_R = \partial^2_R$. The analysis is provided for all $t \in \mathbb{R}_+$ or when specified for all $t \in [0, T]$, with $T < +\infty$. The latter assumption is of main importance to analyze the stability of the scheme, whenever $\text{Im}(\alpha_{\ell}) > 0$, for all $\ell \in \{1, \cdots, N\}$. It is important to recall that beyond $\mathbf{C}^{(0)} \in L^2(\mathbb{R}; \mathbb{C}^N)$ (initial data), we do not make any assumptions (except if specified), regarding the regular-
ity of its regularity. Even if we assume that i) \(\phi_0\) a compact support, and ii) belongs to \(H^2(\mathbb{R}; \mathbb{C}^N) = \{\phi \in L^2(\mathbb{R}; \mathbb{C}^N) : \mathcal{F}^{-1}((1 + |\xi|^2)\mathcal{F}(\phi) \in L^2(\mathbb{R}; \mathbb{C}^N)\}\), then by Paley-Wiener’s theorem for some \(c\) and \(L > 0\) [9]
\[
\|\mathcal{F}(\phi_0)\|_{\infty} \leq ce^{L|\xi|},
\]
we can not conclude regarding the well-posedness of (16).

3.1. Diagonal model

In order to analyze the well-posedness of the system (16), we first consider a diagonal version. The analysis of the following linear version of the system will be justified later on, when we study the stability of semi-implicit numerical schemes. We set the following diagonal matrices (with \(\nabla_R = \partial_R\) below, as the analysis is one-dimensional)
\[
\begin{align*}
\alpha(C, t, R) &= \mathbf{I} \varepsilon(t, R) + (1 - \varepsilon(t, R) + M(C, t, R)) \mathbf{I} + \frac{f(C, t, R)}{M_n}, \\
\beta(C, t, R) &= \frac{1}{M_n} \nabla_R \chi(t, R) + D(C, t, R) \mathbf{I}, \\
\zeta(t, R) &= -\frac{1}{2M_n} \mathbf{I}, \\
f(C, t, R) &= \frac{1}{2} (\nabla_R A(C, t, R) - A^2(C, t, R) \mathbf{I}) + i A(C, t, R) \nabla_R \chi.
\end{align*}
\]

Typically, at time \(t = t_{n+1}\), we define
\[
f(C^n, t_{n+1}, R) := \frac{1}{2} (\nabla_R A(C^n, t_{n+1}, R) - A^2(C^n, t_{n+1}, R) \mathbf{I}) + i A(C^n, t_{n+1}, R) \nabla_R \chi^{n+1}.
\]

We then consider in the following nonlinear model:
\[
\mathbf{i} \partial_t C = \alpha(C, t, R) C + \beta(C, t, R) \nabla_R C + \gamma(t, R) \nabla_R^2 C + \zeta(t, R) \nabla_R^3 C,
\]
with \(\alpha\), and \(\beta\) belong to \(C_0^1(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}^+; \mathbb{C}^{N \times N})\), \(\zeta\) belongs \(C_0^1(\mathbb{R} \times \mathbb{R}^+; \mathbb{R}^{N \times N})\), is \(\mathbf{i}\) (associated to the kinetic operator) is a real-valued function, and \(\gamma \in C_0^1(\mathbb{R} \times \mathbb{R}^+; \mathbb{R}^{N \times N})\).

More generally, we could consider nonlinear function \(\gamma\), \(\gamma(C, t, R)\). However from a practical point of view, as at any given time \(t\), the nonlinearities will be linearized at previous times \(t^- < t\) below, it is sufficient to consider \(\gamma(t, R)\).

Unlike \(\alpha\), \(\beta\) and \(\zeta\) which have a physical meaning, the function \(\gamma\) is artificially introduced to stabilize the model and a corresponding scheme. Notice that the product \(\alpha(C, t, R) C\) (and the others) is a matrix-vector product from \(\mathbb{C}^{N \times N} \times \mathbb{C}^N\) to \(\mathbb{C}^N\). According to the above analysis, the system is well-posed whenever \(\text{Im}(\alpha_{\ell\ell}(C, t, R)) \leq 0\), \(\text{Im}(\beta_{\ell\ell}(C, t, R)) = 0\) and \(\text{Im}(\gamma_{\ell\ell}(t, R)) \geq 0\), for any \(1 \leq \ell \leq N\). This is a simple consequence of the analysis of scalar equations and the fact that System (30) is diagonal. In the following, we will assume that
\(\alpha_{\ell,\text{Inf}}(C, t) \leq \text{Im}(\alpha_{\ell}(C, t)) \leq \alpha_{\ell,\text{Sup}}(C, t) < 0\), as well as \(\text{Im}(\gamma_{\ell}(t, \cdot)) > \gamma_{\ell,\text{Inf}}(t)\) for any \(1 \leq \ell \leq N\). We will also denote \(\{R_j\}_{j \in \mathbb{Z}}\) a sequence of gridpoints in \(\mathbb{R}^*_+,\) and discrete times \(t_{n+1} = t_n + \Delta t_{n+1}\). We also set \(\alpha^n_0 = \alpha(C^{n-1}, t_n, R_j)\), \(\beta^n_0 = \beta(C^{n-1}, t_n, R_j)\), \(\gamma^n_0 = \gamma(t_n, R_j)\), \(\zeta^n_j = \zeta(t_n, R_j)\), and \(C^n_j\) an approximation of \(C(t_n, R_j)\), and \(C\) is assumed smooth. In the following, we denote

