

Semidiscretization in time for nonlinear Schrödinger-waves equations

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Abstract: In this paper, we are concerned with Crank-Nicolson like schemes for:

$$(NLW_\omega) \quad \frac{1}{\omega^2} \partial_t^2 E_\omega - i \partial_t E_\omega - \Delta E_\omega = \lambda |E_\omega|^{2\sigma} E_\omega.$$

We present two schemes for which we give some convergence results. One of the scheme is dissipative and we describe precisely the dissipation. We prove that the solution of the second scheme fits that of (NLW_ω) while the first one compute a average value of the solution.

Key words: Wave equation, Schrödinger Equation, Crank-Nicolson schemes, oscillations.

1 Introduction.

1.1 Setting of the problem.

The aim of this paper is to discuss the behaviour of two schemes for the time-envelope approximation in plasma physics studied in [3]. Let us first recall what is the time-envelope approximation in plasma Physics. In a plasma medium, the electrostatic field E satisfies the following wave equation:

$$\partial_t^2 E + \omega_{pe}^2 E - 3v_{th}^2 \Delta E = \omega_{pe}^2 \frac{\varepsilon_0}{N_0 T_e} |E|^2 E,$$

where ω_{pe} is the electronic plasma pulsation, v_{th} is the thermal velocity of the electrons and ε_0 is the dielectric constant of vacuum. The constants N_0 and T_e are respectively the average density of ions and the electronic temperature. This approximation is valid in the static limit for ions see [7]. Due to the size of the coefficients, solutions to this equation are highly oscillatory and are known as Langmuir waves. Mathematically, these oscillations can be described through the change of function:

$$E(x, t) = \text{Re}(E_{\omega_{pe}} e^{-i\omega_{pe} t}).$$

This leads to the following equation on $E_{\omega_{pe}}$:

$$\partial_t^2 E_{\omega_{pe}} - 2i\omega_{pe} \partial_t E_{\omega_{pe}} - 3v_{th}^2 \Delta E_{\omega_{pe}} = \omega_{pe}^2 \frac{\varepsilon_0}{N_0 T_e} |E_{\omega_{pe}}|^2 E_{\omega_{pe}}.$$

The function $E_{\omega_{pe}}$ is supposed to be the slowly varying part of the electric field. Precisely, in physical text, the assumption that is made is $\partial_t E_{\omega_{pe}} \ll \omega_{pe} E_{\omega_{pe}}$.

After rescaling, this approximation can be shown to be equivalent to perform the limit $\omega \rightarrow \infty$ in [3]:

$$\frac{1}{\omega^2} \partial_t^2 E_\omega - i \partial_t E_\omega - \Delta E_\omega = |E_\omega|^2 E_\omega.$$

We study in fact the more general equation:

$$(NLW_\omega) \quad \frac{1}{\omega^2} \partial_t^2 E_\omega - i \partial_t E_\omega - \Delta E_\omega = \lambda |E_\omega|^{2\sigma} E_\omega.$$

In [3], it is shown that for any initial data $(E_0, E_1) \in H^2(\mathbb{R}^d) \times H^1(\mathbb{R}^d)$ for $d \leq 3$, there exists a unique solution to (NLW_ω) on a maximal existence time $[0, T_\omega[$. Moreover, if E denotes the maximal solution to the nonlinear Schrödinger equation with initial data E_0 defined on $[0, T_0[$:

$$(NLS) \quad -i \partial_t E - \Delta E = \lambda |E|^{2\sigma} E,$$

then on one hand,

$$\liminf_{\omega \rightarrow +\infty} T_\omega \geq T_0,$$

and on the other hand, for any $T < T_0$, E_ω converges to E on $[0, T]$ in $\mathcal{C}([0, T]; H^2)$ while $\partial_t E_\omega$ oscillates at frequency ω^2 around the value $\partial_t E$, except in the compatible case, that is when $E_1 = i(\Delta E_0 + \lambda |E_0|^{2\sigma} E_0)$. In the non-compatible case, $E_\omega - E$ oscillates at frequency ω^2 and these oscillations are of order of magnitude $1/\omega^2$. It follows that the oscillatory part of the solution is physically relevant since it describes the second order term of the solution to (NLW_ω) . It is therefore interesting to compute both the average and the oscillatory parts of the solution. The aim of this paper is to study two kinds of time-discretization to bring to the fore the behavior of the oscillatory and the average parts.

These phenomena can be more easily observed through the following splitting introduced in [2]. Let $E_\omega = F + G$ where the functions F and G are solution to:

$$\begin{cases} \partial_t F = \frac{i\omega^2}{2} \left(1 - \sqrt{1 - \frac{4\Delta}{\omega^2}}\right) F - \frac{1}{i} \left(\sqrt{1 - \frac{4\Delta}{\omega^2}}\right)^{-1} (\lambda |F + G|^{2\sigma} (F + G)) \\ \partial_t G = \frac{i\omega^2}{2} \left(1 + \sqrt{1 - \frac{4\Delta}{\omega^2}}\right) G + \frac{1}{i} \left(\sqrt{1 - \frac{4\Delta}{\omega^2}}\right)^{-1} (\lambda |F + G|^{2\sigma} (F + G)) \end{cases}$$

The initial data for F and G are recovered from E_0 and E_1 (see [2] for details). It is clear on this splitting that F converges to E while G is the oscillatory part of E_ω .

The aim of this paper is to propose some schemes in order to investigate numerically the preceding approximation. We study two schemes of Crank-Nicolson type for (NLW_ω) using this splitting for the associated discrete operators.

1.2 Description of the schemes.

The Crank-Nicolson scheme for (NLS) seems to have been introduced for the first time in [5], while the first results of existence and convergence can be found in [8]. More precised results are given in [1]. All these results are obtained through energy estimates. We will present in next section existence and convergence results for (NLS) using a discrete Duhamel formulation. This formulation allowed us to obtain more precise uniqueness results for the discret problem than in [1] and is well fitted for (NLW_ω) . However, this formulation does not give that the Crank-Nicolson scheme is of second order [1].

The Crank-Nicolson scheme for (NLS) :

$$iu_t + \Delta u = -\lambda |u|^{2\sigma} u, \quad u(x; 0) = u_0(x)$$

reads

$$i \frac{u^{n+1} - u^n}{\delta t} + \frac{1}{2} \Delta(u^{n+1} + u^n) = -\frac{\lambda}{2\sigma + 2} f(u^{n+1}, u^n)(u^{n+1} + u^n),$$

where

$$f(u^{n+1}, u^n) = \frac{|u^{n+1}|^{2\sigma+2} - |u^n|^{2\sigma+2}}{|u^{n+1}|^2 - |u^n|^2}.$$

Analogously, we introduce the two following schemes for (NLW_ω) :

$$(\mathcal{S}_1) \left\{ \begin{array}{l} \frac{1}{\omega^2} \left(\frac{E^{n+1} - 2E^n + E^{n-1}}{\delta t^2} \right) - i \left(\frac{E^{n+1} - E^n}{\delta t} \right) - \frac{1}{2} \Delta(E^{n+1} + E^n) \\ = \frac{\lambda}{2\sigma + 2} \frac{|E^{n+1}|^{2\sigma+2} - |E^n|^{2\sigma+2}}{|E^{n+1}|^2 - |E^n|^2} (E^{n+1} + E^n), \\ E_0 = f, \quad \frac{E^0 - E^{-1}}{\delta t} = g \end{array} \right.$$

and

$$(\mathcal{S}_2) \left\{ \begin{array}{l} \frac{1}{\omega^2} \left(\frac{E^{n+1} - 2E^n + E^{n-1}}{\delta t^2} \right) - i \left(\frac{E^{n+1} - E^{n-1}}{2\delta t} \right) - \frac{1}{2} \Delta(E^{n+1} + E^{n-1}) \\ = \frac{\lambda}{2\sigma + 2} \frac{|E^{n+1}|^{2\sigma+2} - |E^{n-1}|^{2\sigma+2}}{|E^{n+1}|^2 - |E^{n-1}|^2} (E^{n+1} + E^{n-1}), \\ \frac{E_0 + E^{-1}}{2} = f, \quad \frac{E^0 - E^{-1}}{\delta t} = g. \end{array} \right.$$

On one hand, we are able to prove existence, uniqueness and convergence of the discrete sequences E^n for both schemes. There are no conditions on the

relative size of ω and δt for scheme $(\mathcal{S}_2)$ while we need to impose that $\omega^4 \delta t$ is bounded for $(\mathcal{S}_1)$ to derive uniform properties in ω and δt .

On the other hand, one shows that the second schemes is conservative while the first one is dissipative. One of the aim of this paper is to investigate the effect of this dissipation on the discrete solutions; we prove that the discret solution given by $(\mathcal{S}_2)$ behaves like the continuous one, particularly for the oscillatory part (see the numerical experiments at the end of this paper). Moreover the dissipation for $(\mathcal{S}_1)$ is exponentially strong in ω for the oscillatory part of E^n , so that the numerical solution obtained thanks to $(\mathcal{S}_1)$ is the mean value of the solution to (NLW_ω) .

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2 The Crank-Nicolson scheme for the nonlinear Schrödinger equation (NLS) .

The aim of this part is to recall some known results on the Crank-Nicolson scheme for (NLS) and to present the method that we will use to discretize (NLW_ω) .

Let us begin with the inhomogeneous Schrödinger equation:

$$\begin{aligned} iu_t + \Delta u &= f, \\ u(x, 0) &= u_0(x). \end{aligned} \tag{2.1}$$

We will consider the case $x \in \mathbb{R}^d$, $x \in \Pi^d$ (i.e. periodic case), or $x \in \Omega$ (a bounded open set of $\mathbb{R}^d$) with homogeneous Dirichlet or Neuman boundary conditions. We will denote by $S(t) = e^{it\Delta}$ the unitary group generated by $i\partial_t + \Delta$.

The implicit Crank-Nicolson scheme for (2.1) reads as follows:

$$\begin{aligned} i\frac{u^{n+1} - u^n}{\delta t} + \frac{1}{2}\Delta(u^{n+1} + u^n) &= g^{n+1}, \\ u^0 &= u_0(x), \end{aligned} \quad (2.2)$$

where g^{n+1} denotes an approximation of g at time $(n + 1/2)\delta t$. Here the operator Δ denotes either the laplacian for the above precised domain, or a finite difference approximation of this continuous operator. The aim of the following computation is to find a Duhamel-like formulation of (2.2).

Equation (2.2) is equivalent to:

$$u^{n+1} = \left(i + \frac{1}{2}\delta t\Delta\right)^{-1} \left(i - \frac{1}{2}\delta t\Delta\right) u^n + \delta t \left(i + \frac{1}{2}\delta t\Delta\right)^{-1} g^{n+1}. \quad (2.3)$$

Let us introduce

$$A = \left(i + \frac{1}{2}\delta t\Delta\right)^{-1} \left(i - \frac{1}{2}\delta t\Delta\right)$$

and

$$B = \left(i + \frac{1}{2}\delta t\Delta\right)^{-1}.$$

By an obvious induction, one gets

$$u^{n+1} = A^{n+1}u_0 + \sum_{k=0}^n \delta t A^k B g^{n+1-k}. \quad (2.4)$$

On one hand, it is clear that, as in the continuous case, (A^{n+1}) is an unitary operator on any reasonable H^s space.

