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► To cite this version:

Mostafa Abounouh, Hassan Moatassime, Jean-Paul Chehab, Serge Dumont, Olivier Goubet. Discrete Schrödinger equations and dissipative dynamical systems. Communications on Pure and Applied Analysis, 2008, 7 (2), pp.211-227. <10.3934/cpaa.2008.7.211>. <hal-01113776>

HAL Id: hal-01113776

<https://hal.science/hal-01113776v1>

Submitted on 14 Jan 2020

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DISCRETE SCHRÖDINGER EQUATIONS AND DISSIPATIVE DYNAMICAL SYSTEMS

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ABSTRACT. We introduce a Crank-Nicolson scheme to study numerically the long-time behavior of solutions to a one dimensional damped forced nonlinear Schrödinger equation. We prove the existence of a *smooth* global attractor for these discretized equations. We also provide some numerical evidences of this asymptotical smoothing effect.

1. **Introduction.** Weakly damped nonlinear Schrödinger equations provide examples of infinite-dimensional dynamical systems, in the framework described in [18], [10], [17]. For these infinite-dimensional dynamical systems the major issues are: does it exist a *global attractor* for the dissipative dynamical system under consideration ? does this global attractor has finite Hausdorff and fractal dimension ? is this global attractor *regular* ?

Let us give an overview of the previous results for weakly damped nonlinear Schrödinger equations, that are equations that read

$$u_t + \alpha u + iu_{xx} + i|u|^2u = f. \quad (1)$$

Here the unknown $u(t, x)$ maps $\mathbb{R}_t \times \mathbb{T}_x$ into \mathbb{C} . We mean that u is a periodic function with respect to x . Actually $\alpha > 0$ is the damping parameter and the external force f , that does not depend to t , belongs to $L^2(\mathbb{T})$. The pioneering work [6] proved the existence of a finite dimensional *weak* global attractor \mathcal{A} for dissipative NLS. By weak attractor we mean that the attractor attracts the trajectories for the weak topology in the Hilbert space chosen for the mathematical study. Moreover, due to a famous argument due to J.

2000 *Mathematics Subject Classification.* 35B41, 35Q55, 65M06.

Ball, it turns out that this weak attractor is actually a global attractor in the usual sense. Hence the two first issues were successfully addressed. For the issue of the regularity of the attractor, the first result appeared in [7] and states as follows: consider the dynamical system provided by dissipative NLS in $H^1(\mathbb{T})$ with a forcing term in $L^2(\mathbb{T})$, then the global attractor is actually a compact subset of $H^2(\mathbb{T})$. In other words dissipative NLS feature an *asymptotical smoothing effect*, following the terminology introduced in [12].

In this article we would like to address the same issues for discrete nonlinear Schrödinger equations. By discrete nonlinear Schrödinger equations, we mean that we discretize the equation *both* in time and in space and we consider the associated finite-dimensional dynamical system. For discrete nonlinear Schrödinger equations some interesting results are available in the literature but mainly for discretization in space of the equations (nevertheless we refer to the work [3] where a suitable splitting scheme was used for the damped nonlinear Schrödinger equations). We would like to refer to [19] and [5] where the authors consider some discretization in space of the Laplace operator on a finite interval with finite differences and then study the dynamical systems provided by the associated ODE. On the other hand, we would like also to point out the study of discrete nonlinear Schrödinger equations as an infinite-dimensional dynamical system in a lattice in [13]; the authors consider the ODE in the infinite dimensional space $l^2(\mathbb{Z})$ defined at each point $j \in \mathbb{Z}$ by

$$(u_j)_t + \gamma u_j + i(2u_j - u_{j+1} - u_{j-1}) + i|u_j|^2 u_j = f_j. \quad (2)$$

In our article we discretize the Laplace operator with finite differences on a grid of mesh size Δx . We consider also a time discretization provided by a suitable Crank-Nicolson scheme. We prove below that this new scheme fits with the damping and is *unconditionally stable* even for long time. This allow us to prove the existence of a global attractor $\mathcal{A}_{\Delta x}$ for the discrete dynamical system under consideration. Our aim was to give some numerical evidence of the regularity of this attractor. This question is meaningless if one says that we deal with finite dimensional space and that all norms are equivalent. But this matters if we want to have estimates that are uniform in Δx and Δt . Introduce $L_{\Delta x}^2$ and $H_{\Delta x}^s$ spaces as follows. Set A for the discrete Laplace operator in finite differences. Set, for a vector U in \mathbb{C}^N ,

$$\|U\|_{L_{\Delta x}^2}^2 = (\Delta x) \sum_j |u_j|^2, \quad (3)$$

and

$$\|U\|_{H_{\Delta x}^s}^2 = \|(A + Id)^{s/2} U\|_{L_{\Delta x}^2}^2. \quad (4)$$

Our first result states as follows

Theorem 1. *There exists $\mathcal{A}_{\Delta x}$ a compact global attractor for the Discrete Nonlinear Schrödinger equations in $L_{\Delta x}^2$. Moreover $\mathcal{A}_{\Delta x}$ is a bounded subset in $H_{\Delta x}^2$, uniformly in Δt and Δx .*

The results compares with [9] for the continuous case. This results is not obvious since by the inverse inequality, $\|U\|_{H_{\Delta x}^2} \leq c(\Delta x)^{-2} \|U\|_{L_{\Delta x}^2}$, a bounded set in $L_{\Delta x}^2$ is not (uniformly) bounded in $H_{\Delta x}^2$. We give also some numerical evidence for this result. Consider an initial data that is not regular (a shock). Our numerical scheme introduces

no artificial viscosity, and for short interval of times, the solution remains as regular as the shock. But, for the long range, some smoothing occurs.

After the stability issues, come the *consistency*. Consider the ODE provided by (2) on a finite number of j s, corresponding to the discretization of (1) in finite differences. One can prove that this ODE features a global attractor \mathcal{A}_{ODE} (see [19]). We prove in the sequel that for a trajectory in this attractor \mathcal{A}_{ODE} , our scheme is of order 2 in time, uniformly in Δx . We prove also the upper continuity of the attractor, that is if both Δt and Δx converge to 0 then $\mathcal{A}_{\Delta x}$ converges to \mathcal{A} , the continuous attractor. On open question is to estimate the distance between these two attractors. We cannot conclude since we do not now the speed of convergence of trajectories towards \mathcal{A} .