\[
\begin{align*}
\text{Im}(\alpha^{n+1}_{\ell_{i,j}}) & \leq \mathcal{I}_{\alpha_{\ell,\text{Sup}}}^{n+1} := \sup_{j \in \mathbb{Z}} \text{Im}(\alpha^{n+1}_{\ell_{i,j}}) < 0, \\
\text{Im}(\gamma^{n+1}_{\ell_{i,j}}) & \geq \mathcal{I}_{\gamma_{\ell,\text{Inf}}}^{n+1} := \sup_{j \in \mathbb{Z}} \text{Im}(\gamma^{n+1}_{\ell_{i,j}}) > 0, \\
\mathcal{R}\beta^{n+1}_{\ell_{i,j}} & = \sup_{j \in \mathbb{Z}} \text{Re}(\beta^{n+1}_{\ell_{i,j}}),
\end{align*}
\]

where for instance \(\alpha^{n+1}_{\ell_{i,j}} = (\alpha^{n+1}_{i,j})_{\ell_{i,j}}\). In the following, we denote:

\[
\|C^n\|_h = \left( \sum_{\ell=1}^N |C^n_\ell|^2 \right)^{1/2} = \left( \Delta R \sum_{\ell=1}^N \sum_{j \in \mathbb{Z}} |C^n_{\ell,j}|^2 \right)^{1/2},
\]

where \(C^n_{\ell,j}\) is the \(j\)th component of \(C^n\) and \(C_\ell\) is the \(\ell\)th components of \(C\). The \(\ell^2\)-inner product of \(V, W\) in \(\mathbb{C}^N\) as

\[
W^\dagger V = \langle V, W \rangle_{\ell^2(\mathbb{C}^N)} = \sum_{\ell=1}^N V_\ell W_\ell.
\]

Moreover for any diagonal matrix \(M \in \mathbb{C}^{N \times N}\)

\[
W^\dagger VM = \langle MV, W \rangle_{\ell^2(\mathbb{C}^N)} = \sum_{\ell=1}^N \sum_{j=1}^N M_\ell \bar{V}_j W_\ell.
\]

We finally denote \(|u|_2\) the \(\ell^2\)-norm in \(\mathbb{C}^N\). We have

**Theorem 3.1** Assume that \(\|C^0\|_h < +\infty\). Denoting \(t_{n+} = t_n + \Delta t_{n+1}\), we consider the (low-order) semi-implicit splitting scheme

\[
\begin{align*}
C^n_j & = C^n_j + \Delta t_{n+1} \text{Im}(\beta^n_{\ell_{i,j}}) \frac{C^n_{j+1} - C^n_{j-1}}{2\Delta R} - \Delta t_{n+1} \text{Im}(\beta^n_{\ell_{i,j}}) \frac{C^n_{j+1} - C^n_{j-1}}{2\Delta R} - \Delta t_{n+1} \text{Im}(\beta^n_{\ell_{i,j}}) \frac{C^n_{j+1} - C^n_{j-1}}{2\Delta R} \\
C^n_{j+1} & = C^n_j - \Delta t_{n+1} \text{Im}(\alpha^n_{\ell_{i,j}}) \frac{C^n_{j+1} - C^n_{j-1}}{\Delta R^2} - \Delta t_{n+1} \text{Im}(\alpha^n_{\ell_{i,j}}) \frac{C^n_{j+1} - C^n_{j-1}}{\Delta R^2} - \Delta t_{n+1} \text{Im}(\alpha^n_{\ell_{i,j}}) \frac{C^n_{j+1} - C^n_{j-1}}{\Delta R^2},
\end{align*}
\]

approximating (30) where \(\alpha, \beta \in C^1_0(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}_+; \mathbb{C}^{N \times N})\), \(\zeta \in C^1_0(\mathbb{R} \times \mathbb{R}_+; \mathbb{R}^{N \times N})\), and \(\gamma \in C^1_0(\mathbb{R} \times \mathbb{R}_+; i\mathbb{R}^{N \times N})\). We have the following properties.

(i) Assume that i) \(\mathcal{I}_{\alpha_{\ell,\text{Inf}}}(C, t) \leq \text{Im}(\alpha_{\ell}(C, t)) \leq \mathcal{I}_{\alpha_{\ell,\text{Sup}}}(C, t) \leq C < +\infty\) and \(C > 0\), for all \(t > 0\) and for all \(1 \leq \ell \leq N\), and that ii) \(\gamma\) is time-dependent only, and is such that for all \(n \in \mathbb{N}\)

\[
\mathcal{I}_{\gamma^{n+1}_{\ell,\text{Sup}}} \geq \frac{\mathcal{R}\beta^{n+1}_{\ell_{i,j}}}{\mathcal{I}_{\alpha^{n+1}_{\ell_{i,j}}}},
\]

where \(\beta^{n+1}_{\ell_{i,j}}\) is the \((\ell, \ell)\)th entry of the matrix \(\beta^{n+1}_{\ell_{i,j}}\). Then the scheme (19) is unconditionally stable.
Moreover are defined as

\[ A^{n+1} C^{n+1} = B^{n+1} C^n, \]
\[ D^{n+1} C^{n+1} = C^n, \]

where the “infinite” matrix \( A^{n+1} = \{A_{i,j}^{n+1}\}_{i,j} \) and \( B^{n+1} = \{B_{i,j}^{n+1}\}_{i,j} \) (in practice they belong to \( C^{(2J+1)N \times (2J+1)N} \) for some \( J \) such that \( \{R_j\}_{0 \leq j \leq J} \) denote the finite set of grid points) are defined as

\[
\begin{align*}
A_{j,j}^{n+1} &= 1 - 2i\Delta t_{n+1} \frac{\zeta_j^{n+1}}{\Delta R^2}, & B_{j,j}^{n+1} &= 1 + 2i\Delta t_{n+1} \frac{\zeta_j^{n+1}}{\Delta R^2}, \\
A_{j,j-1}^{n+1} &= \Delta t_{n+1} \left( \frac{\text{Im} \beta_j^{n+1}}{\Delta R} + i \frac{\zeta_j^{n+1}}{\Delta R^2} \right), & B_{j,j-1}^{n+1} &= -i \Delta t_{n+1} \frac{\zeta_j^{n+1}}{\Delta R^2}, \\
A_{j,j+1}^{n+1} &= -\Delta t_{n+1} \left( \frac{\text{Im} \beta_j^{n+1}}{\Delta R} - i \frac{\zeta_j^{n+1}}{\Delta R^2} \right), & B_{j,j+1}^{n+1} &= -i \Delta t_{n+1} \frac{\zeta_j^{n+1}}{\Delta R^2}.
\end{align*}
\]