On the other hand, it is also clear that $\|B\|_{H^s \rightarrow H^s} \leq 1$ and that $B \rightarrow -iId$ in the strong topology of the operators. For $t \in [n\delta t, (n+1)\delta t[$ let us denote by $S_{\delta t}(t)$ the operator A^n . Using a spectral decomposition for A it is easy to see that we have a Trotter-Kato formula for $S_{\delta t}(t)$, that is $S_{\delta t} \rightarrow S(t)$ for the strong topology of the operators. For (NLS), equation (2.3) reads:

$$i\frac{u^{n+1} - u^n}{\delta t} + \frac{1}{2}\Delta(u^{n+1} + u^n) = -\frac{\lambda}{2\sigma + 2} f(u^{n+1}, u^n)(u^{n+1} + u^n), \quad (2.5)$$

where

$$f(u^{n+1}, u^n) = \frac{|u^{n+1}|^{2\sigma+2} - |u^n|^{2\sigma+2}}{|u^{n+1}|^2 - |u^n|^2}$$

We next denote by $u_{\delta t}(t)$ the piecewise constant function which value on $[n\delta t, (n+1)\delta t[$ is u^n . With these notations, the discret Duhamel formulation

(2.4) for (2.5) reads:

$$u_{\delta t}((n+1)\delta t) = S_{\delta t}((n+1)\delta t)u_0 - \frac{\lambda}{2\sigma+2} \sum_{k=0}^n \delta t S_{\delta t}(n\delta t - k\delta t) Bf(u_{\delta t}((k+1)\delta t), u_{\delta t}(k\delta t))(u_{\delta t}((k+1)\delta t + u_{\delta t}(k\delta t))). \quad (2.6)$$

We have the following result:

Theorem 2.1

i) Let $u_0 \in H^s$, ($s > \frac{d}{2}$). There exists a constant C independent of δt and u_0 and there exists such that for any $\delta t \leq \frac{1}{C|u_0|_{H^s}^{2\sigma}}$ there exists a unique maximal solution $u_{\delta t}$ of (2.6) in $L^\infty([0, T_{\delta t}]; H^s)$, ($T_{\delta t} = N\delta t$ for some integer N). Moreover, in the 1-D case if $\lambda < 0$ or if $\lambda > 0$ and $\sigma < 2$, one has $T_{\delta t} = +\infty$. In the 2-D case, if $\lambda < 0$ and $\sigma = 1$, then $T_{\delta t} = +\infty$.

ii) Let us denote by u the maximal solution for the (NLS) equation

$$iu_t + \Delta u = -\lambda|u|^{2\sigma}u, \quad u(x; 0) = u_0(x)$$

defined in $\mathcal{C}([0, T_*]; H^s)$. Then one has

$$\liminf_{\delta t \rightarrow 0} T_{\delta t} \geq T_*$$

and $\forall T < T_*$, if δt is sufficiently small, $u_{\delta t}$ belongs to $L^\infty([0, T]; H^s)$ and $u_{\delta t} \rightarrow u$ in $L^\infty([0, T]; H^s)$.

Proof: i) Thanks to the Duhamel formula (2.6), it is clear that the problem can be treated by a fixed point procedure as in the continuous case. So that the local existence part of i) is straightforward. Note that this kind of proof brings out that there exists $T_0 > 0$ and K independent of $\delta t \leq \delta t_0$ such that

$$T_{\delta t} \geq T_0 \text{ and } |u_{\delta t}|_{L^\infty([0, T_0]; H^s)} \leq K \quad (2.7)$$

On the other hand, it is clear that the Crank-Nicolson scheme (2.5) has the following invariant quantities:

$$\begin{aligned} \int |u^n|^2 &= \int |u^0|^2, \quad \forall n \geq 0, \\ \frac{1}{2} \int |\nabla u^n|^2 - \frac{\lambda}{2\sigma+2} \int |u^n|^{2\sigma+2} &= \frac{1}{2} \int |\nabla u^0|^2 - \frac{\lambda}{2\sigma+2} \int |u^0|^{2\sigma+2}, \quad \forall n \geq 0. \end{aligned} \quad (2.8)$$

In the 1-D case, one can apply theorem 2.1 with $s = 1(> \frac{1}{2})$, so that one obtain global existence when $\lambda < 0$ or ($\lambda > 0$ and $\sigma < 2$). In the 2-D case, unfortunatly, we are not able to prove local existence in H^1 so that the only

way to obtain global existence when $\sigma = 1$ and $\lambda < 0$ is to use Brezis-Gallouët technique [4].

ii) Let us write the Duhamel formula for $u(t)$ solution of (NLS) between 0 and $(n+1)\delta t$:

$$u((n+1)\delta t) = S((n+1)\delta t)u_0 + i\lambda \int_0^{(n+1)\delta t} S((n+1)\delta t - \tau)|u|^{2\sigma}u(\tau)d\tau.$$

Substracting this identity from (2.6) and taking the H^s norm leads to

$$\begin{aligned} & |u_{\delta t}((n+1)\delta t) - u((n+1)\delta t)|_{H^s} \\ & \leq |[S_{\delta t}((n+1)\delta t) - S((n+1)\delta t)]u_0|_{H^s} \\ & + \sum_{k=0}^n \left| \int_{k\delta t}^{(k+1)\delta t} S_{\delta t}((n+1)\delta t - k\delta t) B \frac{\lambda}{2\sigma+2} f(u_{\delta t}((k+1)\delta t), u_{\delta t}(k\delta t)) \right. \\ & \quad \left. \times (u_{\delta t}((k+1)\delta t) + u_{\delta t}(k\delta t)) + i\lambda S((n+1)\delta t - \tau)|u|^{2\sigma}u(\tau)d\tau \right|_{H^s}. \end{aligned} \quad (2.9)$$

In order to control the r.h.s of (2.9), one writes each integral on the following form:

$$\begin{aligned} & \left| \int_{k\delta t}^{(k+1)\delta t} S_{\delta t}((n+1)\delta t - k\delta t) B \frac{\lambda}{2\sigma+2} f(u_{\delta t}((k+1)\delta t), u_{\delta t}(k\delta t)) \right. \\ & \quad \left. \times (u_{\delta t}((k+1)\delta t) + u_{\delta t}(k\delta t)) + i\lambda S((n+1)\delta t - \tau)|u|^{2\sigma}u(\tau)d\tau \right|_{H^s} \\ & \leq \left| \int_{k\delta t}^{(k+1)\delta t} [S_{\delta t}((n+1)\delta t - k\delta t) B + iS((n+1)\delta t - k\delta t)] \right. \\ & \quad \left. \times \frac{\lambda}{2\sigma+2} f(u_{\delta t}((k+1)\delta t), u_{\delta t}(k\delta t))(u_{\delta t}((k+1)\delta t) + u_{\delta t}(k\delta t))d\tau \right|_{H^s} \\ & + \left| \int_{k\delta t}^{(k+1)\delta t} [S((n+1)\delta t - \tau) - S((n+1)\delta t - k\delta t)] \lambda |u|^{2\sigma}u(\tau)d\tau \right|_{H^s} \\ & + \left| \int_{k\delta t}^{(k+1)\delta t} S((n+1)\delta t - k\delta t) \lambda \left[\frac{1}{2\sigma+2} f(u_{\delta t}((k+1)\delta t), u_{\delta t}(k\delta t)) \right. \right. \\ & \quad \left. \left. \times (u_{\delta t}((k+1)\delta t) + u_{\delta t}(k\delta t)) - |u|^{2\sigma}u(\tau) \right] d\tau \right|_{H^s} \\ & \equiv I_1^{k,n} + I_2^{k,n} + I_3^{k,n}. \end{aligned}$$

We denote by

$$|u|_{l^\infty(N, H^s)} = \sup_{n=0 \dots N+1} |u(n\delta t)|_{H^s}.$$

Inequality (2.9) can be written as:

$$|u_{\delta t} - u|_{l^\infty(N, H^s)} \leq |(S_{\delta t} - S)u_0|_{l^\infty(N, H^s)} + \sup_{n=0 \dots N} \sum_{k=0}^n I_1^{k,n} + I_2^{k,n} + I_3^{k,n}. \quad (2.10)$$

Since $S_{\delta t} \rightarrow S$ in the strong topology of operators in H^s , one has

$$|(S_{\delta t} - S)u_0|_{l^\infty(N, H^s)} \rightarrow 0 \text{ as } \delta t \rightarrow 0.$$

In the same way, as $B \rightarrow -iI$,

$$\sup_{n=0 \dots N} \sum_{k=0}^n I_1^{k,n} \rightarrow 0 \text{ as } \delta t \rightarrow 0.$$

On the other hand, as the group $S(t)$ is strongly continuous,

$$\sup_{n=0 \dots N} \sum_{k=0}^n I_2^{k,n} \rightarrow 0 \text{ as } \delta t \rightarrow 0.$$

For $I_3^{k,n}$, we write

$$|u|^{2\sigma} u(\tau) = \frac{1}{2\sigma + 2} f(u((k+1)\delta t), u(k\delta t))(u((k+1)\delta t) + u(k\delta t)) + R_k(\tau),$$

so that

$$I_3^{k,n} \leq \int_{k\delta t}^{(k+1)\delta t} \frac{|\lambda|}{2\sigma + 2} |f(u_{\delta t}((k+1)\delta t), u_{\delta t}(k\delta t))(u_{\delta t}((k+1)\delta t) + u_{\delta t}(k\delta t)) - f(u((k+1)\delta t), u(k\delta t))(u((k+1)\delta t) + u(k\delta t))|_{H^s}$$

$$+ \delta t \sup_{\tau \in [k\delta t, (k+1)\delta t]} |R_k(\tau)|_{H^s} \equiv J_k + \delta t G_k(\delta t)$$

As u lies in $\mathcal{C}([0, T]; H^s)$, on has

$$\sum_{k=0}^N \delta t G_k(\delta t) \rightarrow 0 \text{ as } \delta t \rightarrow 0.$$

Due to the form of f , on has

$$J_k \leq \frac{|\lambda|}{2\sigma + 2} \int_{k\delta t}^{(k+1)\delta t} C \left(|u_{\delta t}((k+1)\delta t)|_{H^s}^{2\sigma} + |u_{\delta t}(k\delta t)|_{H^s}^{2\sigma} + |u((k+1)\delta t)|_{H^s}^{2\sigma} + |u(k\delta t)|_{H^s}^{2\sigma} \right)$$

$$\times (|u_{\delta t}((k+1)\delta t) - u((k+1)\delta t)|_{H^s} + |u_{\delta t}(k\delta t) - u(k\delta t)|_{H^s}).$$

Now according to the uniform estimates of $u_{\delta t}$ and u on $[0, N\delta t]$, on has

$$J_k \leq C\delta t (|u_{\delta t}((k+1)\delta t) - u((k+1)\delta t)|_{H^s} + |u_{\delta t}(k\delta t) - u(k\delta t)|_{H^s}).$$

Finally, (2.10) leads to

$$|u_{\delta t} - u|_{l^\infty(N, H^s)} \leq o(1) + CN\delta t |u_{\delta t} - u|_{l^\infty(N, H^s)}. \quad (2.11)$$

Let us write $T_1 = N\delta t$; taking $CT_1 < 1$ leads to

$$|u_{\delta t} - u|_{l^\infty(N, H^s)} \leq o(1).$$

Applying the proof with the new initial data $u(T_1)$, one gets the lower semi-continuity of the existence time $T_{\delta t}$ as $\delta t \rightarrow 0$ and the convergence on $[0, T]$ for any $T < T_*$. $\blacksquare$

Remark 2.1 *We prove in this theorem (part i) the uniqueness of the solution given by the numerical scheme for δt small enough. This was an open question in [1].*

3 Two schemes for (NLW_ω) and their invariants.

Let us recall that for:

$$(NLW_\omega) \begin{cases} \frac{1}{\omega^2} \partial_t^2 E - i \partial_t E - \Delta E = \lambda |E|^{2\sigma} E, \\ E(t=0) = f, \partial_t E(t=0) = g, \end{cases}$$

we introduce the two following schemes.

$$(\mathcal{S}_1) \begin{cases} \frac{1}{\omega^2} \left(\frac{E^{n+1} - 2E^n + E^{n-1}}{\delta t^2} \right) - i \left(\frac{E^{n+1} - E^n}{\delta t} \right) - \frac{1}{2} \Delta(E^{n+1} + E^n) \\ = \frac{\lambda}{2\sigma + 2} \frac{|E^{n+1}|^{2\sigma+2} - |E^n|^{2\sigma+2}}{|E^{n+1}|^2 - |E^n|^2} (E^{n+1} + E^n), \\ E_0 = f, \frac{E^0 - E^{-1}}{\delta t} = g \end{cases}$$

and

$$(\mathcal{S}_2) \begin{cases} \frac{1}{\omega^2} \left(\frac{E^{n+1} - 2E^n + E^{n-1}}{\delta t^2} \right) - i \left(\frac{E^{n+1} - E^{n-1}}{2\delta t} \right) - \frac{1}{2} \Delta(E^{n+1} + E^{n-1}) \\ = \frac{\lambda}{2\sigma + 2} \frac{|E^{n+1}|^{2\sigma+2} - |E^{n-1}|^{2\sigma+2}}{|E^{n+1}|^2 - |E^{n-1}|^2} (E^{n+1} + E^{n-1}), \\ \frac{E_0 + E^{-1}}{2} = f, \frac{E^0 - E^{-1}}{\delta t} = g. \end{cases}$$

For the continuous problem (NLW_ω) , one can prove (see [3]) that the following quantities are constant in time:

$$\int |E|^2 - \frac{2}{\omega^2} \text{Im} \int \bar{E} \partial_t E = C^{st} \quad (3.1)$$

$$\int \left(\frac{1}{\omega^2} |\partial_t E|^2 + |\nabla E|^2 - \frac{\lambda}{\sigma + 1} |E|^{2\sigma+2} \right) = C^{st} \quad (3.2)$$

We now present the discret equivalents of (3.1) and (3.2) for $(\mathcal{S}_1)$ and $(\mathcal{S}_2)$.