For this issue and the issue of lower semi-continuity of attractors, one can conclude only if we now that we have a gradient system and if we know that the continuous flow satisfies the following property: the stationary points, that are in finite numbers, are hyperbolic (see [17] and the references therein). To our knowledge, the precise comparison between a continuous flow and its time discretization requires this kind of property; we would like to refer to [1], [2] where the authors compare the flow and its time discretization in respectively a neighborhood of an hyperbolic fixed point and an hyperbolic periodic orbit. The hyperbolicity properties mean that the stable and unstable manifolds at each point of the invariant set under consideration intersect transversally. This applies for instance for Ginzburg-Landau equation, that is a parabolic regularization of Schrödinger equation. For the sake of completeness, we would like also to point out [14] where the authors gives a complete study of the discretized Ginzburg-Landau equation.

This article is organized as follows. In the second section, we introduce the time discretization and we prove Theorem 1. In a third section we discuss the upper continuity and the consistency properties. In a last section we perform some numerics.

2. The discrete Schrödinger equation.

2.1. A new scheme. Consider the ODE provided by a finite difference approximation (in space) of the periodic NLS equation (1).

Introducing

$$A = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & -1 \\ -1 & 2 & -1 & \ddots & & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & & \ddots & \ddots & \ddots & -1 \\ -1 & 0 & \dots & 0 & -1 & 2 \end{pmatrix}$$

this ODE reads

$$U_t + \alpha U - iAU + i|U|^2 U = F \quad (5)$$

where $(|U|^2 U)_j = |U_j|^2 U_j$, $U \in \mathbb{C}^N$ and where F stands for a finite difference approximation of f . We assume in the following that $\|F\|_{L^2_{\Delta x}}$ is bounded uniformly in Δx .

At a first glance, the classical time discretization of (5) could be

$$\begin{aligned} \frac{U^{n+1} - U^n}{\Delta t} + \alpha \frac{U^{n+1} + U^n}{2} - i A \left(\frac{U^{n+1} + U^n}{2} \right) \\ + \frac{i}{4} (|U^{n+1}|^2 + |U^n|^2) (U^{n+1} + U^n) = F. \end{aligned} \quad (6)$$

In this article, we rather introduce a new scheme ; to begin with, let us observe that (5) is equivalent to

$$\frac{d}{dt} (e^{\alpha t} U) - i A (e^{\alpha t} U) + i |U|^2 (e^{\alpha t} U) = e^{\alpha t} F. \quad (7)$$

We discretize this equation by an Euler scheme of order two to obtain (after multiplication by $e^{-\alpha(n+1)\Delta t}$)

$$\begin{aligned} \frac{U^{n+1} - e^{-\alpha\Delta t} U^n}{\Delta t} - i A \left(\frac{U^{n+1} + e^{-\alpha\Delta t} U^n}{2} \right) + \\ \frac{i}{4} (|U^{n+1}|^2 + |U^n|^2) (U^{n+1} + e^{-\alpha\Delta t} U^n) = \frac{1 + e^{-\alpha\Delta t}}{2} F. \end{aligned} \quad (8)$$

We would like to point out that if $\alpha\Delta t \ll 1$, then since $e^{-\alpha\Delta t} \simeq 1 - \alpha\Delta t$, (8) is equal to (6) up to second order.

2.2. Uniform stability: $L_{\Delta x}^2$ estimate. We now prove that this new scheme is stable in $L_{\Delta x}^2$, uniformly in Δx and time (discrete time $n\Delta t$), assuming that $\alpha\Delta t \ll 1$.

Proposition 1. *Assume that $\alpha\Delta t$ is small enough. There exists $\delta = e^{-\alpha\Delta t} < 1$ such that*

$$\|U^n\|_{L_{\Delta x}^2}^2 \leq \delta^n \|U^0\|_{L_{\Delta x}^2}^2 + (1 - \delta^n) \frac{8}{\alpha^2} \|F\|_{L_{\Delta x}^2}^2 \quad (9)$$

Proof :

Consider the scalar product of (8) with $U^{n+1} + e^{-\alpha\Delta t} U^n$ in the real Hilbert space $\mathbb{C}^N \simeq \mathbb{R}^{2N}$ (endowed with the scalar product in $L_{\Delta x}^2$) to obtain

$$\|U^{n+1}\|_{L_{\Delta x}^2}^2 \leq e^{-2\alpha\Delta t} \|U^n\|_{L_{\Delta x}^2}^2 + \Delta t | \langle F, U^{n+1} + e^{-\alpha\Delta t} U^n \rangle |, \quad (10)$$

where $\langle F, G \rangle = (\Delta x) \sum_j \operatorname{Re}(F_j \overline{G_j})$.

Therefore, by Young's inequality

$$\left(1 - \frac{\alpha\Delta t}{4}\right) \|U^{n+1}\|_{L_{\Delta x}^2}^2 \leq e^{-2\alpha\Delta t} \left(1 + \frac{\alpha\Delta t}{4}\right) \|U^n\|_{L_{\Delta x}^2}^2 + \frac{2\Delta t}{\alpha} \|F\|_{L_{\Delta x}^2}^2 \quad (11)$$

We observe that for $\alpha\Delta t$ small enough we have $\delta \left(1 - \frac{\alpha\Delta t}{4}\right)^{-1} \left(1 + \frac{\alpha\Delta t}{4}\right) \leq 1$. We then obtain

$$\|U^{n+1}\|_{L_{\Delta x}^2}^2 \leq \delta \|U^n\|_{L_{\Delta x}^2}^2 + \frac{4\Delta t}{\alpha} \|F\|_{L_{\Delta x}^2}^2 \quad (12)$$

The discrete Gronwall's lemma gives then

$$\|U^n\|_{L_{\Delta x}^2}^2 \leq \delta^n \|U^0\|_{L_{\Delta x}^2}^2 + (1 - \delta^n) \frac{4\alpha\Delta t}{\alpha^2(e^{\alpha\Delta t} - 1)} \|F\|_{L_{\Delta x}^2}^2, \quad (13)$$

that completes the proof of the Proposition. \square

2.3. Well-posedness of scheme. (8) defines an implicit scheme. This problem is well-posed if we are able to prove that the Picard iteration scheme $w^k \rightarrow w^{k+1}$ on \mathbb{C}^N defined by

$$\frac{w^{k+1} - e^{-\alpha\Delta t}U^n}{\Delta t} - \frac{iA}{2}(w^{k+1} + e^{-\alpha\Delta t}U^n) + \frac{i}{4}(|w^k|^2 + |U^n|^2)(w^{k+1} + e^{-\alpha\Delta t}U^n) = \frac{1 + e^{-\alpha\Delta t}}{2}F \quad (14)$$

with $w^0 = 0$ is convergent. It is an exercise (proceeding as in section 2.2) to prove that

$$\sup_k \|w^k\|_{L^2_{\Delta x}}^2 \leq \frac{8}{\alpha^2} \|F\|_{L^2_{\Delta x}}^2. \quad (15)$$

On the one hand, estimates (15) ensures that the non linear mapping $w^k \rightarrow w^{k+1}$, that is continuous, send the ball of radius $\frac{2\sqrt{2}}{\alpha} \|F\|_{L^2_{\Delta x}}$ into itself. The Brouwer fixed point theorem applies and then leads to the existence of a fixed point U^{n+1} .