Moreover

\[
\begin{align*}
D_{j,j}^{n+1} &= 1 + i\Delta t_{n+1} (\alpha_j^{n+1} - \frac{2\gamma_j^{n+1}}{\Delta R^2}), \\
D_{j,j-1}^{n+1} &= i\Delta t_{n+1} \left( - \frac{\text{Re} (\beta_j^{n+1})}{\Delta R} + \frac{\gamma_j^{n+1}}{\Delta R^2} \right), \\
D_{j,j+1}^{n+1} &= i\Delta t_{n+1} \left( \frac{\text{Re} (\beta_j^{n+1})}{\Delta R} + \frac{\gamma_j^{n+1}}{\Delta R^2} \right), \\
d_j^{n+1} &= (D_{j,j}^{n+1} - 1)/\Delta t_{n+1} = i\left( \alpha_j^{n+1} - \frac{2\gamma_j^{n+1}}{\Delta R^2} \right), \\
e_j^{n+1} &= D_{j,j-1}^{n+1}/\Delta t_{n+1} = i\left( - \frac{\text{Re} (\beta_j^{n+1})}{\Delta R} + \frac{\gamma_j^{n+1}}{\Delta R^2} \right), \\
f_j^{n+1} &= D_{j,j+1}^{n+1}/\Delta t_{n+1} = i\left( \frac{\text{Re} (\beta_j^{n+1})}{\Delta R} + \frac{\gamma_j^{n+1}}{\Delta R^2} \right).
\end{align*}
\]

And, we finally set

\[
\begin{align*}
d_{l,j}^{n+1} &= \left( d_j^{n+1} \right)_{\ell}, \\
e_{l,j}^{n+1} &= \left( e_j^{n+1} \right)_{\ell}, \\
f_{l,j}^{n+1} &= \left( f_j^{n+1} \right)_{\ell}.
\end{align*}
\]

The first part of the scheme is standard (Crank-Nicolson for the Schrödinger part, and implicit scheme for the (real) transport term [7]), for any \( \Delta t_{n+1} > 0 \),

\[ \|C^n\|_h \leq \|C^n\|_h. \]

However, the other part of the scheme is less standard and requires a special care on the choice of \( \gamma \) (which is a free function). In order to study the stability of the second part of the scheme, we multiply the scheme by \( (C_j^{n+1})^\dagger \), and we get

\[
\Delta R \sum_{j \in \mathbb{Z}} C_j^{n+1} (C_j^{n+1})^\dagger = \Delta R \sum_{j \in \mathbb{Z}} D_{j,j}^{n+1} (C_j^{n+1})^2 + D_{j,j-1}^{n+1} (C_{j-1}^{n+1})^\dagger + D_{j,j+1}^{n+1} (C_{j+1}^{n+1})^\dagger.
\]
so that
\[
\|C^{n+1}\|_h^2 = -\Delta t_{n+1}\Delta R \sum_{j \in \mathbb{Z}} \text{Re}(d_j^{n+1}C_j^{n+1}C_j^{n+1}) + 2\Re(e_j^{n+1}C_j^{n+1}C_j^{n+1}) + \Delta R \sum_{j \in \mathbb{Z}} \text{Re}(f_j^{n+1}C_j^{n+1}C_j^{n+1}),
\]
(21)
and by Cauchy Schwarz
\[
\|C^{n+1}\|_h^2 \leq \|C^n\|_h\|C^{n+1}\|_h \\
\leq \Delta t_{n+1}(\|d^{n+1}\|_\infty + \|e^{n+1}\|_\infty + \|f^{n+1}\|_\infty)\|C^{n+1}\|_h + \|C^n\|_h\|C^{n+1}\|_h,
\]
where we have denoted for any matrix sequence \(\{M_j\}_{j \in \mathbb{Z}} \in \mathbb{C}^{N \times N}:
\[
\|M\|_\infty = \sup_{j \in \mathbb{Z}} \max_{1 \leq \ell \leq N} \|M_j\|_{\ell \ell}.
\]
However the last inequality does not allow to prove the stability of the scheme. As a consequence, we have to go back to (21). We next focus on the first statement of the proposition.