Proposition 3.1

i) Let $(E^n)_{-1 \leq n \leq N}$ be the solution of $(\mathcal{S}_1)$, one has

$$\begin{aligned}
& \int |E^{n+1}|^2 - \frac{2}{\omega^2} \mathcal{I}m \int \overline{E}^{n+1} \left(\frac{E^{n+1} - E^n}{\delta t} \right) \\
&= \int |E^0|^2 - \frac{2}{\omega^2} \mathcal{I}m \int \overline{E}^0 \left(\frac{E^0 - E^{-1}}{\delta t} \right) \\
&+ \frac{1}{\omega^2} \int \sum_{k=0}^n \delta t \mathcal{I}m \left[\left(\frac{E^{k+1} - E^k}{\delta t} \right) \left(\frac{\overline{E}^k - \overline{E}^{k-1}}{\delta t} \right) \right]
\end{aligned} \tag{3.3}$$

and

$$\begin{aligned}
& \int \left(\frac{1}{\omega^2} \left| \frac{E^{n+1} - E^n}{\delta t} \right|^2 + |\nabla E^{n+1}|^2 - \frac{\lambda}{\sigma+1} |E^{n+1}|^{2\sigma+2} \right) \\
&+ \delta t \int \sum_{k=0}^n \frac{1}{\omega^2} \delta t \left| \frac{E^{k+1} - 2E^k + E^{k-1}}{\delta t^2} \right|^2 \\
&= \int \left(\frac{1}{\omega^2} \left| \frac{E^0 - E^{-1}}{\delta t} \right|^2 + |\nabla E^0|^2 - \frac{\lambda}{\sigma+1} |E^0|^{2\sigma+2} \right).
\end{aligned} \tag{3.4}$$

ii) Let $(E^n)_{-1 \leq n \leq N}$ be the solution of $(\mathcal{S}_2)$, one has

$$\begin{aligned}
& \int \frac{1}{2} (|E^{n+1}|^2 + |E^n|^2) - \frac{2}{\omega^2} \mathcal{I}m \int \overline{E}^{n+1} \left(\frac{E^{n+1} - E^n}{\delta t} \right) \\
&= \int \frac{1}{2} (|E^0|^2 + |E^{-1}|^2) - \frac{2}{\omega^2} \mathcal{I}m \int \overline{E}^0 \left(\frac{E^0 - E^{-1}}{\delta t} \right)
\end{aligned} \tag{3.5}$$

and

$$\begin{aligned}
& \int \left\{ \frac{1}{\omega^2} \left| \frac{E^{n+1} - E^n}{\delta t} \right|^2 + \frac{1}{2} (|\nabla E^{n+1}|^2 + |\nabla E^n|^2) \right\} \\
&- \frac{\lambda}{2\sigma+2} \int (|E^{n+1}|^{2\sigma+2} + |E^n|^{2\sigma+2}) \\
&= \int \left\{ \frac{1}{\omega^2} \left| \frac{E^0 - E^{-1}}{\delta t} \right|^2 + \frac{1}{2} (|\nabla E^0|^2 + |\nabla E^{-1}|^2) \right\} \\
&- \frac{\lambda}{2\sigma+2} \int (|E^0|^{2\sigma+2} + |E^{-1}|^{2\sigma+2}).
\end{aligned} \tag{3.6}$$

Proof: The proofs are standard, we omit them.

Remark 3.1 *It is clear that $(\mathcal{S}_2)$ has exactly the same invariants as the continuous problem, while the last term of the l.h.s of (3.4) is clearly a temporal diffusion term of order of magnitude $\frac{\delta t}{\omega^2}$. We will come back on this diffusion term in the last part of the paper.*

4 Splitting of the schemes $(\mathcal{S}_1)$ and $(\mathcal{S}_2)$

In the continuous case, the following splitting was introduced in [2] for (NLW_ω) :

$$E = F + G,$$

$$\partial_t F = i \frac{\omega^2}{2} \left(1 - \sqrt{1 - \frac{4\Delta}{\omega^2}} \right) F + i \left(\sqrt{1 - \frac{4\Delta}{\omega^2}} \right)^{-1} \lambda |E|^{2\sigma} E, \quad (4.1)$$

$$\partial_t G = i \frac{\omega^2}{2} \left(1 + \sqrt{1 - \frac{4\Delta}{\omega^2}} \right) G - i \left(\sqrt{1 - \frac{4\Delta}{\omega^2}} \right)^{-1} \lambda |E|^{2\sigma} E. \quad (4.2)$$

One can compute explicitly the initial data for F and G from f and g (see [2]). The principle of this splitting is the following one: the function G contains all the oscillatory part of the solution (see the operator $i \frac{\omega^2}{2} \left(1 + \sqrt{1 - \frac{4\Delta}{\omega^2}} \right)$, but of course the order of magnitude of $G(0)$ is $\frac{1}{\omega^2}$. On the other hand, F converges to the solution of (NLS) .

The aim of this section is to present a similar splitting for $(\mathcal{S}_1)$ and $(\mathcal{S}_2)$. In analogy with (4.1) and (4.2), we search a splitting for $(\mathcal{S}_1)$ and $(\mathcal{S}_2)$ of the form:

$$E^n = F^n + G^n$$

$$\frac{F^{n+1} - F^n}{\delta t} = i\alpha \left(\frac{F^{n+1} + F^n}{2} \right) + \gamma_1 \left(\frac{1}{\delta t} + i \frac{\alpha}{2} \right) f^{n+1} \quad (4.3)$$

$$\frac{G^{n+1} - G^n}{\delta t} = i\beta \left(\frac{G^{n+1} + G^n}{2} \right) + \gamma_2 \left(\frac{1}{\delta t} + i \frac{\beta}{2} \right) f^{n+1}, \quad (4.4)$$

where f^{n+1} denotes the r.h.s of $(\mathcal{S}_1)$ or $(\mathcal{S}_2)$.

Let (X_1, X_2) be the roots of the characteristic equation of (S_1) or (S_2) . These characteristic equations are:

For (S_1)

$$X^2 \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2} \right) + X \left(\frac{-2}{\omega^2 \delta t^2} + \frac{i}{\delta t} - \frac{\Delta}{2} \right) + \frac{1}{\omega^2 \delta t^2} = 0, \quad (4.5)$$

for (S_2)

$$X^2 \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{2\delta t} - \frac{\Delta}{2} \right) + X \left(\frac{-2}{\omega^2 \delta t^2} \right) + \left(\frac{1}{\omega^2 \delta t^2} + \frac{i}{2\delta t} - \frac{\Delta}{2} \right) = 0. \quad (4.6)$$

(Of course X_1 and X_2 are operators.)

If we look to the homogeneous problem associated to (4.3) and (4.4), we get

$$F^{n+1} = \left(1 - i\frac{\alpha}{2}\delta t\right)^{-1} \left(1 + i\frac{\alpha}{2}\delta t\right) F^n$$

and by identification, one finds

$$X_1 = \left(1 - i\frac{\alpha}{2}\delta t\right)^{-1} \left(1 + i\frac{\alpha}{2}\delta t\right). \quad (4.7)$$

In the same way, one gets for X_2

$$X_2 = \left(1 - i\frac{\beta}{2}\delta t\right)^{-1} \left(1 + i\frac{\beta}{2}\delta t\right). \quad (4.8)$$

The nature of the operators α and β will give us some informations on the behaviour of the schemes. We still have to determine (γ_1, γ_2) . We deal with both schemes separately.

4.1 Splitting for (S_1)

Using (4.7) and (4.8), one writes

$$F^{n+1} = X_1 F^n + \gamma_1 X_1 f^{n+1}, \quad (4.9)$$

$$G^{n+1} = X_2 G^n + \gamma_2 X_2 f^{n+1}. \quad (4.10)$$

Rewritting these identities for F^n and G^n gives

$$F^n = X_1 F^{n-1} + \gamma_1 X_1 f^n, \quad (4.11)$$

$$G^n = X_2 G^{n-1} + \gamma_2 X_2 f^n. \quad (4.12)$$

so that (4.9) and (4.10) yield

$$F^{n+1} = X_1(X_1 F^{n-1} + \gamma_1 X_1 f^n) + \gamma_1 X_1 f^{n+1}, \quad (4.13)$$

$$G^{n+1} = X_2(X_2 G^{n-1} + \gamma_2 X_2 f^n) + \gamma_2 X_2 f^{n+1}. \quad (4.14)$$

Plugging (4.11)-(4.14) into (S_1) and using the fact that X_1 and X_2 verify the characteristic equation (4.5) leads to

$$\begin{aligned} & \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2}\right) (\gamma_1 X_1 + \gamma_2 X_2) f^{n+1} \\ & + \left\{ \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2}\right) (\gamma_1 X_1^2 + \gamma_2 X_2^2) \right. \\ & \left. + \left(\frac{-2}{\omega^2 \delta t^2} + \frac{i}{\delta t} - \frac{\Delta}{2}\right) (\gamma_1 X_1 + \gamma_2 X_2) \right\} f^n = f^{n+1} \end{aligned}$$

So we have to solve

$$\left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2}\right) (\gamma_1 X_1 + \gamma_2 X_2) = 1$$

$$\left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2}\right) (\gamma_1 X_1^2 + \gamma_2 X_2^2) + \left(\frac{-2}{\omega^2 \delta t^2} + \frac{i}{\delta t} - \frac{\Delta}{2}\right) (\gamma_1 X_1 + \gamma_2 X_2) = 0$$

The solution of which is $\gamma_1 = -\gamma_2$ and

$$\gamma_1 = \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2}\right)^{-1} (X_1 - X_2)^{-1}.$$

We have proved

Proposition 4.1

It is equivalent to solve (S_1) with E_1 and E_0 given or to solve

$$\begin{cases} F^{n+1} = X_1 F^n + \gamma X_1 f^{n+1}, \\ G^{n+1} = X_2 G^n - \gamma X_2 f^{n+1}, \end{cases}$$

$$E^n = F^n + G^n,$$

$$f^{n+1} = \frac{\lambda}{2\sigma + 2} \frac{|E^{n+1}|^{2\sigma+2} - |E^n|^{2\sigma+2}}{|E^{n+1}|^2 - |E^n|^2} (E^{n+1} + E^n),$$

$$\begin{cases} F^0 = (X_2 - X_1)^{-1} X_1 (X_2 E^{-1} - E^0), \\ G^0 = (X_2 - X_1)^{-1} X_2 (E^0 - X_1 E^{-1}). \end{cases}$$