On the other hand, if one prefers to establish the uniqueness of the fixed point, we rather use the following statement, assuming some kind of CFL condition on $\frac{\Delta t}{\Delta x}$.

Lemma 1. : Assume that $\frac{\Delta t}{\Delta x}$ is small enough. Then the mapping $w^k \rightarrow w^{k+1}$ is a contraction and the Banach fixed point theorem applies. Then we have the existence and uniqueness of a fixed point U^{n+1} .

Proof :

Consider (14) at step $k-1$ and subtract this equation to (14) at step k . We thus obtain the following equation for $Z_k = w^{k+1} - w^k$

$$\begin{aligned} & Z_k - \frac{i\Delta t}{2}AZ_k + \frac{i\Delta t}{4}(|U^n|^2)Z_k \\ & + \frac{i\Delta t}{4}(|w^k|^2 - |w^{k-1}|^2)U^n e^{-\alpha\Delta t} \\ & + \frac{i\Delta t}{4}(|w^k|^2 Z_k + (|w^k|^2 - |w^{k-1}|^2)w^k) = 0. \end{aligned} \quad (16)$$

Let us now multiply this equation by Z_k in the real Hilbert space $L^2_{\Delta x}$ and to obtain

$$\begin{aligned} \|Z_k\|_{L^2_{\Delta x}}^2 &= \frac{\Delta t}{4} \langle w^k \overline{Z_{k-1}} U^n e^{-\alpha\Delta t}, iZ_k \rangle \\ &+ \frac{\Delta t}{4} \langle \overline{w^{k-1}} Z_{k-1} U^n e^{-\alpha\Delta t}, iZ_k \rangle \\ &+ \frac{\Delta t}{4} \langle w^k \overline{Z_{k-1}} w^k, iZ_k \rangle + \frac{\Delta t}{4} \langle \overline{w^{k-1}} Z_{k-1} w^k, iZ_k \rangle \end{aligned} \quad (17)$$

and then, by straightforward inequalities

$$\begin{aligned} \|Z_k\|_{L^2_{\Delta x}}^2 &\leq (\Delta t \|Z_k\|_{L^2_{\Delta x}} \|Z_{k-1}\|_{L^2_{\Delta x}}) \\ &\cdot (\|w^{k-1}\|_{L^\infty_{\Delta x}} + \|w^k\|_{L^\infty_{\Delta x}}) (\|U^n\|_{L^\infty_{\Delta x}} + \|w^k\|_{L^\infty_{\Delta x}} + \|w^{k-1}\|_{L^\infty_{\Delta x}}) \end{aligned} \quad (18)$$

We now recall the following well-known inverse inequality

Lemma 2. : $\|f\|_{L_{\Delta x}^\infty} \leq \frac{1}{(\Delta x)^{\frac{1}{2}}} \|f\|_{L_{\Delta x}^2}$.

Then, the uniform upper bound for w^k , U^n on $L_{\Delta x}^2$ leads to : there exists $c > 0$ such that

$$\|Z_k\|_{L_{\Delta x}^2} \leq c \left(\frac{\Delta t}{\Delta x} \right) \|Z_{k-1}\|_{L_{\Delta x}^2} \quad (19)$$

The results follows promptly. \square

2.4. Existence for the discrete global attractor. At this stage we have defined a nonlinear mapping $S : U^n \rightarrow U^{n+1}$ that maps continuously $L_{\Delta x}^2 \simeq \mathbb{C}^N$ into itself and that possesses a bounded absorbing set in $L_{\Delta x}^2$.

Since we are dealing with finite dimensional space, we have that the continuous map S is compact, then Theorem I.1.1 in [18] applies and we obtain

Proposition 2. *There exists $\mathcal{A}_{\Delta x}$ a compact set in $L_{\Delta x}^2$ that is a global attractor for the dynamical system defined by the Discrete Nonlinear Schrödinger Equation.*

At this point, we would like to emphasize the following point : the "size" of the global attractor does not depend on the mesh size of the space discretization Δx . This contrasts with the following fact : when we deals with the classical scheme (6), one can prove the existence of an absorbing ball whose size tends to infinity when $\Delta x \rightarrow 0$.

2.5. Discrete regularity for the attractor. We first state and prove

Proposition 3. : $\mathcal{A}_{\Delta x}$ is a bounded subset in $H_{\Delta x}^1$, uniformly in Δx .

Proof :

Multiply (8) by $i(U^{n+1} - e^{-\alpha\Delta t}U^n)$ in the Hilbert space $L_{\Delta x}^2$ to obtain

$$\begin{aligned} & \|A^{\frac{1}{2}}U^{n+1}\|_{L_{\Delta x}^2}^2 - e^{-2\alpha\Delta t} \|A^{\frac{1}{2}}U^n\|_{L_{\Delta x}^2}^2 \\ &= \frac{1}{2} \langle (|U^n|^2 + |U^{n+1}|^2)(U^{n+1} + e^{-\alpha\Delta t}U^n), U^{n+1} - e^{-\alpha\Delta t}U^n \rangle \\ &+ (1 + e^{-\alpha\Delta t}) \langle iF, U^{n+1} - e^{-\alpha\Delta t}U^n \rangle. \end{aligned} \quad (20)$$

Let us observe that the first term in the r.h.s. of (20) reads also

$$\begin{aligned} & \sum_{j=1}^N \Delta x (|U_j^{n+1}|^4 - e^{-2\alpha\Delta t} |U_j^n|^4) \\ &+ (1 - \delta^2) \sum_{j=1}^N \Delta x (|U_j^n|^2 |U_j^{n+1}|^2). \end{aligned} \quad (21)$$

Introducing

$$J(U^{n+1}) = \|A^{\frac{1}{2}}U^{n+1}\|_{L_{\Delta x}^2}^2 - \frac{1}{2} \|U^{n+1}\|_{L_{\Delta x}^4}^4 + (1 + \delta) \langle iF, U^{n+1} \rangle, \quad (22)$$

We thus obtain

$$J(U^{n+1}) \leq \delta^2 J(U^n) + \frac{1-\delta^2}{2} \sum_{j=1}^N \Delta x (|U_j^n|^2 |U_j^{n+1}|^2). \quad (23)$$

We now use the following discrete Gagliardo-Nirenberg inequality :

Lemma 3. : $\forall v \in \mathbb{C}^N$, $\|v\|_{L_{\Delta x}^4}^4 \leq 2\|v\|_{L_{\Delta x}^2}^3 \|v\|_{H_{\Delta x}^1}$.