Proof of Statement 1. We notice that
\[
\|C^{n+1}\|_h^2 = -\Delta t_{n+1}\Delta R \sum_{j \in \mathbb{Z}} \text{Re}(d_j^{n+1}C_j^{n+1}C_j^{n+1}) + 2\Re(e_j^{n+1}C_j^{n+1}C_j^{n+1}) + \Delta R \sum_{j \in \mathbb{Z}} \text{Re}(f_j^{n+1}C_j^{n+1}C_j^{n+1}).
\]
(22)
Thus
\[
\|C^{n+1}\|_h^2 \leq \|C^n\|_h\|C^{n+1}\|_h + \Delta t_{n+1}\Delta R \sum_{j \in \mathbb{Z}} \sum_{\ell = 1}^N \text{Im}(\alpha_{\ell j}^{n+1} - \frac{2\gamma_{\ell j}^{n+1}}{\Delta R^2})|C_{\ell j}^{n+1}|^2 \\
+ \text{Im}(\frac{\gamma_{\ell j}^{n+1}}{\Delta R^2}(C_{\ell j}^{n+1}C_{\ell j}^{n+1} + C_{\ell j}^{n+1}C_{\ell j}^{n+1})) \\
+ \text{Im}(\frac{\text{Re}(\beta_{\ell j}^{n+1})}{\Delta R}(C_{\ell j}^{n+1}C_{\ell j}^{n+1} - C_{\ell j}^{n+1}C_{\ell j}^{n+1})).
\]
\[
\leq \|C^n\|_h\|C^{n+1}\|_h + \Delta t_{n+1}\Delta R \sum_{j \in \mathbb{Z}} \sum_{\ell = 1}^N \text{Im}(\alpha_{\ell j}^{n+1} - \frac{2\gamma_{\ell j}^{n+1}}{\Delta R^2})|C_{\ell j}^{n+1}|^2 \\
+ \frac{\text{Im}(\gamma_{\ell j}^{n+1})}{\Delta R^2} \text{Re}(C_{\ell j}^{n+1}C_{\ell j}^{n+1} + C_{\ell j}^{n+1}C_{\ell j}^{n+1}) \\
+ \frac{\text{Re}(\beta_{\ell j}^{n+1})}{\Delta R} \text{Im}(C_{\ell j}^{n+1}C_{\ell j}^{n+1} - C_{\ell j}^{n+1}C_{\ell j}^{n+1}).
\]
For smooth solutions \(C\), where \(C_j^n = C(t_n, R_j)\), we set
\[
C_{j+1,\ell}^{n+1} := C_{\ell j}^{n+1} \pm \Delta R \partial_R C_{\ell j}^{n+1} + \Delta R^2 \partial_R^2 C_{\ell j}^{n+1}/2 \pm O(\Delta R^3),
\]
then
\[
\|C^{n+1}\|_h^2 \leq \|C^n\|_h\|C^{n+1}\|_h + \Delta t_{n+1}\Delta R \sum_{j \in \mathbb{Z}} \sum_{\ell = 1}^N \text{Im}(\alpha_{\ell j}^{n+1} - \frac{2\gamma_{\ell j}^{n+1}}{\Delta R^2})|C_{\ell j}^{n+1}|^2 \\
+ \frac{2\text{Im}(\gamma_{\ell j}^{n+1})}{\Delta R^2}(|C_{\ell j}^{n+1}|^2 + \Delta R^2 \text{Re}(\partial_R^2 C_{\ell j}^{n+1}C_{\ell j}^{n+1}/2 + O(\Delta R^4)) \\
- \frac{2\text{Re}(\beta_{\ell j}^{n+1})}{\Delta R} \text{Im}(\partial_R C_{\ell j}^{n+1}C_{\ell j}^{n+1} + O(\Delta R^2)) \\
\leq \|C^n\|_h\|C^{n+1}\|_h + \Delta t_{n+1}\Delta R \sum_{j \in \mathbb{Z}} \sum_{\ell = 1}^N \text{Im}(\alpha_{\ell j}^{n+1})|C_{\ell j}^{n+1}|^2 \\
+ \frac{\text{Im}(\gamma_{\ell j}^{n+1})}{\Delta R^2} \text{Re}(\partial_R^2 C_{\ell j}^{n+1}C_{\ell j}^{n+1} + O(\Delta R^2)) \\
- \frac{2\text{Re}(\beta_{\ell j}^{n+1})}{\Delta R} \text{Im}(\partial_R C_{\ell j}^{n+1}C_{\ell j}^{n+1} + O(\Delta R^2)).
\]
By integration by parts, we get
\[
\|C^{n+1}\|_{h}^{2} \leq \|C^{n}\|_{h} \|C^{n+1}\|_{h} + \Delta t_{n+1} \Delta R \sum_{j \in \mathbb{Z}} \sum_{\ell=1}^{N} \text{Im}(\alpha_{\ell,j}^{n+1}) |C_{\ell,j}^{n+1}|^{2} + O(\Delta R^{2})
\]
\[-\text{Im}(\alpha_{\ell,j}^{n+1}) \partial_{R}C_{\ell,j}^{n+1} |^{2} - \text{Im}(\partial_{R}C_{\ell,j}^{n+1}) |^{2} + 2 \text{Re}(\beta_{\ell,j}^{n+1}) \partial_{R}C_{\ell,j}^{n+1} |^{2} \).

As
\[
\text{Im}(\alpha_{\ell,j}^{n+1}) \leq \sup_{j \in \mathbb{Z}} \text{Im}(\alpha_{\ell,j}^{n+1}), \quad \text{Im}(\gamma_{\ell,j}^{n+1}) \geq I_{\gamma_{\ell,j}^{n+1}} > 0,
\]
we get
\[
\|C^{n+1}\|_{h}^{2} \leq \|C^{n}\|_{h} \|C^{n+1}\|_{h} + \Delta t_{n+1} \sum_{\ell=1}^{N} \left( I_{\alpha_{\ell,j}^{n+1}} \|C^{n+1}\|_{h} - I_{\gamma_{\ell,j}^{n+1}} \|\partial_{R}C^{n+1}\|_{h} \right)
\]- \sup_{j \in \mathbb{Z}} \text{Im}(\partial_{R}C_{\ell,j}^{n+1}) \text{Re}(\partial_{R}C_{\ell,j}^{n+1} |C_{\ell,j}^{n+1}|^{2}) + 2 \text{Re}(\beta_{\ell,j}^{n+1}) \partial_{R}C_{\ell,j}^{n+1} |^{2}
\|C^{n+1}\|_{h} + O(\Delta R^{2})
\].