The operators X_1 and X_2 are solution to the characteristic equation (4.5) and:

$$\gamma = \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2}\right)^{-1} (X_1 - X_2)^{-1}.$$

Proof: The only thing that we have to find is the value of the initial data for F and G . One has

$$F^0 + G^0 = E^0$$

and for all n

$$X_2 F^{n+1} + X_1 G^{n+1} = X_1 X_2 (F^n + G^n).$$

Applying this identity with $n = -1$ leads to

$$F^0 + G^0 = E^0,$$

$$X_2 F^0 + X_1 G^0 = X_1 X_2 E^{-1},$$

which leads to the result. ■

4.2 Splitting for (S_2)

The same technique works for (S_2) . The case of (S_2) is easier since one find explicit and usefull values for X_1 and X_2 . One gets:

Proposition 4.2

It is equivalent to solve (S_2) with E_1 and E_0 given or to solve

$$\begin{cases} F^{n+1} = X_1 F^n + \gamma X_1 f^{n+1}, \\ G^{n+1} = X_2 G^n - \gamma X_2 f^{n+1}, \\ E^n = F^n + G^n, \end{cases}$$

$$f^{n+1} = \frac{\lambda}{2\sigma + 2} \frac{|E^{n+1}|^{2\sigma+2} - |E^{n-1}|^{2\sigma+2}}{|E^{n+1}|^2 - |E^{n-1}|^2} (E^{n+1} + E^{n-1}),$$

$$\begin{cases} F^0 = (X_2 - X_1)^{-1} X_1 (X_2 E^{-1} - E^0), \\ G^0 = (X_2 - X_1)^{-1} X_2 (E^0 - X_1 E^{-1}). \end{cases}$$

Moreover the operators X_1 and X_2 which are the solutions to the characteristic equation (4.6) are given by:

$$X_{1,2} = \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{2\delta t} - \frac{\Delta}{2} \right)^{-1} \left(\frac{1}{\omega^2 \delta t^2} \mp \frac{i}{2} \sqrt{\frac{1}{\delta t^2} + \Delta^2 - \frac{4\Delta}{\omega^2 \delta t^2}} \right).$$

and

$$\gamma = \left(i \sqrt{\frac{1}{\delta t^2} + \Delta^2 - \frac{4\Delta}{\omega^2 \delta t^2}} \right)^{-1}$$

Remark 4.1 *The modulus of X_1 or X_2 for (S_2) is equal to one. So that the operators α and β in (4.3) and (4.4) for (S_2) are self adjoint and therefore $i\alpha$ and $i\beta$ are skew-adjoint and generate unitary groups on any H^s .*

On the contrary, this is not the case for (S_1) .

5 Existence and convergence.

Using these frameworks, we will prove existence and convergence for (S_1) and (S_2) , for fixed ω .

5.1 Study of (S_1) .

We work on the version of (S_1) given in proposition 4.1:

$$\begin{aligned} F^{n+1} &= X_1 F^n + \gamma X_1 f^{n+1}, \\ G^{n+1} &= X_2 G^n - \gamma X_2 f^{n+1}. \end{aligned} \tag{5.1}$$

This result is:

Theorem 5.1

- Let $(F_0^{\delta t}, G_0^{\delta t}) \in (H^s)^2 (s > \frac{d}{2})$ that may depend on δt and such that

$$(F_0^{\delta t}, G_0^{\delta t}) \rightarrow (\tilde{F}_0, \tilde{G}_0) \text{ as } \delta t \rightarrow 0 \text{ in } H^s.$$

There exists a constant δt_0 depending only on $|(\tilde{F}_0, \tilde{G}_0)|_{H^s}$ such that for any $\delta t \leq \delta t_0$, there exists a unique maximal solution to (5.1) with $F^0 = F_0^{\delta t}, G^0 = G_0^{\delta t}$ defined on the interval $[0, T_{\delta t}]$ (with $T_{\delta t} = N\delta t$ for some integer N).

- Let (F, G) be the solution of (4.1), (4.2) with the initial data $F(0) = \tilde{F}_0, G(0) = \tilde{G}_0$ and T_∞ its existence time.

One has $\liminf_{\delta t \rightarrow 0} T_{\delta t} \geq T_\infty$ and for all $T < T_\infty$,

$$(F^{\delta t}, G^{\delta t}) \rightarrow (F, G) \text{ in } L^\infty([0, T]; H^s)$$

where $(F^{\delta t}, G^{\delta t})$ is the piecewise constant function which value at point $t = n\delta t$ is (F^n, G^n) .

Proof: It will be exactly the same as for (NLS) (see part 2). The only points that we have to prove are:

- The operator $\frac{\gamma}{\delta t}$ is bounded and converges strongly to $i \left(\sqrt{1 - \frac{4\Delta}{\omega^2}} \right)^{-1}$.
- The discret groups $X_1^{\frac{T}{\delta t}}$ and $X_2^{\frac{T}{\delta t}}$ are bounded and converge to $e^{i\frac{\omega^2}{2} \left(1 - \sqrt{1 - \frac{4\Delta}{\omega^2}} \right) T}$ and $e^{i\frac{\omega^2}{2} \left(1 + \sqrt{1 - \frac{4\Delta}{\omega^2}} \right) T}$ respectively.

The proof goes through three lemmas.

Lemma 5.1

The operators X_1 and X_2 have their norm uniformly bounded in ω and δt .

Proof: One has the following explicit expressions for X_1 and X_2 :

$$X_{1,2} = \frac{1}{2} \left\{ \frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2} \right\}^{-1} \left\{ - \left(\frac{-2}{\omega^2 \delta t^2} + \frac{i}{\delta t} - \frac{\Delta}{2} \right) \pm \left(\sqrt{\frac{\mu + \sqrt{\mu^2 + \frac{\Delta^2}{\delta t^2}}}{2}} + i \sqrt{\frac{-\mu + \sqrt{\mu^2 + \frac{\Delta^2}{\delta t^2}}}{2}} \right) \right\} \quad (5.2)$$

where

$$\mu = \frac{\Delta^2}{4} - \frac{1}{\delta t^2} + \frac{4\Delta}{\omega^2 \delta t^2}.$$

We first remark that the operator

$$\left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{\Delta}{2} \right)^{-1} \left(\frac{-2}{\omega^2 \delta t^2} + \frac{i}{\delta t} - \frac{\Delta}{2} \right)$$

is bounded independently of ω and δt . We still have to prove that the second part of $X_{1,2}$ is bounded. Let us call it Y and use a spectral representation of Δ (Fourier transform in $\mathbb{R}^d$, diagonalization in $\Omega \subset \mathbb{R}^d$).

$$\hat{Y} = \left(\sqrt{\frac{\hat{\mu} + \sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{2}} + i \sqrt{\frac{-\hat{\mu} + \sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{2}} \right) \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} + \frac{\xi^2}{2} \right)^{-1}$$

and letting $z = \frac{\xi^2 \delta t}{2}$, one gets

$$|\hat{Y}|^4 = \left\{ \left(z^2 - 1 - \frac{8z}{\omega^2 \delta t} \right)^2 - 4z^2 \right\} \left\{ 1 + \left(\frac{1}{\omega^2 \delta t} + z \right)^2 \right\}^{-2}.$$

One has

$$|\hat{Y}|^4 \leq c + \frac{\left(z^2 - 1 - \frac{z}{\omega^2 \delta t} \right)^2}{\left(1 + \left(\frac{1}{\omega^2 \delta t} + z^2 \right)^2 \right)^2}.$$

On the other hand

$$\frac{\left| z^2 - 1 - \frac{z}{\omega^2 \delta t} \right|}{1 + \left(\frac{1}{\omega^2 \delta t} + z \right)^2} \leq \frac{z^2 + 1 + \frac{z}{\omega^2 \delta t}}{1 + \frac{1}{\omega^4 \delta t^2} + z^2 + \frac{2z}{\omega^2 \delta t}} \leq 1,$$

thereby proving lemma 5.1. ■

Proposition 5.1

Let K such that $\omega^2 \delta t^{\frac{1}{2}} \leq K$. Then there exists a constant $c(K)$ such that

$$|X_1^{\frac{T}{\delta t}}| + |X_2^{\frac{T}{\delta t}}| \leq c(K).$$

Proof: We will use the invariants of (S_1) given in proposition 3.1. Let us denote by $S_0^{\delta t}(n\delta t)f$ the solution to

$$\frac{1}{\omega^2} \left(\frac{E^{n+1} - 2En + En + 1}{\delta t^2} \right) - i \left(\frac{E^{n+1} - E^n}{\delta t} \right) - \frac{1}{2} \Delta(E^{n+1} + E^n) = 0,$$

$$E^0 = f, \quad \frac{E^0 - E^{-1}}{\delta t} = 0, \tag{5.3}$$

and by $S_1^{\delta t}(n\delta t)g$ the solution to

$$\begin{aligned} \frac{1}{\omega^2} \left(\frac{E^{n+1} - 2En + En + 1}{\delta t^2} \right) - i \left(\frac{E^{n+1} - E^n}{\delta t} \right) - \frac{1}{2} \Delta(E^{n+1} + E^n) &= 0, \\ E^0 &= 0, \quad \frac{E^0 - E^{-1}}{\delta t} = g. \end{aligned} \tag{5.4}$$

We now compute X_1^n and X_2^n in terms of $S_0^{\delta t}$ and $S_1^{\delta t}$.

It is clear that there exists two operators A and B such that

$$S_0^{\delta t}(n\delta t) = AX_1^{n+1} + BX_2^{n+1}.$$

Writting $S_0(0) = Id$ and $\frac{S_0^{\delta t}(0) - S_0^{\delta t}(-\delta t)}{\delta t} = 0$, one gets

$$A = (X_1 - X_2)^{-1}(1 - X_2) \text{ and } B = (X_2 - X_1)^{-1}(1 - X_1)$$

so that

$$S_0^{\delta t}(n\delta t) = (X_1 - X_2)^{-1}(1 - X_2)X_1^{n+1} + (X_2 - X_1)^{-1}(1 - X_1)X_2^{n+1}. \quad (5.5)$$

On the same way, one obtains

$$S_1^{\delta t}(n\delta t) = \delta t \left((X_1 - X_2)^{-1}X_2X_1^{n+1} + (X_2 - X_1)^{-1}X_1X_2^{n+1} \right). \quad (5.6)$$

One can solve the system formed by (5.5) and (5.6) in X_1^{n+1}, X_2^{n+1} :

$$X_1^{n+1} = X_1S_0^{\delta t}(n\delta t) - \frac{1 - X_1}{\delta t}S_1^{\delta t}(n\delta t) \quad (5.7)$$

and

$$X_2^{n+1} = X_2S_0^{\delta t}(n\delta t) - \frac{1 - X_2}{\delta t}S_1^{\delta t}(n\delta t). \quad (5.8)$$

Since we know that the operators X_1 and X_2 are uniformly bounded, we need to show that $S_0^{\delta t}$ is uniformly bounded on H^s and we have to find some bound on $\frac{1 - X_{1,2}}{\delta t}S_1^{\delta t}(n\delta t)$.

The proof goes through two lemmas.

Lemma 5.2

There exists a constant c independent of ω and δt such that:

$$\left| \frac{1 - X_k}{\delta t}f \right|_{H^s} \leq c \left(\omega |f|_{H^{s+1}} + \omega^2 |f|_{H^s} \right).$$

for $k = 1, 2$.