Now and in the sequel we denote by K a constant that depends only on α and $\|F\|_{L_{\Delta x}^2}$; K may vary from one line to one another.

We infer from the uniform upper bound in $L_{\Delta x}^2$ and from (22) that there exists K such that

$$J(U^{n+1}) \geq \frac{1}{2} \|A^{\frac{1}{2}} U^{n+1}\|_{L_{\Delta x}^2}^2 - K. \quad (24)$$

On the other hand, there exists (another) K such that

$$(1 - \delta^2) \sum_{j=1}^N \Delta x (|U_j^n|^2 |U_j^{n+1}|^2) \leq K \Delta t (1 + \|A^{\frac{1}{2}} U^{n+1}\|_{L_{\Delta x}^2}^{1/2} \|A^{\frac{1}{2}} U^n\|_{L_{\Delta x}^2}^{1/2}). \quad (25)$$

We now infer from (23)-(25) that

$$J(U^{n+1}) \leq \delta J(U^n) + K \Delta t. \quad (26)$$

Then, proceeding as in the proof of Proposition 1 (see (9)), we obtain

$$J(U^n) \leq \delta^n J(U^0) + \frac{K \Delta t}{1 - \delta} \leq \delta^n J(U^0) + \frac{2K}{\alpha}. \quad (27)$$

We now consider a discrete trajectory U^n that belongs to the global attractor $\mathcal{A}_{\Delta x}$ that is bounded in $L_{\Delta x}^2$. Let us recall that the global attractor consists in complete orbits and that therefore we can go backward in time.

There exists then K that depends only on α , $\|F\|_{L_{\Delta x}^2}$ such that, due to inverse inequality,

$$J(U^0) \leq \delta^n J(U^{-n}) + K \leq K \left(\delta^n (1 + \frac{1}{(\Delta x)^2}) + 1 \right). \quad (28)$$

Let $n \rightarrow +\infty$ concludes the proof of the Proposition, using once again (24). \square

Remark 1. *The proof of this proposition shows that there exists an absorbing ball in $H_{\Delta x}^1$ that captures all the trajectories in $L_{\Delta x}^2$, but with a discrete time that depends on Δx .*

We now complete the proof of Theorem 1 by the following statement

Proposition 4. $\mathcal{A}_{\Delta x}$ is a bounded subset in $H_{\Delta x}^2$, uniformly in Δx .

Proof : Introduce $Z^{n+1} = \frac{U^{n+1} - e^{-\alpha \Delta t} U^n}{\Delta t}$ that plays the role of the time derivative of U^n . We infer from (8) that

$$\begin{aligned} \frac{Z^{n+1} - e^{-\alpha \Delta t} Z^n}{\Delta t} &= \frac{i}{2} A (Z^{n+1} + e^{-\alpha \Delta t} Z^n) \\ &+ \frac{i}{4} (|U^{n+1}|^2 + |U^n|^2) (U^{n+1} + e^{-\alpha \Delta t} U^n) \\ &- \frac{i}{4} (|U^{n-1}|^2 + |U^n|^2) (U^n + e^{-\alpha \Delta t} U^{n-1}) = 0. \end{aligned} \quad (29)$$

Multiply this equation by $Z^{n+1} + e^{-\alpha\Delta t}Z^n$ in the Hilbert space $L_{\Delta x}^2$ to obtain

$$\begin{aligned} \|Z^{n+1}\|_{L_{\Delta x}^2}^2 &\leq e^{-2\alpha\Delta t}\|Z^n\|_{L_{\Delta x}^2}^2 + c(\Delta t) \left(\|U^n\|_{L_{\Delta x}^\infty}^2 + \|U^{n-1}\|_{L_{\Delta x}^\infty}^2 \right) \left(\|Z^{n+1}\|_{L_{\Delta x}^2}^2 \right. \\ &\quad \left. + e^{-\alpha\Delta t}\|Z^n\|_{L_{\Delta x}^2}^2 \right) \left(\|U^{n-1}\|_{L_{\Delta x}^2}^2 + \|U^n\|_{L_{\Delta x}^2}^2 + \|U^{n+1}\|_{L_{\Delta x}^2}^2 \right). \end{aligned} \quad (30)$$

Since we know that $\mathcal{A}_{\Delta x}$ is bounded in $H_{\Delta x}^1$, uniformly in Δx , proceeding as in the proof of Proposition 1 (see (9)) we obtain that there exists K that depends on α , $\|F\|_{L_{\Delta x}^2}$ such that

$$\|Z^{n+1}\|_{L_{\Delta x}^2}^2 \leq \delta\|Z^n\|_{L_{\Delta x}^2}^2 + K\Delta t, \quad (31)$$

since

Lemma 4. $\forall v \in \mathbb{C}^N$, $\|v\|_{L_{\Delta x}^\infty} \leq c\|v\|_{H_{\Delta x}^1}$.

Therefore $\frac{U^{n+1} - e^{-\alpha\Delta t}U^n}{\Delta t}$ remains in a bounded set of $L_{\Delta x}^2$. Then $U^{n+1} + e^{-\alpha\Delta t}U^n$ remains bounded in $H_{\Delta x}^2$, uniformly in Δx , i.e. $\exists K = K(\alpha, \|F\|_{L_{\Delta x}^2})$;

$$\begin{aligned} K &\geq \|U^{n+1} + e^{-\alpha\Delta t}U^n\|_{H_{\Delta x}^2} \\ &\geq \left[\|U^{n+1}\|_{H_{\Delta x}^2} - e^{-\alpha\Delta t}\|U^n\|_{H_{\Delta x}^2} \right]. \end{aligned} \quad (32)$$

Then, for any n

$$\|U^{n+1}\|_{H_{\Delta x}^2} \leq e^{-\alpha\Delta t}\|U^n\|_{H_{\Delta x}^2} + K, \quad (33)$$

and then

$$\begin{aligned} \|U^0\|_{H_{\Delta x}^2} &\leq e^{-n\alpha\Delta t}\|U^{-n}\|_{H_{\Delta x}^2} + K \\ &\leq e^{-n\alpha\Delta t} \left(1 + \frac{4}{(\Delta x)^2} \right) \|U^{-n}\|_{L_{\Delta x}^2} + K. \end{aligned} \quad (34)$$

If U^n is a complete trajectory that is bounded in $L_{\Delta x}^2$, $n \rightarrow +\infty$ completes the proof of the Theorem.