Now we have to prove that overall \(\|C^{n+1}\|_{h} \leq \|C^{n}\|_{h}\). Unlike the coefficient \(\alpha\) which is purely physical, \(\gamma\) is a free matrix-valued function which is designed to stabilize the scheme. We set \(\eta_{\ell}^{n+1} > 0\) such that \(0 < \eta_{\ell}^{n+1} |\mathcal{R}_{\ell,j}^{n+1}| < -I_{\alpha_{\ell,j}^{n+1}}\), so that
\[
I_{\alpha_{\ell,j}^{n+1}} |C_{\ell,j}^{n+1}|^{2} + 2 |\mathcal{R}_{\ell,j}^{n+1}| |\partial_{R}C_{\ell,j}^{n+1}| C_{\ell,j}^{n+1} |h| \leq \left( I_{\alpha_{\ell,j}^{n+1}} + \eta_{\ell}^{n+1} |\mathcal{R}_{\ell,j}^{n+1}| \right) |C_{\ell,j}^{n+1}|^{2}
\] \[+ \frac{|\mathcal{R}_{\ell,j}^{n+1}|}{\eta_{\ell}^{n+1}} |\partial_{R}C_{\ell,j}^{n+1}|^{2}.
\]

So far, we have proven that
\[
\|C^{n+1}\|_{h}^{2} \leq \|C^{n}\|_{h} \|C^{n+1}\|_{h} + \Delta t_{n+1} \sum_{\ell=1}^{N} \left( \frac{|\mathcal{R}_{\ell,j}^{n+1}|}{\eta_{\ell}^{n+1}} + I_{\gamma_{\ell,j}^{n+1}} \right) |\partial_{R}C_{\ell,j}^{n+1}|^{2}
\] \[+ \Delta t_{n+1} |\partial_{R}C_{\ell,j}^{n+1}| |\partial_{R}C_{\ell,j}^{n+1}| C_{\ell,j}^{n+1} |h| + O(\Delta R^{2})
\].

Now, we can select \(\gamma\) accordingly, that is such that
\[
\frac{|\mathcal{R}_{\ell,j}^{n+1}|}{\eta_{\ell}^{n+1}} - I_{\gamma_{\ell,j}^{n+1}} < 0.
\]
As \(\eta_{\ell}^{n+1} < -I_{\alpha_{\ell,j}^{n+1}} / |\mathcal{R}_{\ell,j}^{n+1}|\), this corresponds to take \(\gamma\) such that
\[
I_{\gamma_{\ell,j}^{n+1}} > -\frac{|\mathcal{R}_{\ell,j}^{n+1}|^{2}}{I_{\alpha_{\ell,j}^{n+1}}}.
\]
In addition, we need to control the \(|\partial_{R}C_{\ell,j}^{n+1}|^{2}\) term. A natural choice is to take \(\gamma\)-space dependent, which allows for removing this contribution. As a consequence, if \(\gamma\) is time-dependent only, and is such that
\[
I_{\gamma_{\ell,j}^{n+1}} > -\frac{|\mathcal{R}_{\ell,j}^{n+1}|^{2}}{I_{\alpha_{\ell,j}^{n+1}}}.
\]
Then \( \| C^{n+1} \|_h^2 \leq \| C^n \|_h^2 \), and as a consequence, for any \( \Delta t_{n+1} > 0 \), the scheme (19) is unconditionally \( \ell^2 \)-stable, that is by induction

\[
\| C^{n+1} \|_h^2 \leq \| C^n \|_h \leq \cdots \leq \| C^0 \|_h.
\]

This concludes the proof of the first statement of the theorem. Let us now focus on the second statement.

Proof of Statement 2. We naturally have \( \| C^n \|_h = \| C^n \|_h \), and also for \( \text{Im} \beta \) and \( \zeta \) constant: \( \| C^n \|_h = \| C^n \|_h \). Let us focus, on the second part of the scheme. We multiply the scheme by \( (C_j^n)^t \), sum over \( Z \), and take the real part. As \( \text{Re}(d_j) = 0 \), this leads to

\[
\Delta R \sum_{j \in Z} \sum_{\ell = 1}^N \text{Re}(C_{t_j}^\ell C_{t_j}^{n+1}) = -\Delta t_{n+1} \sum_{j \in Z} \sum_{\ell=1}^N \text{Re}(\beta_{t_{\ell j}}^{n+1}) \text{Im}(C_{t_{\ell j}}^{n+1} C_{t_{\ell j}}^n - C_{t_{\ell j}}^{n+1} C_{t_{\ell j}}^n) + \| C^n \|_h^2
\]

By Cauchy Schwarz, we get

\[
\| C^n \|_h \| C^{n+1} \|_h \geq \Delta t_{n+1} \Delta R \sum_{j \in Z} \sum_{\ell=1}^N | \text{Re}(\beta_{t_{\ell j}}^{n+1}) \text{Im}(\partial_R C_{t_{\ell j}}^{n+1} C_{t_{\ell j}}^n) | + \| C^n \|_h^2
\]

so that

\[
\| C^{n+1} \|_h^2 > \| C^n \|_h^2,
\]

as \( \text{Re}(\beta) \neq 0 \). This concludes the proof. \( \square \)

In fact the condition on \( \text{Im} \alpha \) can be relaxed, and we get the following corollary, if we consider the IVP for \( t \in [0, T] \).