Proof: We use a spectral representation of $-\Delta$ on formula (5.2) to get:

$$\begin{aligned} 1 - \hat{X}_k &= \frac{\frac{-i}{\delta t} + 3\frac{\xi^2}{2}}{2 \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} + \frac{\xi^2}{2} \right)} - \varepsilon \frac{\left(\sqrt{\frac{\hat{\mu} + \sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{2}} + i \sqrt{\frac{-\hat{\mu} + \sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{2}} \right)}{2 \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} + \frac{\xi^2}{2} \right)} \\ &\equiv M + N \end{aligned}$$

with $\varepsilon = \pm 1$ and $\hat{\mu} = \left(\frac{\xi^4}{4} - \frac{1}{\delta t^2} - \frac{4\xi^2}{\omega^2 \delta t^2} \right)$.

• Estimate of M :

$$M = \frac{\delta t}{2} \frac{\left(-i + \frac{3\xi^2 \delta t}{2} \right)}{\left(i\delta t + \frac{\xi^2 \delta t^2}{2} + \frac{1}{\omega^2} \right)},$$

so that

$$\frac{M}{\delta t} = \frac{\omega^2}{2} \frac{\left(-i + \frac{3\xi^2 \delta t}{2}\right)}{\left(1 + i\delta t \omega^2 + \frac{\xi^2}{2} \delta t^2 \omega^2\right)}$$

that is

$$\begin{aligned} \frac{|M|^2}{\delta t^2} &= \frac{\omega^4}{4} \frac{1 + \frac{9\xi^4 \delta t^2}{4}}{\left(1 + \frac{\xi^2}{2} \delta t^2 \omega^2\right)^2 + \delta t^2 \omega^4} \\ &\leq \frac{\omega^4}{4} + \frac{\omega^2 \xi^2 \left(\frac{9\omega^2 \xi^2 \delta t^2}{16}\right)}{\xi^2 \omega^2 \delta t^2}, \end{aligned}$$

and then,

$$\frac{|M|^2}{\delta t^2} \leq \frac{\omega^4}{4} + \frac{9}{16} \omega^2 \xi^2. \quad (5.9)$$

• Estimate of N :

$$4|N|^2 = \frac{\sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{\frac{1}{\delta t^2} + \left(\frac{\xi^2}{2} + \frac{1}{\omega^2 \delta t^2}\right)^2},$$

so that,

$$\frac{4|N|^2}{\delta t^2} = \frac{\sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{1 + \left(\frac{\xi^2}{2} \delta t + \frac{1}{\omega^2 \delta t}\right)^2} \leq \frac{|\hat{\mu}| + \frac{\xi^2}{\delta t}}{1 + \left(\frac{\xi^2 \delta t}{2} + \frac{1}{\omega^2 \delta t}\right)^2}$$

And with the expression of μ , one gets:

$$\begin{aligned} 4 \frac{|N|^2}{\delta t^2} &\leq \frac{\left(\frac{\xi^4}{4} + \frac{1}{\delta t^2} + \frac{4\xi^2}{\omega^2 \delta t^2} + \frac{\xi^2}{\delta t}\right)}{\left(1 + \frac{\xi^4 \delta t^2}{4} + \frac{1}{\omega^4 \delta t^2} + \frac{\xi^2}{\omega^2}\right)}, \\ &\leq \frac{\left(\frac{3\xi^4}{4} + \frac{3}{2\delta t^2} + \frac{4\xi^2}{\omega^2 \delta t^2}\right)}{\left(1 + \frac{\xi^4 \delta t^2}{4} + \frac{1}{\omega^4 \delta t^2} + \frac{\xi^2}{\omega^2}\right)}, \\ &\leq \omega^2 \xi^2 \left(\frac{\frac{3\xi^2}{4\omega^2} + \frac{4}{\omega^4 \delta t^2}}{\frac{\xi^2}{\omega^2} + \frac{1}{\omega^4 \delta t^4}}\right) + \frac{\frac{3}{2\delta t^2}}{\frac{1}{\omega^4 \delta t^2}}. \end{aligned}$$

That is:

$$4 \frac{|N|^2}{\delta t^2} \leq 4\omega^2 \xi^2 + \frac{3}{2} \omega^4. \quad (5.10)$$

One obtains with (5.9) and (5.10)

$$\frac{|1 - \hat{X}_k|}{\delta t} \leq c(\omega|\xi| + \omega^2), \quad k = 1, 2,$$

so that lemma 5.2 is proved. ■

Since we need an estimate on $\frac{1-X_{1,2}}{\delta t} S_1^{\delta t}(n\delta t)$, in view of lemma 5.2, we need to bound $\omega^2 S_1^{\delta t}$ and $\omega(-\Delta)^{\frac{1}{2}} S_1^{\delta t}$. These properties are fulfilled in the continuous case as S_1 is a smoothing operator.

Lemma 5.3

$\exists c > 0$ such that $\forall T > 0$, for any n such that $n\delta t \leq T, \forall f \in H^1$, one has:

$$\left| S_0^{\delta t}(n\delta t)f \right|_{H^1} \leq c(1 + T^{\frac{1}{2}}) |f|_{H^1},$$

and $\forall g \in L^2$,

$$\left| \omega \nabla S_1^{\delta t}(n\delta t)g \right|_{L^2} \leq |g|_{L^2}$$

and

$$\left| \omega^2 S_1^{\delta t}(n\delta t)g \right|_{L^2} \leq c(1 + T^{\frac{1}{2}} \omega^2(\delta t)^{\frac{1}{2}}) |g|_{L^2}.$$

Proof: For $S_0^{\delta t}$, we rewrite (3.3) and (3.4):

$$\begin{aligned} & \int \left| S_0^{\delta t}((n+1)\delta t)f \right|^2 \\ & - \frac{2}{\omega^2} \text{Im} \int \overline{S_0^{\delta t}((n+1)\delta t)f} \left(\frac{S_0^{\delta t}((n+1)\delta t)f - S_0^{\delta t}(n\delta t)f}{\delta t} \right) = \\ & \int |f|^2 \\ & + \frac{\delta t}{\omega^2} \text{Im} \int \sum_{k=0}^n \left(\frac{S_0^{\delta t}((k+1)\delta t)f - S_0^{\delta t}(k\delta t)f}{\delta t} \right) \left(\frac{\overline{S_0^{\delta t}(k\delta t)f} - \overline{S_0^{\delta t}((k-1)\delta t)f}}{\delta t} \right) \end{aligned} \quad (5.11)$$

and

$$\begin{aligned} & \frac{1}{\omega^2} \int \left| \frac{S_0^{\delta t}((n+1)\delta t)f - S_0^{\delta t}(n\delta t)f}{\delta t} \right|^2 + \int \left| \nabla S_0^{\delta t}((n+1)\delta t)f \right|^2 \\ & = \int |\nabla f|^2 \end{aligned} \quad (5.12)$$

$$- \frac{\delta t}{\omega^2} \int \sum_{k=0}^n \delta t \left| \frac{S_0^{\delta t}((k+1)\delta t)f - 2S_0^{\delta t}(k\delta t)f + S_0^{\delta t}((k-1)\delta t)f}{\delta t^2} \right|^2.$$

From (5.12), it is clear that $|\nabla S_0^{\delta t}((n+1)\delta t)f|_{L^2}$ and $\frac{1}{\omega} \left| \frac{S_0^{\delta t}((n+1)\delta t)f - S_0^{\delta t}(n\delta t)f}{\delta t} \right|_{L^2}$ are bounded by $|\nabla f|_{L^2}$. The equation (5.11) becomes:

$$\begin{aligned} & \int |S_0^{\delta t}((n+1)\delta t)f|^2 \leq \int |f|^2 \\ & + \frac{1}{\omega^2} \int |S_0^{\delta t}((n+1)\delta t)f|^2 + \frac{1}{\omega^2} \int \left| \frac{S_0^{\delta t}((n+1)\delta t)f - S_0^{\delta t}(n\delta t)f}{\delta t} \right|^2 \\ & + \frac{\delta t}{\omega^2} \left| \mathcal{I}m \int \sum_{k=0}^n \left(\frac{S_0^{\delta t}((k+1)\delta t)f - 2S_0^{\delta t}(k\delta t)f + S_0^{\delta t}((k-1)\delta t)f}{\delta t} \right) \right. \\ & \quad \left. \left(\frac{\overline{S_0^{\delta t}(k\delta t)f} - \overline{S_0^{\delta t}((k-1)\delta t)f}}{\delta t} \right) \right| \end{aligned}$$

The last term of the right hand side of this estimate is bounded thanks to the diffusion term of (5.12), and one obtains:

$$\begin{aligned} & \left(1 - \frac{1}{\omega^2}\right) |S_0^{\delta t}((n+1)\delta t)f|_{L^2}^2 \leq |\nabla f|_{L^2}^2 + \int |f|^2 + \\ & \frac{\delta t^2}{\omega^2} \sum_{k=0}^n \left| \frac{S_0^{\delta t}((k+1)\delta t)f - 2S_0^{\delta t}(k\delta t)f + S_0^{\delta t}((k-1)\delta t)f}{\delta t^2} \right|_{L^2} \\ & \quad \left| \frac{S_0^{\delta t}(k\delta t)f - S_0^{\delta t}((k-1)\delta t)f}{\delta t} \right|_{L^2} \end{aligned}$$

That is

$$\begin{aligned} & \left(1 - \frac{1}{\omega^2}\right) |S_0^{\delta t}((n+1)\delta t)f|_{L^2}^2 \leq |f|_{H^1}^2 + \\ & \frac{\delta t^2}{\omega^2} \left\{ \sum_{k=0}^n \left| \frac{S_0^{\delta t}((k+1)\delta t)f - 2S_0^{\delta t}(k\delta t)f + S_0^{\delta t}((k-1)\delta t)f}{\delta t^2} \right|_{L^2}^2 \right\}^{\frac{1}{2}} \\ & \quad \left\{ \sum_{k=0}^n \left| \frac{S_0^{\delta t}(k\delta t)f - S_0^{\delta t}((k-1)\delta t)f}{\delta t} \right|_{L^2}^2 \right\}^{\frac{1}{2}} \\ & \leq |f|_{H^1} + \frac{\delta t}{\omega} |\nabla f|_{L^2} \left\{ \sum_{k=0}^n \left| \frac{S_0^{\delta t}(k\delta t)f - S_0^{\delta t}((k+1)\delta t)f}{\delta t^2} \right|_{L^2}^2 \right\}^{1/2} \\ & \leq |f|_{H^1} + n^{1/2} \delta t |\nabla f|_{L^2}^2, \end{aligned}$$

thanks to (5.12).