Remark 2. *This result is sharp. The assumption $\|F\|_{L_{\Delta x}^2} < +\infty$ uniformly in (Δx) implies that the stationary solutions belongs only to $H_{\Delta x}^2$.*

3. Consistency and convergence of the attractors.

3.1. Existence and regularity of the attractor for the ODE. To begin with, we recall some results for the continuous attractor that were established in [8].

Theorem 2. *Consider a trajectory $u(t)$ that is included in the continuous attractor \mathcal{A} . Then there exists a constant K that depends only on $\alpha, \|f\|_{L^2(\mathbb{T})}$ such that for any t in \mathbb{R}*

$$\|u(t)\|_{H^2(\mathbb{T})} + \|u_t(t)\|_{H^4(\mathbb{T})} + \|u_{tt}(t)\|_{H^4(\mathbb{T})} \leq K. \quad (35)$$

At a first glance, this result is surprising and means that along the invariant set the time derivative of the solution is more regular than the solution itself. Actually, one can go further in the regularity in t of the solutions of a PDE along an invariant set (see [11]). On the other hand, the estimate (35) provides upper bound for the distance between approximate inertial manifolds and \mathcal{A} (see [8] and the references therein).

We now go back to our numerical scheme. Consider (5) as a dynamical system in $L^2_{\Delta x}$. One can prove the existence of a global attractor \mathcal{A}_{ODE} as in [19] for instance. Moreover, in the spirit of Theorem 2, one can prove

Theorem 3. *Consider a trajectory $U(t)$ that is included in the attractor \mathcal{A}_{ODE} . Then there exists a constant K that depends only on $\alpha, \|F\|_{L^2_{\Delta x}}$ such that for any t in \mathbb{R}*

$$\|AU(t)\|_{L^2_{\Delta x}} + \|A^2U_t(t)\|_{L^2_{\Delta x}} + \|A^2U_{tt}(t)\|_{L^2_{\Delta x}} \leq K. \quad (36)$$

Since the proof of this theorem is just a suitable adaptation of the article [8] using discrete norms as in previous section, we omit it for the sake of conciseness.

3.2. Consistency. Consider $U(t)$ a complete trajectory that is embedded in the attractor \mathcal{A}_{ODE} . Set $V^n = U(n\Delta t)$. We define the consistency error as

$$\begin{aligned} \eta_n = & \frac{V^{n+1} - e^{-\alpha\Delta t}V^n}{\Delta t} - iA \left(\frac{V^{n+1} + e^{-\alpha\Delta t}V^n}{2} \right) + \\ & \frac{i}{4} (|V^{n+1}|^2 + |V^n|^2) (V^{n+1} + e^{-\alpha\Delta t}V^n) - \frac{1 + e^{-\alpha\Delta t}}{2} F. \end{aligned} \quad (37)$$

We now state and prove

Proposition 5. *There exists K that depends only on the data $\alpha, \|F\|_{L^2_{\Delta x}}$ and that does not depend on Δx such that*

$$\|\eta_n\|_{L^2_{\Delta x}} \leq K(\Delta t)^2.$$

Proof: Integrate (5) between $n\Delta t$ and $(n+1)\Delta t$ to obtain (recalling that $\delta = e^{-\alpha\Delta t}$)

$$V^{n+1} - \delta V^n = \int_{n\Delta t}^{(n+1)\Delta t} e^{s-\alpha(n+1)\Delta t} (F + iAU(s) - iU^2(s)\bar{U}(s)) ds. \quad (38)$$

We now invoke the well-known trapezoid formula to estimate the r.h.s of (38)

Lemma 5. *Consider $g(t)$ a smooth function. Then $|\int_a^b g(s)ds - \frac{b-a}{2}(g(b) + g(a))| \leq c(b-a)^3 \sup_t |\ddot{g}(t)|$.*

We thus obtain

$$\begin{aligned} & \int_{n\Delta t}^{(n+1)\Delta t} e^{\alpha s - \alpha(n+1)\Delta t} (F + iAU(s) - iU^2(s)\bar{U}(s)) ds = \\ & \frac{\Delta t}{2} (F + iAV^{n+1} - i|V^{n+1}|^2V^{n+1} + \delta(F + iAV^n - i|V^n|^2V^n)) + \zeta_n, \end{aligned} \quad (39)$$

where

$$\|\zeta_n\|_{L^2_{\Delta x}} \leq c(\Delta t)^3 e^{-\alpha(n+1)\Delta t} \sup_{t \in [n\Delta t, (n+1)\Delta t]} \|\partial_t^2 (e^{\alpha t}(-iF + AU - |U|^2U)(t))\|_{L^2_{\Delta x}}.$$

Therefore, using Theorem 3, it is an exercise to prove that

$$e^{-\alpha(n+1)\Delta t} \sup_{t \in [n\Delta t, (n+1)\Delta t]} \|\partial_t^2 (e^{\alpha t}(-iF + AU - |U|^2U)(t))\|_{L^2_{\Delta x}} \leq K.$$

To complete the consistency estimate, we have to majorize in $L^2_{\Delta x}$ the difference

$$(|V^{n+1}|^2 V^{n+1} + \delta |V^n|^2 V^n) - \left(\frac{|V^{n+1}|^2 + |V^n|^2}{2} \right) (V^{n+1} + \delta V^n) = \frac{1}{2} (|V^{n+1}|^2 - |V^n|^2) (V^{n+1} - \delta V^n). \quad (40)$$

Since by Theorem 3 the time derivative U_t is uniformly bounded, we bound this term by $K(\Delta t)^2$.

This completes the proof of the proposition. \square

3.3. Upper semi-continuity of the attractors. Introduce I the interpolation operator that maps the continuous space into the discrete one by $(Iu)_j = \frac{1}{\Delta x} \int_{(j-1/2)\Delta x}^{(j+1/2)\Delta x} u(y) dy$. We rather use this " L^2 " interpolation operator instead of the classical one since we only assume that f belongs to $L^2(\mathbb{T})$. Anyway $(Iu)_j \sim u(j\Delta x)$ if u is regular enough. The aim of this section is to establish that when both Δt and Δx converges to 0, then the Hausdorff semi-distance $\sup_{a \in \mathcal{A}} \inf_{b \in \mathcal{A}_{\Delta x}} \|Ia - b\|_{L^2_{\Delta x}}$ converges to 0.