**Corollary 3.1** Assume that \( \| C^0 \|_h < +\infty \). We consider the (low-order) semi-implicit splitting scheme (19) approximating (30), for \( t \in [0, T] \) with \( T = \sum_{n=1}^N \Delta t_n \), and where \( \alpha, \beta \in C_0^1(\mathbb{C}^N \times \mathbb{R} \times [0, T]; \mathbb{C}^N \times \mathbb{N}), \) \( \zeta \in C_0^1(\mathbb{R} \times [0, T]; \mathbb{R}^N \times \mathbb{R}^N), \) and \( \gamma \in C_0^1(\mathbb{R} \times [0, T]; i\mathbb{R}^N \times \mathbb{R}^N) \). Assume that:

- there exists \( M > 0 \), such that \( \mathcal{I} \alpha_{t, \text{inf}}(C, t) \leq \text{Im}(\alpha_{t}(C, t, \cdot)) \leq \mathcal{I} \alpha_{t, \text{sup}}(C, t) \leq M \) for all \( t > 0 \) and for all \( 1 \leq \ell \leq N \),
- \( \gamma \) is time-dependent only, and is such that for all \( n \in \mathbb{N} \)

\[
\mathcal{I} \gamma_{t_{\ell j}}^{n+1} \geq \frac{|\mathcal{R} \gamma_{t_{\ell j}}^{n+1}|^2}{|\mathcal{I} \alpha_{t_{\ell j}}^{n+1}|}.
\]

Then the scheme (19) is unconditionally stable.

**Proof.** The proof is identical to Proposition 3.1, except that we now prove that there exists a constant \( C_1 = C_1(M) \), such that for \( N \) such that \( \sum_{n=1}^N \Delta t_n = T < +\infty \):

\[
\| C^{n+1} \|_h \leq \| C^n \|_h (1 + C_1 \Delta t_{n+1})
\]
Then using a discrete Gronwall inequality, there exists $C_2(M,T) > 0$ such that for all $n \leq N$
\[ \|C_{n+1}\|_h \leq \|C_0\|_h e^{C_2 T}. \]
This concludes the proof. □

From a practical point of view, we then have to add a matrix $\gamma$ such that (23) in order to stabilize the scheme.

3.2. Masking $Re(\nabla \chi/\chi)$ and $Im(\alpha_{\ell \ell}) > 0$

A simple alternative to the stabilization approach is, as suggested in [6], to cancel the real part of $Re(\nabla \chi/\chi)$ and potentially $Im(\alpha)$ which are responsible for the instability of the scheme, and the ill-posedness of the model. Starting from
\[ i\partial_t C = \alpha(C,t,R)C + \beta(C,t,R)\nabla R C + \zeta(t,R)\nabla^2 R C \]
we set $\tilde{\beta} \in C^1(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}^+; i\mathbb{R}^{N \times N})$ and $\tilde{\alpha} \in C^1(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}^+; \mathbb{R}^{N \times N})$ such that, for all $\ell \in \{1, \ldots, N\}$
\[ \tilde{\beta}(C,t,R) := i \text{Im}(\beta)(C,t,R), \quad \alpha_{\ell \ell}(C,t,R) := \begin{cases} \tilde{\alpha}_{\ell \ell}(C,t,R), & \text{if } \text{Im}(\alpha_{\ell \ell})(C,t,R) \leq 0 \\ \text{Re}(\alpha_{\ell \ell}(C,t,R)), & \text{if } \text{Im}(\alpha_{\ell \ell})(C,t,R) > 0. \end{cases} \]

We then consider the following system
\[ i\partial_t C = \tilde{\alpha}(C,t,R)C + \tilde{\beta}(C,t,R)\nabla R C + \zeta(t,R)\nabla^2 R C. \] (25)

In this case, it is no more necessary to introduce an artificial diffusion. In fact, using standard analysis, we can prove:

**Proposition 3.1** Assume that $\|C_0\|_h < +\infty$. We deduce that stability of the following schemes approximating (25) respectively on $\mathbb{R}^+ \times \mathbb{R}$ and $[0,T] \times \mathbb{R}$.

(i) Denoting $\tilde{\alpha}^n_j = \tilde{\alpha}(C^{-1},t_n,R_j), \quad \tilde{\beta}^n_j = \tilde{\beta}(C^{-1},t_n,R_j)$, the following semi-implicit scheme:
\[ C_{j+1}^{n+1} = C_j^n + \Delta t_{n+1}\tilde{\alpha}^n_j \frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2\Delta R} - \Delta t_{n+1}i\tilde{\beta}^n_j \frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2\Delta R^2}, \]
\[ -\Delta t_{n+1}i\tilde{\beta}^n_j \frac{C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}}{2\Delta R^2} - \Delta t_{n+1}i\tilde{\zeta}^n_j \frac{C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}}{2\Delta R^2}, \]
approximating (25) on $\mathbb{R}^+ \times \mathbb{R}$, where $\tilde{\alpha} \in C_0^1(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}^+; \mathbb{C}^{N \times N}), \tilde{\beta} \in C_0^1(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}^+; \mathbb{R}^{N \times N}), \tilde{\zeta} \in C_0^1(\mathbb{R} \times \mathbb{R}^+; \mathbb{R}^{N \times N})$ is unconditionally stable. However (26) is consistent with (25), but not with (24) in general.

(ii) Moreover, the following semi-implicit scheme:
\[ C_{j+1}^{n+1} = C_j^n + \Delta t_{n+1}\tilde{\alpha}^n_j \frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2\Delta R} - \Delta t_{n+1}i\tilde{\beta}^n_j \frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2\Delta R^2}, \]
\[ -\Delta t_{n+1}i\tilde{\beta}^n_j \frac{C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}}{2\Delta R^2} - \Delta t_{n+1}i\tilde{\zeta}^n_j \frac{C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}}{2\Delta R^2}, \] (27)
approximating (25) on $[0, T] \times \mathbb{R}$, with $T < \infty$, where $\alpha \in C^1_0(\mathbb{C}^N \times \mathbb{R} \times [0, T]; \mathbb{C}^{N \times N})$, $
abla \beta \in C^1_0(\mathbb{C}^N \times \mathbb{R} \times [0, T]; \mathbb{R}^{N \times N})$, $\zeta \in C^1_0(\mathbb{R} \times [0, T]; \mathbb{R}^{N \times N})$ is unconditionally stable. However (27) is consistent with (25), but not with (24) in general.