For $S_1^{\delta t}$, we rewrite (3.3) and (3.4) again:

$$\begin{aligned}
& \int \left| S_1^{\delta t}((n+1)\delta t)g \right|^2 \\
& - \frac{2}{\omega^2} \mathcal{I}m \int \overline{S_1^{\delta t}((n+1)\delta t)g} \left(\frac{S_1^{\delta t}((n+1)\delta t)g - S_1^{\delta t}(n\delta t)g}{\delta t} \right) \\
& = \frac{\delta t^2}{\omega^2} \mathcal{I}m \int \sum_{k=0}^n \left(\frac{S_1^{\delta t}((k+1)\delta t)g - 2S_1^{\delta t}(k\delta t)g + S_1^{\delta t}((k-1)\delta t)g}{\delta t^2} \right) \\
& \quad \times \left(\frac{\overline{S_1^{\delta t}(k\delta t)g} - \overline{S_1^{\delta t}((k-1)\delta t)g}}{\delta t} \right)
\end{aligned} \tag{5.13}$$

and

$$\begin{aligned}
& \int \frac{\left| S_1^{\delta t}((n+1)\delta t)g - S_1^{\delta t}(n\delta t)g \right|^2}{\omega^2 \delta t^2} + \int \left| \nabla S_1^{\delta t}((n+1)\delta t)g \right|^2 \\
& \delta t^2 \int \sum_{k=0}^n \frac{\left| S_1^{\delta t}((k+1)\delta t)g - 2S_1^{\delta t}(k\delta t)g + S_1^{\delta t}((k-1)\delta t)g \right|^2}{\omega^2 \delta t^4} \\
& = \frac{1}{\omega^2} \int |g|^2.
\end{aligned} \tag{5.14}$$

It is clear from (5.14) that

$$\left| \omega \nabla S_1^{\delta t} g \right|_{L^2} \leq |g|_{L^2}.$$

On the other hand, multiplying (5.13) by ω^4 gives:

$$\begin{aligned}
& \omega^4 \left| S_1^{\delta t}((n+1)\delta t)g \right|_{L^2}^2 \leq \frac{\omega^4}{2} \left| S_1^{\delta t}((n+1)\delta t)g \right|_{L^2}^2 \\
& + 2 \left| \frac{S_1^{\delta t}((n+1)\delta t)g - S_1^{\delta t}(n\delta t)g}{\delta t} \right|_{L^2}^2 \\
& + \omega^2 \delta t \sum_{k=0}^n \delta t \left| \frac{S_1^{\delta t}((k+1)\delta t)g - 2S_1^{\delta t}(k\delta t)g + S_1^{\delta t}((k-1)\delta t)g}{\delta t^2} \right|_{L^2} \\
& \quad \times \left| \frac{\overline{S_1^{\delta t}(k\delta t)g} - \overline{S_1^{\delta t}((k-1)\delta t)g}}{\delta t} \right|_{L^2},
\end{aligned}$$

so that

$$\begin{aligned}
& \frac{\omega^4}{2} \left| S_1^{\delta t}((n+1)\delta t)g \right|_{L^2}^2 \leq 2|g|_{L^2} \\
& + \omega^2 \delta t^2 \left\{ \sum_{k=0}^n \left| \frac{S_1^{\delta t}((k+1)\delta t)g - 2S_1^{\delta t}(k\delta t)g + S_1^{\delta t}((k-1)\delta t)g}{\delta t^2} \right|_{L^2}^2 \right\}^{1/2}
\end{aligned}$$

$$\times \left\{ \sum_{k=0}^n \left| \frac{S_1^{\delta t}(k\delta t)g - S_1^{\delta t}((k-1)\delta t)g}{\delta t} \right|_{L^2}^2 \right\}^{1/2}.$$

The r.h.s of this inequality is controlled via (5.14) by

$$\begin{aligned} \frac{\omega^4}{2} |S_1^{\delta t}((n+1)\delta t)g|_{L^2}^2 &\leq 2|g|_{L^2} + \omega^2 \delta t |g|_{L^2} \left(\sum_{k=0}^n |g|_{L^2}^2 \right)^{1/2}, \\ &\leq 2|g|_{L^2} + (\omega^2 \delta t^{1/2}) (n\delta t)^{1/2} |g|_{L^2}, \end{aligned}$$

which leads to the result. ■

Lemma 5.2 with lemma 5.3 finish the proof of proposition 5.1.

We moreover need a uniform bound on γ .

Lemma 5.4

One has:

$$\forall f \in H^s, |\gamma f|_{H^s} \leq \delta t |f|_{H^s}.$$

Proof : We take a spectral representation of γ , given thanks to proposition 4.1:

$$\hat{\gamma} = \left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} + \frac{\xi^2}{2} \right)^{-1} (\hat{X}_1 - \hat{X}_2)^{-1}$$

One gets,

$$(\hat{\gamma})^{-1} = \sqrt{\frac{\hat{\mu} + \sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{2}} + i \sqrt{\frac{-\hat{\mu} + \sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}}}{2}}$$

Hence

$$|\hat{\gamma}|^{-2} = \sqrt{\hat{\mu}^2 + \frac{\xi^4}{\delta t^2}},$$

that is

$$|\hat{\gamma}|^{-4} = \left(\frac{\xi^4}{4} - \frac{4\xi^2}{\omega^2 \delta t^2} \right)^2 + \frac{1}{\delta t^4} + \frac{\xi^4}{2\delta t^2} + \frac{8\xi^2}{\omega^2 \delta t^4} \geq \frac{1}{\delta t^4}.$$

■

Let us recall that for equations (5.1):

$$F^{n+1} = X_1 F^n + \gamma X_1 f^{n+1},$$

$$G^{n+1} = X_2 G^n - \gamma X_2 f^{n+1},$$

we have proved that, X_1 and X_2 are uniformly bounded operators, that $X_k^{\frac{T}{\delta t}}$ are bounded uniformly in δt and in ω under the condition $\omega^2 \delta t^{\frac{1}{2}} \leq K$ by proposition 5.1. Moreover $\frac{\gamma}{\delta t}$ is bounded. Applying the technique presented for (NLS) in section 2, one gets the existence part of theorem 5.1 .

For the convergence part, it is enough to show that: $X_1^{\frac{T}{\delta t}}$ and $X_2^{\frac{T}{\delta t}}$ converge respectively to $e^{i\frac{\omega^2}{2}(1-\sqrt{1-\frac{4\Delta}{\omega^2}})T}$ and $e^{i\frac{\omega^2}{2}(1+\sqrt{1-\frac{4\Delta}{\omega^2}})T}$ for the strong topology of operators and that $\frac{\gamma}{\delta t}X_{1,2} \rightarrow -\frac{1}{i}(\sqrt{1-\frac{4\Delta}{\omega^2}})^{-1}$ for the same topology. In order to find an asymptotic expression for X_1 and X_2 , we build it by the characteristic equation (after taking a spectral representation).

$$X^2 \left(\frac{1}{\omega^2} - i\delta t + \frac{\xi^2}{2}\delta t^2 \right) + X \left(\frac{-2}{\omega^2} + i\delta t + \frac{\xi^2}{2}\delta t^2 \right) + \frac{1}{\omega^2} = 0$$

Plugging

$$X_{1,2} = 1 + c_{1,2}\delta t + d_{1,2}\delta t^2,$$

one gets by identification

$$\frac{(c_{1,2})^2}{\omega^2} - ic_{1,2} + \xi^2 = 0,$$

that is

$$c_{1,2} = i\frac{\omega^2}{2} \left(1 \mp \sqrt{1 + \frac{4\xi^2}{\omega^2}} \right).$$

Hence

$$\hat{X}_{1,2}^{\frac{T}{\delta t}} \rightarrow e^{i\frac{\omega^2}{2} \left(1 \mp \sqrt{1 + \frac{4\xi^2}{\omega^2}} \right) T}.$$

On the other hand

$$\begin{aligned} \hat{\gamma} &= - \left(\frac{1}{\omega^2\delta t^2} - \frac{i}{\delta t} + \frac{\xi^2}{2} \right)^{-1} \left(i\omega^2\delta t\sqrt{1 + \frac{4\xi^2}{\omega^2}} + o(\delta t) \right)^{-1} \\ &= - \left(\frac{1}{\omega^2\delta t} - i + \frac{\xi^2}{2}\delta t \right)^{-1} \left(i\omega^2\sqrt{1 + \frac{4\xi^2}{\omega^2}} + o(1) \right)^{-1} \\ &= - \frac{\delta t}{i\sqrt{1 + \frac{4\xi^2}{\omega^2}}} + o(\delta t). \end{aligned}$$

Therefore

$$\frac{\hat{\gamma}}{\delta t} \xrightarrow{\delta t \rightarrow 0} -\frac{1}{i} \frac{1}{\sqrt{1 + \frac{4\xi^2}{\omega^2}}}.$$

which ends the proof of theorem 5.1. ■

Remark 5.1

One can obtain convergence results as $\omega \rightarrow +\infty$, $\delta t \rightarrow 0$ as long as the stability condition $\omega^2\delta t^{\frac{1}{2}}$ is satisfied. See section 6 for comments.

Remark 5.2

Using lemma 5.3, one could work directly on the initial scheme (S_1) . However, we think that it is more interesting to characterize the behaviour of F and G which are respectively the Schrödinger and the oscillatory part of the solution.

5.2 Study of (S_2) .

The case of (S_2) is easier. The result is the same that the one of theorem 5.1:

Theorem 5.2

- Let $(F_0^{\delta t}, G_0^{\delta t}) \in (H^s)^2 (s > \frac{d}{2})$ that may depend on δt and such that

$$(F_0^{\delta t}, G_0^{\delta t}) \rightarrow (\tilde{F}_0, \tilde{G}_0) \text{ as } \delta t \rightarrow 0 \text{ in } H^s.$$

There exists a constant δt_0 depending only $|(\tilde{F}_0, \tilde{G}_0)|_{H^s}$ such that for any $\delta t \leq \delta t_0$, there exists a unique maximal solution to (5.1) with $F^0 = F_0^{\delta t}, G^0 = G_0^{\delta t}$ defined on the interval $[0, T_{\delta t}]$ (with $T_{\delta t} = N\delta t$ for some integer N).

- Let (F, G) be the solution of (4.3), (4.4) with the initial data $F(0) = \tilde{F}_0, G(0) = \tilde{G}_0$ and T_∞ its existence time.

One has $\liminf_{\delta t \rightarrow 0} T_{\delta t} \leq T_\infty$ and for all $T < T_\infty$,

$$(F^{\delta t}, G^{\delta t}) \rightarrow (F, G) \text{ in } L^\infty([0, T]; H^s)$$

where $(F^{\delta t}, G^{\delta t})$ is the piecewise constant function which value at point $t = n\delta t$ is (F^n, G^n) .

On one hand, since X_1 and X_2 are unitary operators, the semigroups $X_1^{\frac{T}{\delta t}}, X_2^{\frac{T}{\delta t}}$ are uniformly bounded.

On the other hand γ is given by

$$\hat{\gamma} = -i \frac{1}{\sqrt{\xi^4 + \frac{1}{\delta t^2} + \frac{4\xi^2}{\omega^2 \delta t^2}}}$$

which is obviously bounded by δt and

$$\frac{\hat{\gamma}}{\delta t} \rightarrow -i \frac{1}{\sqrt{1 + \frac{4\xi^2}{\omega^2}}}.$$

We still have to prove the convergence of the semigroups $X_{1,2}^{\frac{T}{\delta t}}$ toward their continuous counterparts.

Let us write

$$\hat{X}_{1,2}^{\frac{T}{\delta t}} = e^{\frac{T}{\delta t} \log \left(\frac{\frac{1}{\omega^2} \mp \frac{i}{2} \sqrt{\left(1 + \frac{4\xi^2}{\omega^2}\right) \delta t^2 + \xi^4 \delta t^4}}{\frac{1}{\omega^2} - i \frac{\delta t}{2} + \frac{\xi^2}{2} \delta t^2} \right)},$$

that is

$$\hat{X}_{1,2}^{\frac{T}{\delta t}} \sim e^{\frac{T}{\delta t} \log \left(\left(1 \mp \frac{i\omega^2}{2} \sqrt{1 + \frac{4\xi^2}{\omega^2}} \delta t\right) \left(1 + i \frac{\omega^2 \delta t}{2}\right) \right)} \text{ as } \delta t \rightarrow 0,$$

and then

$$\hat{X}_{1,2}^{\frac{T}{\delta t}} \sim e^{iT \frac{\omega^2}{2} \left(1 \mp \sqrt{1 + \frac{4\xi^2}{\omega^2}}\right)}.$$

The result follows. ■

Remark 5.3

The bounds on $X_1, X_2, X_1^{\frac{T}{\delta t}}, X_2^{\frac{T}{\delta t}}, \gamma$ are uniform with respect to δt and ω without any stability condition, so that any convergence result as $\omega \rightarrow +\infty, \delta t \rightarrow 0$ on $X_1^{\frac{T}{\delta t}}$ and $X_2^{\frac{T}{\delta t}}$ can be adapted to (S_2) . Of course, since $X_1^{\frac{T}{\delta t}}$ and $X_2^{\frac{T}{\delta t}}$ are unitary on L^2 , there is no diffusion in (S_2) .