The idea is to use \mathcal{A}_{ODE} and the following triangle inequality

$$\sup_{a \in \mathcal{A}} \inf_{b \in \mathcal{A}_{\Delta x}} \|Ia - b\|_{L^2_{\Delta x}} \leq \sup_{c \in \mathcal{A}_{ODE}} \inf_{b \in \mathcal{A}_{\Delta x}} \|c - b\|_{L^2_{\Delta x}} + \sup_{a \in \mathcal{A}} \inf_{c \in \mathcal{A}_{ODE}} \|c - Ia\|_{L^2_{\Delta x}}. \quad (41)$$

Consider the first term in the r.h.s of (41). Consider $U(t)$ a complete trajectory in \mathcal{A}_{ODE} . Set $G(U^n, U^{n+1}) = F - \frac{i}{4}(|U^n|^2 + |U^{n+1}|^2)(\delta U^n + U^{n+1})$. Then, if $V^n = U(n\Delta t)$ and $\varepsilon_n = U^n - V^n$,

$$\frac{\varepsilon_{n+1} - \delta \varepsilon_n}{\Delta t} + \frac{i}{2} A(\varepsilon_{n+1} + \delta \varepsilon_n) = G(U^n, U^{n+1}) - G(V^n, V^{n+1}) + \eta_n, \quad (42)$$

where η_n is the consistency error. Using the upper bounds on the attractors given in Theorems 1 and 3, one can prove that $\|G(U^n, U^{n+1}) - G(V^n, V^{n+1})\|_{L^2_{\Delta x}} \leq K\|\varepsilon_{n+1} + \delta \varepsilon_n\|_{L^2_{\Delta x}}$. Actually U^n is not in the discrete attractor, but since $U^0 = V^0$ is in $H^2_{\Delta x}$ and since the equation features also an $H^2_{\Delta x}$ absorbing set, we may assume that U^n is bounded in $H^2_{\Delta x}$.

Considering then the scalar product of 42 with $\varepsilon_{n+1} + \delta \varepsilon_n$ in $L^2_{\Delta x}$ we thus obtain

$$\|\varepsilon_{n+1}\|_{L^2_{\Delta x}}^2 - \delta^2 \|\varepsilon_n\|_{L^2_{\Delta x}}^2 \leq K\Delta t \left(\|\varepsilon_{n+1} + \delta \varepsilon_n\|_{L^2_{\Delta x}}^2 + \|\eta_n\|_{L^2_{\Delta x}}^2 \right), \quad (43)$$

and then, by the consistency estimate of Lemma 5,

$$\|\varepsilon_{n+1}\|_{L^2_{\Delta x}} \leq \delta^2 \frac{1 + K\Delta t}{1 - K\Delta t} \|\varepsilon_n\|_{L^2_{\Delta x}} + K(\Delta t)^3. \quad (44)$$

Using $\delta^2 \frac{1 + K\Delta t}{1 - K\Delta t} \leq e^{2(K-\alpha)\Delta t} = \beta$ for Δt small enough, we then have by the discrete Gronwall lemma, (and with $\varepsilon_0 = 0$)

$$\|\varepsilon_n\|_{L^2_{\Delta x}} \leq \beta^n K \frac{(\Delta t)^3}{\beta - 1} \leq \tilde{K} \beta^n (\Delta t)^2. \quad (45)$$

We now infer from (45)

Proposition 6.

$$\lim_{\Delta t \rightarrow 0} \sup_{c \in \mathcal{A}_{ODE}} \inf_{b \in \mathcal{A}_{\Delta x}} \|c - b\|_{L^2_{\Delta x}} = 0. \quad (46)$$

Proof: Consider $U(t)$ a complete trajectory in \mathcal{A}_{ODE} as above. Consider estimate (45) between $U(0)$ and $U^n = S^n(U(-n\Delta t))$, where S stands for the discrete semi-group that is defined by $U^{n+1} = SU^n$ where U^{n+1} solves (8). Consider $\varepsilon > 0$. To the very definition of a global attractor we know that there exists b in $\mathcal{A}_{\Delta x}$ such that for n large enough

$$\|b - S^n(U(-n\Delta t))\|_{L^2_{\Delta x}} \leq \varepsilon. \quad (47)$$

Fix then n in (45) and let $\Delta t \rightarrow 0$ that gives $\|b - U(0)\|_{L^2_{\Delta x}} \leq \varepsilon$. Since ε is arbitrary the proof of the Proposition is completed. \square

It remains to compare the attractors \mathcal{A} and \mathcal{A}_{ODE} . We give an overview of this process that is more or less standard. Consider a complete trajectory $u(t)$ in the global attractor \mathcal{A} . We apply the interpolation operator I to the equation (1). This gives,

$$(Iu)_t + \alpha Iu + iI(u_{xx}) + iI(|u|^2 u) = If = F. \quad (48)$$

Let us point out that the operator I and ∂_x do not commute; this shows in the consistency error as follows

$$\eta(t) = i(AIu - I(u_{xx})) + i(|Iu|^2 Iu - I(|u|^2 u)); \quad (49)$$

observe that due to standard results and since $u(t)$ is bounded in $H^2(\mathbb{T})$, then $\|\eta(t)\|_{L^2_{\Delta x}} = O(1)$ when $\Delta x \rightarrow 0$, uniformly in t .

Introduce now $V(t) = U(t) - Iu(t)$ that solves

$$V_t + \alpha V - iAV = \eta + i(|Iu|^2 Iu - |U|^2 U). \quad (50)$$

Considering the scalar product in $L^2_{\Delta x}$ with w , we thus obtain, since $\| |Iu|^2 Iu - |U|^2 U \|_{L^2_{\Delta x}} \leq K \|V\|_{L^2_{\Delta x}}$ in the global attractor that $\|V(t)\|_{L^2_{\Delta x}} \leq e^{Kt} \sup_t \|\eta(t)\|_{L^2_{\Delta x}}$. We conclude then as in the proof of Proposition 6.

4. Numerical experiments.

4.1. Implementation of the scheme. The implementation of the Crank-Nicolson scheme needs a fixed point problem to be solved at each time step. Let Id be the Identity matrix. If we set

$$\begin{aligned} \Phi(U, U^n) &= \left(Id - i\frac{\Delta t}{2} A \right)^{-1} \left\{ e^{-\alpha \Delta t} \left(Id + i\frac{\Delta t}{2} A \right) U^n - \frac{i\Delta t}{4} (|U|^2 + |U^n|^2) (U + e^{-\alpha \Delta t} U^n) \right. \\ &\quad \left. + \left(\frac{1 + e^{-\alpha \Delta t}}{2} F \right) \right\} \end{aligned}$$

then the time marching scheme reduces to solve the fixed point problem

$$U = \Phi(U, U^n) \quad (51)$$

at the n -th time step. Lemma 1 insures that there exists a unique fixed point if $\alpha \Delta t$ is small enough, the proof uses the classical Banach fixed point theorem. In practice, for this NLS equation, the convergence of the Picard iterates is obtained by taking only very small values of Δt , typically $\Delta t \simeq 10^{-4}$. This is dramatic since we are looking to