Sketch of the proof. We do not detail the proof as it is based on same technique as above, where however it is no more necessary to control the real part of $\nabla \beta$ which is null. Basically we multiply by $C^{n+1}_j$ and we sum over $\mathbb{Z}$. As i) the kinetic operator is approximated by a Crank-Nicolson scheme, ii) the transport operator is implicated, iii) the reaction algebraic operator ($\alpha$-based) is such that $\text{Im}(\alpha_{\ell \ell}) \leq 0$ for all $\ell \in \{1, \cdots, N\}$, we show by standard energy method that $\|C^{n+1}_j\|_h \leq \|C^n_j\|_h$. □

3.3. About the consistency of the “masked” semi-implicit scheme.

Masking the sources of instability also modifies the equivalent equation, and more generally impacts the consistency of the scheme. In order to maintain the consistency of the scheme, while maintaining (to a certain extent....) its stability, we proceed as in [6]. In order to solve (24), we split the equation as follows from any time $t_n$ to $t_{n+1} = t_n + \Delta t_{n+1}$ and we also denote $t_{n^*} = t_n + \Delta t_{n+1}$, $t_{n^{**}} = t_n + 2\Delta t_{n+1}$: a first order splitting reads (higher order splitting methods can easily be derived)

$$
\begin{cases}
\quad i \partial_t C = \tilde{\alpha}(C^n, t, R) C + \nabla R C + \zeta(t, R) \nabla^2 R C, \quad C(t_n, \cdot) = C^n, \quad t \in [t_n, t_{n^*}], \\
\quad i \partial_t C = (\alpha(C^n, t, R) - \tilde{\alpha}(C^n, t, R)) C, \quad C(t_{n^*}, \cdot) = C^{n^*}, \quad t \in [t_n, t_{n^{**}}], \\
\quad i \partial_t C = (\beta(C^n, t, R) - \tilde{\beta}(C^n, t, R)) \nabla R C, \quad C(t_{n^{**}}, \cdot) = C^{n^{**}}, \quad t \in [t_n, t_{n+1}].
\end{cases}
$$

As the matrices $\alpha$, $\tilde{\alpha}$ are diagonal, we formally have for all $\ell \in \{1, \cdots, N\}$ :

$$
C^{n^{**}} = \exp \left( \int_{t_n}^{t_{n^{**}}} \text{Im}(\alpha(C^n, s, R)) \frac{1 - \text{sign}(\text{Im}(\alpha(C^n, s, R)))}{2\Delta t_{n^*}} \text{ds} \right) C^{n^*}.
$$

Notice that there exists $C > 0$

$$
\|C^{n^{**}}\|_h \leq \|C^n\|_h (1 + C\Delta t_{n+1}).
$$

The last equation reads

$$
\partial_t C = -i \text{Re}(\beta(C^n, t, R)) \nabla R C, \quad C(t_n, \cdot) = C^{n^{**}}, \quad t \in [t_n, t_{n+1}].
$$

This equation is ill-posed. However, we can approximate it as follows (on an infinite domain), the equation formally reads

$$
\partial_t C = \text{Re}(\beta(C^n, t, R))[\nabla R]C, \quad C(t_n, \cdot) = C^{n^{**}}, \quad t \in [t_n, t_{n+1}],
$$

where

$$
[\nabla R]C = F_R^{-1}(i\xi R F_R(C(\xi))) , \quad (28)
$$
and where $\mathcal{F}_R$ (resp. $\mathcal{F}_R^{-1}$) denotes the Fourier transform (resp. inverse Fourier transform). Formula (28) is nothing by the pseudodifferential or symbolic representation of the operator $\nabla_R$. We then formally rewrite

$$C^{n+1} = \exp \left( \int_{t_n}^{t_{n+1}} \text{Re}(\beta(C^n, t, R))[[\nabla_R]] \right) C^{n*}.$$  

In practice the operator $[[\cdot]]$ is computed using the Fast Fourier Transform. Notice that if $\text{Re}\beta = 0$, then for $t \in [0, T]$, and $T = \sum_{n=1}^N \Delta t_n$, there exists $C(T) > 0$

$$\|C^{n+1}\|_h \leq \|C^0\|_h (1 + C \Delta t_{n+1})^n,$$

$$\leq \|C^0\|_h e^{CT}.$$  

If $\text{Im}(\alpha_{\ell\ell}) < M < 0$, for any $\ell \in \{1, \cdots, N\}$, the corresponding $\exp(-Mt)$-term, gives some control to find $T^* = T^*(M) < T$, such that

$$\|C^{n+1}\|_h > \|C^{n*}\|_h$$

but

$$\|C^{n+1}\|_h \leq \|C^n\|_h e^{CT^*} \leq \|C^n\|_h e^{CT^*}.$$  

We then have

**Proposition 3.2** Assume that $\|C^0\|_h < +\infty$, then the following scheme :

$$C^n_{\ell} = C^n_{\ell} + \Delta t_{n+1} \frac{\beta^{n+1}_{\ell} C^{n+1}_{\ell} - C^{n+1}_{\ell-1}}{2\Delta R} - \Delta t_{n+1} i\alpha^{n+1}_{\ell} C^{n+1}_{\ell} - \Delta t_{n+1} 2\Delta R^2 \frac{C^{n+1}_{\ell+1} - 2C^{n+1}_{\ell} + C^{n+1}_{\ell-1}}{2\Delta R^2} - \Delta t_{n+1} i\zeta^{n+1}_{\ell} C^{n+1}_{\ell+1} - 2C^{n}_{\ell} + C^{n}_{\ell-1}$$