6 Final remarks and numerical experiments

6.1 Diffusion and oscillations

Let us recall the splitting for the continuous problem (4.1)-(4.2):

$$\begin{cases} \partial_t F = \frac{i\omega^2}{2} \left(1 - \sqrt{1 - \frac{4\Delta}{\omega^2}}\right) F - \frac{1}{i} \left(\sqrt{1 - \frac{4\Delta}{\omega^2}}\right)^{-1} (\lambda |F + G|^{2\sigma} (F + G)) \\ \partial_t G = \frac{i\omega^2}{2} \left(1 + \sqrt{1 - \frac{4\Delta}{\omega^2}}\right) G + \frac{1}{i} \left(\sqrt{1 - \frac{4\Delta}{\omega^2}}\right)^{-1} (\lambda |F + G|^{2\sigma} (F + G)) \end{cases}$$

We have $|G(0)|_{H^s} \leq \frac{C}{\omega^2}$ (see [2]). It is clear that

$$e^{i\frac{\omega^2}{2} \left(1 - \sqrt{1 - \frac{4\Delta}{\omega^2}}\right) t} \xrightarrow{\omega \rightarrow +\infty} e^{i\Delta t},$$

$$e^{i\frac{\omega^2}{2} \left(1 + \sqrt{1 - \frac{4\Delta}{\omega^2}}\right) t} - e^{i\omega^2 t} e^{-i\Delta t} \xrightarrow{\omega \rightarrow +\infty} 0.$$

Therefore F is the part of the solution that converges to the solution of (NLS) . The function G is an oscillatory part of the solution, the amplitude of these oscillations are $\frac{1}{\omega^2}$ while the frequency is $\frac{\omega^2}{2\pi}$. The question is: how the scheme take into account this behaviour? Let us consider first the expression (4.3) and (4.4) of the schemes:

$$\frac{F^{n+1} - F^n}{\delta t} = i\alpha \left(\frac{F^{n+1} + F^n}{2} \right) + \gamma \left(\frac{1}{\delta t} + i\frac{\alpha}{2} \right) f^{n+1}, \quad (6.1)$$

$$\frac{G^{n+1} - G^n}{\delta t} = i\beta \left(\frac{G^{n+1} + G^n}{2} \right) - \gamma \left(\frac{1}{\delta t} + i\frac{\beta}{2} \right) f^{n+1}. \quad (6.2)$$

From (4.7) and (4.8) one finds

$$\alpha = \frac{2i}{\delta t} (1 + X_1)^{-1} (1 - X_1),$$

$$\beta = \frac{2i}{\delta t} (1 + X_2)^{-1} (1 - X_2).$$

For the scheme (S1), under the condition $\omega^2 \delta t = 1$ (which does not satisfy the stability condition $\omega^4 \delta t \leq K$), one obtains at the first order when $\delta t \rightarrow 0$ that $X_2 \rightarrow \frac{1+i}{2}$, and $X_1 \rightarrow 1$, so that the linear part on G^n can be written as

$$G^{n+1} = \frac{1+i}{2} G^n \text{ and } G(T) = \frac{1}{(\sqrt{2})^{T/\delta t}} e^{\frac{i\pi}{4} \frac{T}{\delta t}} G(0),$$

or

$$G(T) = \frac{1}{(\sqrt{2})^{T\omega^2}} e^{\frac{i\pi}{4} T\omega^2} G(0).$$

On the other hand, under the condition $\omega^4 \delta t = 1$, one finds that

$$X_2 = 1 + i\delta t^{1/2} + (-i\Delta - 1)\delta t + O(\delta t^{3/2}), \quad X_1 = 1 + O(\delta t),$$

so that

$$X_2^{T/\delta t} \sim e^{\frac{iT}{\delta t^{1/2}}} e^{-i\Delta T} e^{-T},$$

that is

$$X_2^{T/\delta t} \sim e^{iT\omega^2} e^{-i\Delta T} e^{-T},$$

and we recover the correct behaviour for G^n on short time scale; the oscillations are however damped exponentially in time.

On the contrary, for scheme (S2), let us take $\omega^2 = \frac{1}{\delta t}$: in order to capture the oscillations at the frequency ω^2 , one has to take δt at least smaller than $\frac{1}{\omega^2}$.

Then

$$\hat{X}_1 = \frac{\frac{1}{\delta t} - \frac{i}{2} \sqrt{\frac{1}{\delta t^2} + \xi^4 + \frac{4\xi^2}{\delta t}}}{\frac{1}{\delta t} - \frac{i}{2\delta t} + \frac{\xi^2}{2}},$$

that is

$$\hat{X}_1 = \frac{1 - \frac{i}{2} \sqrt{1 + \xi^4 \delta t^2 + 4\xi^2 \delta t}}{\left(1 - \frac{i}{2}\right) + \frac{\xi^2}{2} \delta t},$$

As $\delta t \rightarrow 0$ one gets

$$\hat{X}_1 \sim \frac{1 - \frac{i}{2} (1 + 2\xi^2 \delta t)}{\left(1 - \frac{i}{2}\right) + \frac{\xi^2}{2} \delta t}.$$

Therefore

$$\begin{aligned} 1 - \hat{X}_1 &\sim \frac{\left(1 - \frac{i}{2}\right) + \xi^2 \frac{\delta t}{2} - 1 + \frac{i}{2} (1 + 2\xi^2 \delta t)}{\left(1 - \frac{i}{2}\right) + \xi^2 \frac{\delta t}{2}}, \\ &= \frac{\xi^2 \delta t \left(\frac{1}{2} + i\right)}{\left(1 - \frac{i}{2}\right) + \xi^2 \frac{\delta t}{2}} \end{aligned}$$

and

$$\begin{aligned} 1 + \hat{X}_1 &= \frac{\left(1 - \frac{i}{2}\right) + \xi^2 \frac{\delta t}{2} + 1 - \frac{i}{2} (1 + 2\xi^2 \delta t)}{\left(1 - \frac{i}{2}\right) + \xi^2 \frac{\delta t}{2}}, \\ &= \frac{(2 - i) + \xi^2 \delta t \left(\frac{1}{2} - i\right)}{\left(1 - \frac{i}{2}\right) + \xi^2 \frac{\delta t}{2}}. \end{aligned}$$

Therefore, after straightforward computations, one gets

$$\alpha \sim -\xi^2.$$

In the same way, one finds

$$\hat{X}_2 \sim \frac{1 + \frac{i}{2}(1 + 2\xi^2\delta t)}{\left(1 - \frac{i}{2}\right) + \xi^2\frac{\delta t}{2}}.$$

Therefore,

$$\begin{aligned} 1 - \hat{X}_2 &\sim \frac{1 - \frac{i}{2} + \xi^2\frac{\delta t}{2} - 1 - \frac{i}{2}(1 + 2\xi^2\delta t)}{\left(1 - \frac{i}{2}\right) + \xi^2\frac{\delta t}{2}}, \\ &\sim \frac{i}{\left(1 - \frac{i}{2}\right) + \xi^2\frac{\delta t}{2}}. \end{aligned}$$

On the same way,

$$\begin{aligned} 1 + \hat{X}_2 &= \frac{\left(1 - \frac{i}{2}\right) + \xi^2\frac{\delta t}{2} + 1 + \frac{i}{2}(1 + 2\xi^2\delta t)}{\left(1 - \frac{i}{2}\right) + \xi^2\frac{\delta t}{2}}, \\ &\sim \frac{2}{\left(1 - \frac{i}{2}\right) + \xi^2\frac{\delta t}{2}}, \end{aligned}$$

so that

$$\beta \sim -\omega^2.$$

Therefore F^n converges to the solution of (NLS) while the equation on G^n is asymptotically

$$\frac{G^{n+1} - G^n}{\delta t} + i\omega^2 \left(\frac{G^{n+1} + G^n}{2} \right) = h.o.t.$$

The scheme (S_2) captures the oscillations with the good frequency. Note that the condition on the time step: $\delta t \leq \frac{1}{\omega^2}$ is natural to obtain precise enough results.

6.2 Numerical results.

We have computed solutions to (S_1) and (S_2) in 1D, with $\sigma = 2$ using a finite differences discretization of $-\Delta$ in order to illustrate the above described behaviour. For $\sigma = 2, \lambda > 0$ one has blowing up solutions for (NLW_ω) if ω is not too large (see [3]) and also for (NLS). We did not try to refine in time and space near the numerical blow up. We compute on the interval $[-5, 5]$ with $\delta x = 10^{-2}$. At each time step, one has to solve a nonlinear system:

$$\begin{aligned} \frac{1}{\omega^2} \left(\frac{E^{n+1} - 2E^n + E^{n-1}}{\delta t^2} \right) - i \left(\frac{E^{n+1} - E^n}{\delta t} \right) - A_h \left(\frac{E^{n+1} + E^n}{2} \right) = \\ \frac{|E^{n+1}|^4 + |E^n|^4 + |E^n|^2 |E^{n+1}|^2}{3} \left(\frac{E^{n+1} + E^n}{2} \right), \end{aligned} \tag{6.3}$$

E^n and E^{n-1} are given by the previous time steps.
To find E^{n+1} , we use a fixed point procedure to solve

$$\left(\frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{1}{2} A_h \right) X = \frac{|X|^4 + |E^n|^4 + |E^n|^2 |X|^2}{3} \left(\frac{X + E^n}{2} \right) + H^n.$$

We consider the iteration k :

$$\left\{ \frac{1}{\omega^2 \delta t^2} - \frac{i}{\delta t} - \frac{1}{2} A_h - \left(\frac{|X_k|^4 + |E^n|^4 + |E^n|^2 |X_k|^2}{6} \right) \right\} X_{k+1} = \frac{|X_k|^4 + |E^n|^4 + |E^n|^2 |X_k|^2}{6} E^n + H^n$$

This semi-implicit procedure has the advantage to preserve, at each internal step, the invariant (3.3) for (S_1) (or (3.5) for (S_2)), and therefore it is more stable than the explicit version.

- About blowing up : if ω is large enough, the solution of (NLW_ω) seems to blow up allways before that of (NLS) and the existence time T_ω seems to be an increasing function of ω . See figure 1 for which:

$$E(0) = 4e^{-20x^2} \text{ and } \partial_t E(0) = e^{-20x^2}, \delta t = 10^{-5}.$$

In all the figures, the t-scale is multiplied by 10^3 .

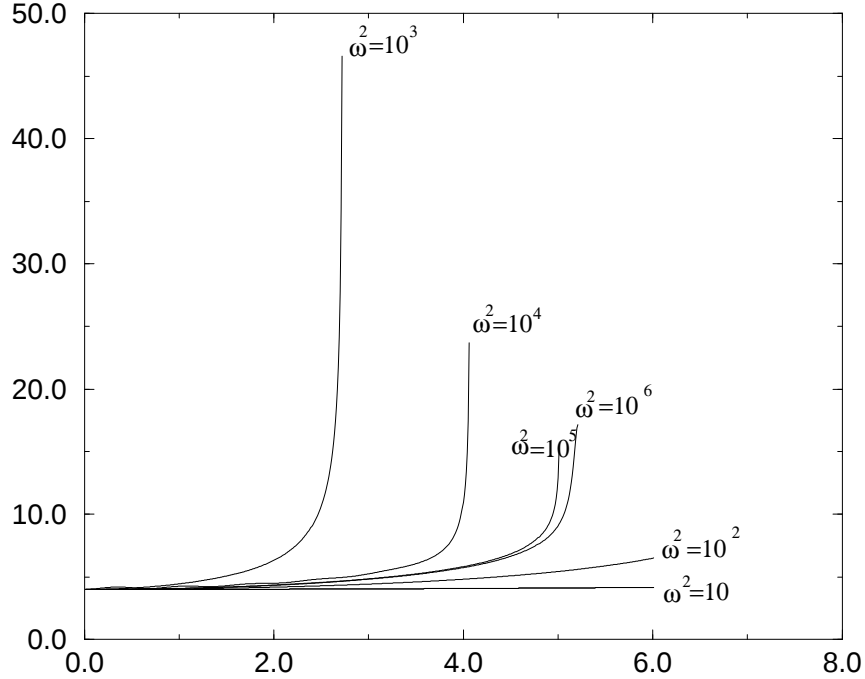


Figure 1: $|E_\omega(0, t)|$ for $\omega^2 = 10, 10^2, 10^3, 10^4, 10^5, 10^6$ computed by $(S1)$.