the long time numerical behavior of the solution. Anyway, this effective restriction on the time step is really artificial because the scheme is supposed to be unconditionally stable. For this reason, we propose to solve (51) by accelerating the (Picard) sequence

$$\begin{aligned} U^{(0)} &= U^n \\ \text{for } m &= 0, \dots \\ U^{(m+1)} &= \Phi(U^{(m)}, U^n), \end{aligned} \quad (52)$$

enhancing in that way the stability region, allowing then to take larger values of Δt . To this end, we use the Δ^k acceleration procedure, see [4] and the references therein. In two words, the Δ^k procedure consists in replacing the Picard iterates by

$$\begin{aligned} U^{(0)} &= U^n \\ \text{for } m &= 0, \dots \\ U^{(m+1)} &= U^{(m)} - (-1)^k \alpha_m^k \Delta_\Phi^k U^{(m)}; \end{aligned} \quad (53)$$

where $\Delta_\Phi^k U^{(m)} = \sum_{j=0}^k C_j^k (-1)^{k-j} \Phi^{(j)}(U^{(m)}, U^n)$, $C_j^k = \frac{k!}{j!(k-j)!}$ is the binomial coefficient and $\Phi^{(j)}$ denotes the j -th composition of Φ with itself. The parameter α_m^k is computed such as minimizing the euclidian norm of the linearized part of the residual $r^{(m+1)} = u^{(m+1)} - \Phi(U^{(m)}, U^n)$. We have

$$\alpha_m^k = (-1)^k \frac{\langle \Delta_\Phi^1 U^{(m)}, \Delta_\Phi^{k+1} U^{(m)} \rangle}{\langle \Delta_\Phi^{k+1} U^{(m)}, \Delta_\Phi^{k+1} U^{(m)} \rangle} \quad (54)$$

see [4]. These acceleration procedure have been applied with success for solving nonlinear eigenvalue problem and presently, for the NLS scheme, we obtain good results with the Δ^1 (Lemaréchal's) and the Δ^2 (Marder-Weitzner) methods; we can take Δt up to 1.10^{-1} and after a transient time very few iterations are needed for solving (51) with a good accuracy. To achieve the description of the implementation of the scheme (8), we mention that the evaluation of Φ necessitates the solution of a linear system with the matrix $Id - i\frac{\Delta t}{2}A$. Since this matrix is independant of t , this is done by a QR factorization method.

4.2. Discrete smoothing. We address here the following issue : consider $U \in \mathbb{C}^N$, that could be the sampling of a function at points $j\Delta x$. How to check that this sampling corresponds to a function that belongs to H^1 ?

In a perfect world, we just have to check that the sequence :

$$\alpha_N = \frac{1}{\Delta x} \sum_{j=1}^N (u_{j+1} - u_j)^2 \quad (55)$$

remains bounded when $N \rightarrow +\infty$. In the real world of numerics, we can deal with large N 's but hardly pretend that $\Delta x = \frac{1}{N} \rightarrow 0$.

Therefore we shall use in the sequel the following ansatz : consider a periodic function

to compute the coarser grid approximation, we make use of the formula

$$\sigma(x) = \sigma(2x) + \frac{1}{2}(\sigma(2x+1) + \sigma(2x-1)). \quad (60)$$

Therefore U expands / splits as follows

$$\begin{aligned} u(x) &= \left(\sum_{j=1}^m U_{2j} \sigma \left(\frac{x}{\Delta x} - 2j \right) \right) + \left(\sum_{j=1}^m U_{2j+1} \sigma \left(\frac{x}{\Delta x} - 2j - 1 \right) \right) \\ &= \sum_{j=1}^m U_{2j} \sigma \left(\frac{x}{2\Delta x} - j \right) - \frac{1}{2} \sum_{j=1}^m U_{2j} \left(\sigma \left(\frac{x}{\Delta x} - 2j + 1 \right) + \sigma \left(\frac{x}{\Delta x} - 2j - 1 \right) \right) \\ &\quad + \sum_{j=1}^m U_{2j+1} \sigma \left(\frac{x}{\Delta x} - 2j - 1 \right) \\ &= \underbrace{\left(\sum_{j=1}^m U_{2j} \sigma \left(\frac{x}{2\Delta x} - j \right) \right)}_{\text{approximation on the coarse grid}} \\ &\quad + \underbrace{\left(\sum_{j=1}^m \left(U_{2j+1} - \frac{U_{2j} + U_{2j+2}}{2} \right) \sigma \left(\frac{x}{\Delta x} - 2j - 1 \right) \right)}_{\text{difference}} \end{aligned} \quad (61)$$

This corresponds to

$$\begin{array}{ccccccc} \otimes & - & - & - & X & - & - & - & \otimes & - & - & - & X & - & - & - & \otimes \\ \downarrow 1 & & & & & & & & -\frac{1}{2} \searrow & \downarrow 1 & \swarrow & -\frac{1}{2} & & & & & \\ \odot & - & - & - & X & - & - & - & \odot & - & - & - & X & - & - & - & \odot \end{array}$$

We now define the incremental unknown as

$$z_j = U_{2j+1} - \frac{U_{2j} + U_{2j+2}}{2}, \quad (62)$$

We compute recursively the incremental unknowns corresponding to nested grids from a coarser grid to the finest one. The criterion reads

$$\sum_{k=1} 4^{ks} \|w_k\|_{L^2}^2 < +\infty \quad (63)$$

where w_k is the incremental unknown corresponding to the grid of mesh size 2^{-k} . Actually, if we compute the convergence radius ρ of the series $\sum \|w_k\|_{L^2}^2 Z^k$ in \mathbb{C} , then $\rho = 4^s$.

4.4. Preliminary tests. Before to go further on the investigation of the *discrete regularity* of the solutions of our discrete nonlinear Schrödinger equations, we will check that both the Fourier and multigrid approach allow us to compute successfully the discrete regularity of the following test functions:

- $f_1(x) = \begin{cases} -1 & \text{if } x \in [0, \frac{1}{2}[\\ 1 & \text{if } x \in [\frac{1}{2}, 1[\end{cases}$
- $f_2(x) = |x - \frac{1}{2}|$
- $f_3(x) = x^2(1 - x)^2$
- $f_4(x) = \sin(2\pi x)$.