$$C^{n+1} = \exp \left( \int_{t_n}^{t_{n+1}} \text{Im}(\alpha(s, R)) \frac{1 - \text{sign}(\text{Im}(\alpha(C^n, s, R)))}{2\Delta t_{n+1}} \right.  
+ \text{Re}(\beta(C^n, s, R))[[\nabla_R]] ds \right) C^{n*},$$

is consistent with (24), and $\|C^{n*}\|_h \leq \|C^n\|_h$. Moreover if

- $\text{Re}\beta = 0$ for all $t \in [0, T]$, there exists $C = C(T, M) > 0$ the scheme is unconditionally stable, that is for any $n \leq N$:

$$\|C^n\|_h < \|C^0\|_h e^{CT}.$$  

- If $\text{Im}(\alpha_{\ell\ell}) < M < 0$ for any $\ell \in \{1, \cdots, N\}$, there exists $T^* < T$, such that if $\sum_{n=1}^{N^*} \Delta t_n = T^*$, we have

$$\|C^n\|_h < \|C^0\|_h e^{CT^*}.$$  

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3.4. Non-Diagonal model

In this section, we no more assume that the system is diagonal. This complexifies the analysis of stability as it is no more possible to directly reduce the analysis to scalar problems. However, it is still possible to conclude on the unconditional instability. We set

\[
\begin{align*}
\alpha(C,t,R) &= I \epsilon(t,R) - \epsilon(t,R) I + M(t,R) + \frac{f(C,t,R)}{M_n}, \\
\beta(C,t,R) &= \frac{1}{M_n} \nabla_R \chi (t,R) + D(t,R), \\
\zeta(t,R) &= -\frac{1}{2M_n} I, \\
f(C,t,R) &= \frac{1}{2} (I \nabla_R A(C,t,R) - A^2(C,t,R) I) + i A(C,t,R) I \nabla_R \chi.
\end{align*}
\]

We then define

\[
f(C^n,t_{n+1},R) := \frac{1}{2} (I \nabla_R A(C^n,t_{n+1},R) - A^2(C^n,t_{n+1},R) I) + i A(C^n,t_{n+1},R) I \nabla_R \chi^{n+1},
\]

and consider in the following equation

\[
\mathbf{i} \partial_t \mathbf{C} = \alpha(C,t,R) \mathbf{C} + \beta(C,t,R) \nabla_R \mathbf{C} + \gamma(t,R) \nabla^2_R \mathbf{C} + \zeta(t,R) \nabla^2_R \chi,
\]

with \(\alpha\), and \(\beta\) belong to \(C^1_0(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}_+; \mathbb{C}^{N \times N})\), \(\zeta\) belongs \(C^1_0(\mathbb{R} \times \mathbb{R}_+; \mathbb{R}^{N \times N})\), that is \(\zeta\) (associated to the kinetic operator) is a real-valued function, and \(\gamma \in C^1_0(\mathbb{R} \times \mathbb{R}_+; i \mathbb{R}^{N \times N})\). The main difference with the diagonal case is that \(M\) and \(D\) are non-diagonal matrices. As in the non-diagonal, we have

**Proposition 3.3** Denoting \(t_{n \ast} = t_n + \Delta t_{n+1}\), we consider the (low-order) semi-implicit splitting scheme (19), approximating (30) where \(\alpha, \beta \in C^1_0(\mathbb{C}^N \times \mathbb{R} \times \mathbb{R}_+; \mathbb{C}^{N \times N})\), \(\zeta \in C^1_0(\mathbb{R} \times \mathbb{R}_+; \mathbb{R}^{N \times N})\), and \(\gamma \in C^1_0(\mathbb{R} \times \mathbb{R}_+; i \mathbb{R}^{N \times N})\). Assume that i) \(||C^0||_h < +\infty\), ii) \(\text{Im}(\alpha(t,C,t,R)) = 0\) for all \(t > 0\) and that iii) \(\gamma\) is identically null, then the scheme (19) is unconditionally unstable.

4. Conclusion

In this paper, we have proposed a mathematical analysis of toy-models derived from the conditional equation within the Exact Factorization of the time-dependent Schrödinger equation. We have exhibited some mathematical issues in this equation, and proposed some cures to fix them. The analysis was combined with the numerical analysis of basic numerical approximation schemes. In a more general framework (multidimensional and nonlinear), we have then derived and analyzed a stable numerical scheme which is a good candidate for approximating the full conditional equation (1) and (3). We below list some important properties of the schemes developed above.
• The schemes derived above are low-order in space and time. Basically, it can be shown [10] that the spatial discretization of the kinetic operator is first order accurate (except when the coefficients are constant, it is then second-order), as well as the transport operator. Overall, the time discretization is first order accurate. With such low order schemes, it is necessary to use very small spatial and time (when stability allows...) step discretizations.

• The equivalent equation of the scheme contains a diffusion term $\gamma \Delta C$ which overall, at least partially, stabilizes the scheme but also regularizes the solution.

• Although, the system is nonlinear (quasilinear) using semi-implicit schemes allow for “locally” linearize in time.

• Other possible sources of instability: whenever $\text{Im}(\alpha_{ell}) \geq 0$, the above schemes are unstable, as the equation is ill-posed (instability of the solution with respect with the initial data).

• In order to stabilize the scheme, the strategy developed in Section 3.1 can then be explored.

In forthcoming paper, we will propose some realistic simulations with the full EF model.

References