• About oscillations: for $\omega^2 = 10^5$, $\delta t = 10^{-5}$, $E(0) = 4e^{-20x^2}$ and $\partial_t E(0) = e^{-20x^2}$ one can see oscillations with the correct amplitude and frequency by the scheme (S_2) while there are no oscillation on the solution computed by (S_1) see figure 2 and figure 3.

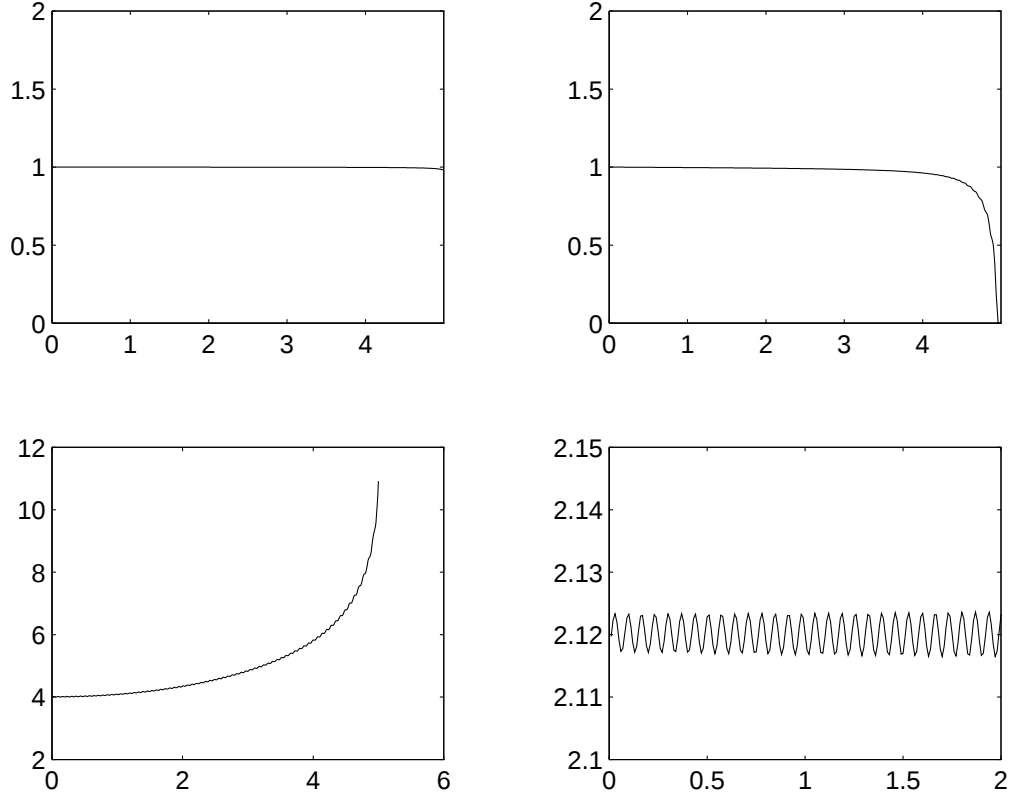


Figure 2: Scheme (S_2) , noncompatible initial data, upper left: Invariant (3.2), upper right: Invariant (3.1), bottom left $|E_\omega(0, t)|$, bottom right $|E_\omega|_{L^2}(t)$.

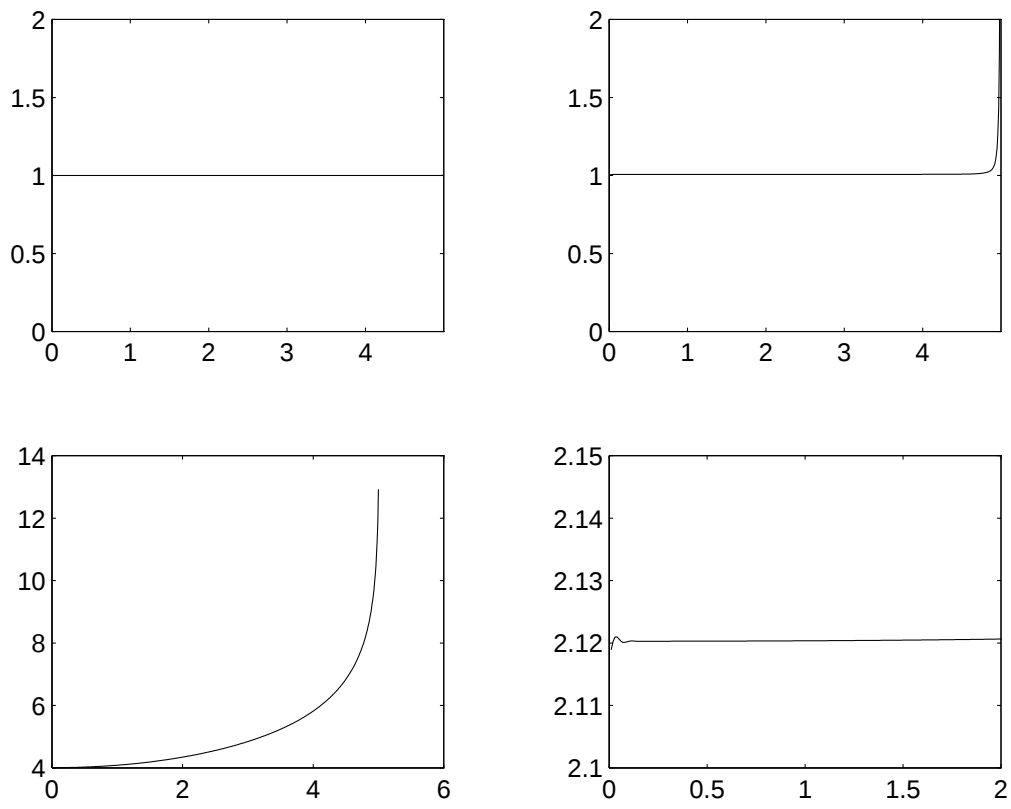


Figure 3: Scheme (S1), noncompatible initial data upper left: Invariant (3.2), upper right: Invariant (3.1), bottom left $|E_\omega(0, t)|$, bottom right $|E_\omega|_{L^2}(t)$.

If one choose

$$\partial_t E(0) = i(\Delta E(0) + |E(0)|^4 E(0)),$$

that is for compatible initial data that ensure that $G(0) = O(\frac{1}{\omega^4})$, these oscillations disappear, see figure 4.

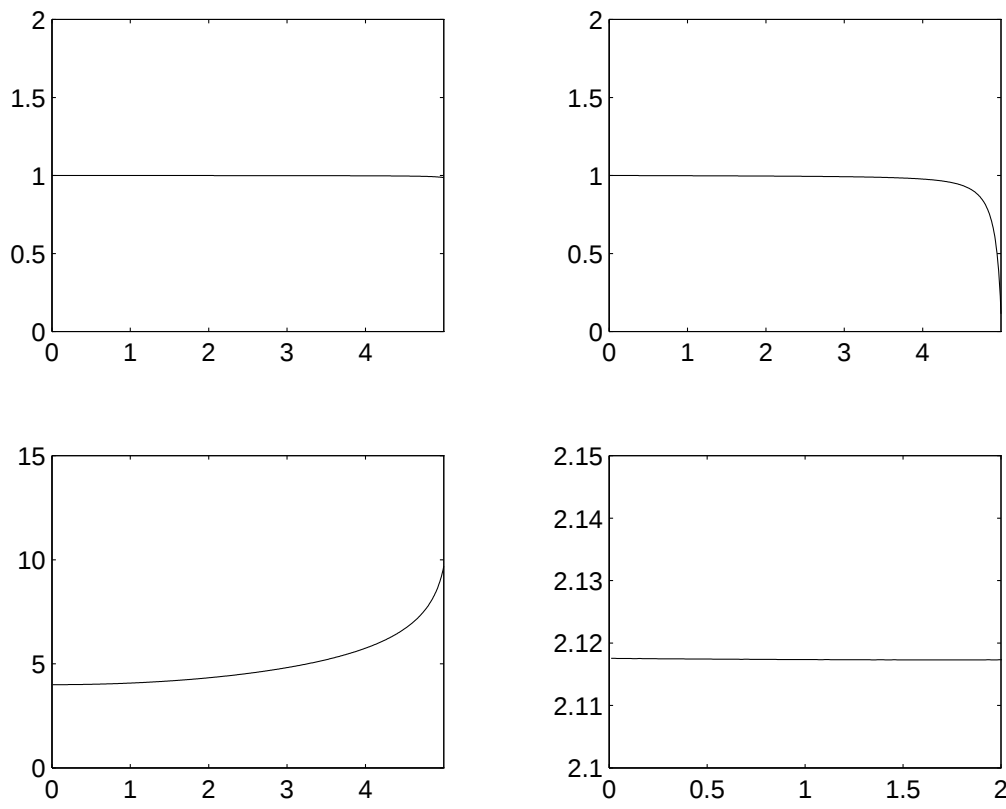


Figure 4: Scheme $(S2)$, compatible initial data, upper left: Invariant (3.2), upper right: Invariant (3.1), bottom left $|E_\omega(0, t)|$, bottom right $|E_\omega|_{L^2}(t)$.

For $\omega = 10^6$ the solution given by $(S1)$ is close to that of the nonlinear Schrödinger equation given by the Crank-Nicolson scheme. However, the behavior near the blow-up time of the solution given by $(S2)$ for ω large is highly oscillatory so that $(S2)$ is not appropriate in this case. Therefore, both schemes can be useful: $(S1)$ can be used in order to compute the mean value of the solution to (NLW_ω) until the blow-up time and $(S2)$ in order to compute the oscillations that exist in the physical solution.

References

- [1] G. D. Akrivis, V. A. Dougalis and O. A. Karakashian, *On fully discret Galerkin methods of second order temporal accuracy for the nonlinear Schrödinger equation* Numer. Math. 59, 31-53, (1991).
- [2] L. Bergé, B. Bidegaray, T. Colin, *A perturbative analysis of the time-envelope approximation in strong Langmuir turbulence*, Physica D, vol. 95, No 3-4, pp 351-379 (1996).
- [3] L. Bergé, T. Colin, *A singular perturbation problem for an envelope equation in plasma physics*, Physica D 84, 437-459, (1995).
- [4] H. Brezis, T. Gallouët, *Nonlinear Schrödinger evolution equations*, Nonlinear Analysis TMA, vol 4, No4, 677-681, (1980).
- [5] M. Delfour, M. Fortin and G. Payne, *Finite difference solutions of a nonlinear Schrödinger equation*, J. comput. Phys. 44, 277-288, (1981).
- [6] J. Ginibre, G. Velo, *On a class of nonlinear Schrödinger equations Part I,II*. J. Funct. Anal. 32, 1979, p1-32, 33-71; *part III* Ann. Inst. H Poincaré, A 28, 1978, p287-316; *The global Cauchy problem for the nonlinear Schrödinger equation revisited*. Ann. Inst. H. Poincaré, Anal. Non Linéaire 2,1985 ,p309-402.
- [7] D.R. Nicholson *Introduction to plasma theory*. J. Wiley and Sons Eds., New-York, 177-181 (1983).
- [8] J. M. Sanz-Serna, *Methods for the numerical solution of the nonlinear Schrödinger equation* Mathematics of computation, 43, 167, 21-27 (1984).