We proceed to the computations on a grid with $N=128$ points (x_i, y_i) for $1 \leq i \leq N$ such that $x_i = ih$, $\Delta x = \frac{1}{N}$, and $y_i = f_l(x_i)$ with the four functions $f_l; l = 1, 2, 3, 4$. defined above. We aim to compute the regularity index s_l of each function f_l , both with Fourier analysis and multigrid approaches. Then f_l belongs to $H_{\Delta x}^s$ with

	Fourier analysis	Multigrid approach
f_1	s=0.6049	s=0.50
f_2	s=1.6357	s=1.50
f_3	s=3.7917	s=2.00
f_4	s=10.000	s=1.9834

These results show that we are able to give a satisfactory measurement of the regularity index for a given function, but with a limitation of our multigrid approach. Actually, since our incremental unknowns behaves as wavelet coefficients with a wavelet that has two vanishing moments, we cannot go further than 2 in the regularity measurement process. Moreover, we can explain the error on the measurement of the regularity of the analytical function f_4 in the Fourier analysis setting by round up errors in the numerical computations.

4.5. Numerical evidences for the regularity of solutions to discrete Schrödinger equation. We compute below the discrete regularity of a solution of (8) and we plot the evolution of this discrete regularity with respect to time. The computations are performed for different forcing terms f and for various initial data u_0 . In the computations below $\alpha = 0.01$ and the time step Δt is equal to 10^{-2} .

The figures in the sequel represent the regularity of the solution as a function of time, both with Fourier and multigrid approaches. All the example below give evidence of robustness and stability of our Crank-Nicolson scheme for long-time computations.

- To begin with, we are given a smooth forcing term $f = 0$ and a smooth initial data $u_0 = \sin(2\pi x)$. We observe that in that case there is no loss of regularity along the process (see Fig 1). Once again, the measurement of regularity is limited when using multigrids.
- We now introduce a forcing term f that is the Heaviside function (regularity $H^{\frac{1}{2}+}$). $\alpha = 0.01$. For $u_0 = 1$, we observe that after a transient time the regularity of the solution converges to the predicted regularity of the attractor that should be $s = 2, 5^+$.
- In the next example with keep the Heaviside function as forcing term and we chose an initial data that has very low regularity (say L^2); to plot a low regular initial

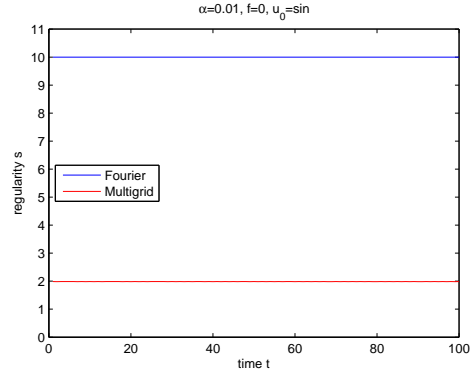


FIGURE 1. Regularity of $u(t, \cdot)$ when $\alpha = 0.01$, $f = 0$, $u_0(x) = \sin(2\pi x)$.

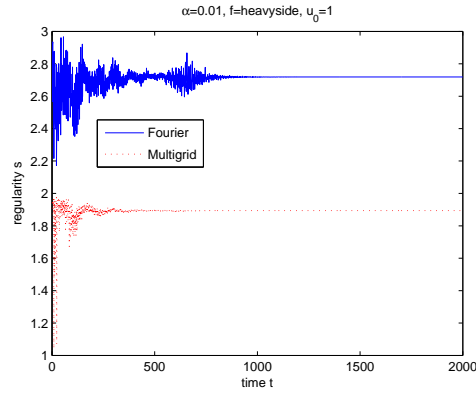


FIGURE 2. Regularity of $u(t, \cdot)$ when $\alpha = 0.01$, $f = \text{Heaviside}$, $u_0 \equiv 1$.

data we perform a random function u_0 . The results are very interesting. After a transient time the solution forget the low regular initial data and its regularity converges to the expected regularity of the attractor as in the example above.

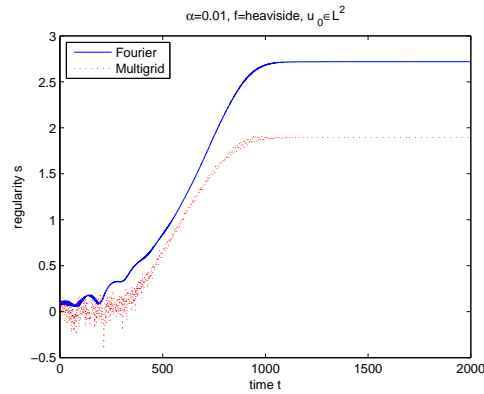


FIGURE 3. Regularity of $u(t, \cdot)$ when $\alpha = 0.01$, $f = \text{Heaviside}$, $u_0 \in L^2$.

- In that example the forcing term is a L^2 function obtained with a random procedure and the initial data is smooth. The regularity of the solution converges towards the expected value of the regularity of the attractor that is 2 in this case.

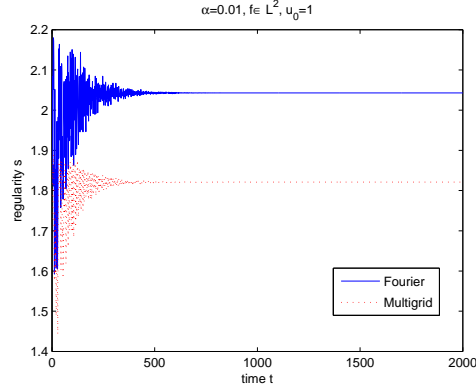


FIGURE 4. Regularity of $u(t, \cdot)$ when $\alpha = 0.01$, $f \in L^2$, $u_0 \equiv 1$.

- This example is similar with the previous one, but we are given here a non-smooth initial data u_0 that is the Heaviside function. Once again, the regularity of the solution converges towards the expected value of the regularity of the attractor that is 2 in this case.

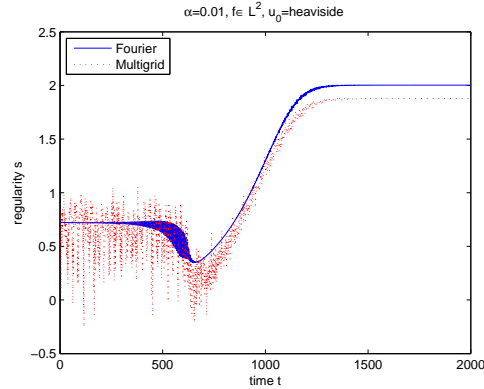


FIGURE 5. Regularity of $u(t, \cdot)$ when $\alpha = 0.01$, $f \in L^2$, u_0 Heaviside.

Acknowledgements. This work initiated when the two last authors were visiting the University Cadi Ayyad of Marrakech and has been partially supported by the research programs "Dissipation and asymptotique" and "Couplage Fluide-Sable" by CNRS (France) and CNRST (Marocco), and also by the INRIA research program MASOH (Modélisation, Analyse et Simulation d'Ondes Hydrodynamiques).

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