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CRANK-NICOLSON SCHEME FOR A LOGARITHMIC SCHRÖDINGER EQUATION

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ABSTRACT. We discuss here a classical Crank-Nicolson numerical scheme to approximate the solutions of a nonlinear equation Schrödinger that reads

$$u_t - i\partial_x(\nu(x)\partial_x u) - iu \log |u|^2 = 0.$$

1. INTRODUCTION

We consider here numerical approximations of an evolution logarithmic equation that reads

$$(1) \quad u_t - i\partial_x(\nu(x)\partial_x u) - iu \log |u|^2 = 0.$$

The unknown $u(t, x)$ maps $\mathbb{R} \times \mathbb{R}$ into \mathbb{C} . This evolution equation has two singularities. First, we consider a discontinuity at $x = 0$ that reads $\nu(x) = \nu_+ > 0$ if $x > 0$ and $\nu_- > 0$ if $x < 0$. Then we have to handle a nonlinearity whose derivative is not bounded at 0.

We first discuss logarithmic Schrödinger equations (here in one dimension). For $\nu(x) = 1$ constant and λ in $\{-1, 1\}$, these equations that read in one dimension,

$$(2) \quad u_t - iu_{xx} = i\lambda u \log |u|^2,$$

are models in nonlinear wave mechanics or in nonlinear optics (see [10] and the references therein). According to the terminology introduced in [10], the case $\lambda =$

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-1 corresponds to the *defocusing* case, while the case $\lambda = 1$ to the *focusing case*. Formally an energy that reads

$$\int_{\mathbb{R}} |u_x|^2 dx - \lambda |u|^2 \log |u|^2 dx,$$

is conserved along the flow of the solutions of (2). Despite the fact that the second term in the energy above has no definite sign, it was rigorously proved in [10] that the nonlinearity enhanced the classical decay dispersion estimate (over the linear case), and then this equation has to be called defocusing. Here we are interested in the focusing case that was introduced and studied in [11].

Here beyond the classical case we are interested in the case of some impurity in the material that affects the propagation of the wave. Various models of impurity has been studied in the literature. Let us first point out the case where the classical dispersion operator iu_{xx} is perturbed by a Dirac mass at 0 and replaced by $iu_{xx} + iZu\delta_0$ for some constants Z (see [17], [19], [20] and the references therein). In the present article we also have a singularity at the origin but that corresponds to a discontinuity of the parameter ν with respect to x . The problem of the study of the corresponding linear operator has been addressed in [3] and [9]. Let us point out that this problem differs from the one where we have rough coefficients, that are time dependent but space independent, in front of the dispersion operator (see [2], [14] and the references therein).

In the present article we are interested in the approximation of the solution of the equation by a classical Crank-Nicolson scheme. We keep for the theoretical aspects the space variable x continuous. To begin with, as in the articles [4], [5], we introduce a regularized version of the equation, replacing the logarithmic nonlinearity by a regularized version at $u = 0$. This regularization depends on a small parameter ε . We note that the Crank-Nicolson scheme provides an order 2 in time approximation of the solution of the regularized equation, but the drawback is that the error estimates depend on some functions of ε^{-1} . Our main result is to provide a precise error estimate depending on τ and ε . These results compare, with better estimates in ε^{-1} , to a semi-implicit Crank-Nicolson type order 2 scheme used in [4], [5]; in these articles were also studied suitable splitting schemes.

This article outcomes as follows. In a first section we handle the initial value problem for our non standard logarithmic Schrödinger equation. In a second section we introduce and discuss the properties of the Crank-Nicolson scheme applied to our equation. In a third section we provide some numerical illustrations. We end this article by the proof of the main result that is the error estimate for the Crank-Nicolson the scheme.

We complete this introduction by introducing some notations. A generic constant C is independent of ε , τ but may depend on the solution and of the time t . Besides, C may change from one line to one another without notice.

2. INITIAL VALUE PROBLEM FOR LOGARITHMIC EQUATION

In this section we study the initial value problem for equation (1) above, following the method introduced and described in [11] and [12].

2.1. A linear unbounded operator. Consider $A = -\partial_x(\nu(x)\partial_x \cdot)$ the unbounded operator defined as, for u, v in $H^1(\mathbb{R})$

$$(3) \quad (Au, v)_{L^2(\mathbb{R})} = \operatorname{Re} \int_{\mathbb{R}} \nu(x) u_x(x) \bar{v}_x(x) dx.$$

It is standard to prove that the domain of A is

$$(4) \quad D(A) = \{u \in H^1(\mathbb{R}) \cap H^2(\mathbb{R} - \{0\}); \nu_+ u_x(0^+) = \nu_- u_x(0^-)\}.$$

Besides due to (3), we have that $D(A^{\frac{1}{2}}) = H^1(\mathbb{R})$ and that $(Au, u)_{L^2(\mathbb{R})}$ defines a seminorm that is equivalent to the Poincaré seminorm, i.e.

$$(5) \quad \min(\nu_-, \nu_+) \int_{\mathbb{R}} |u_x(x)|^2 dx \leq (Au, u)_{L^2(\mathbb{R})} \leq \max(\nu_-, \nu_+) \int_{\mathbb{R}} |u_x(x)|^2 dx.$$

The operator A is a nonnegative self-adjoint unbounded operator and then classical functional calculus applies and the powers A^m are well-defined (see [21] and the references therein). Moreover the solution of the equation for $\tau \in \mathbb{R}$

$$(6) \quad v + i\tau Av = u,$$

satisfies $\|v\|_{L^2(\mathbb{R})} = \|u\|_{L^2(\mathbb{R})}$ and $(Av, v)_{L^2(\mathbb{R})} = (Au, u)_{L^2(\mathbb{R})}$.

2.2. Handling the initial value problem. Formally there are two quantities that are conserved along the flow of the solutions of (1), the mass $\|u\|_{L^2(\mathbb{R})}$ and the energy

$$(7) \quad E(u) = \int_{\mathbb{R}} \nu(x) |u_x(x)|^2 dx - \int_{\mathbb{R}} |u(x)|^2 \log |u(x)|^2 dx.$$

Following [11] we seek solutions whose energy is finite. The nonnegative part of the energy is

$$\int_{\mathbb{R}} \nu(x) |u_x(x)|^2 dx - \int_{\{|u| \leq 1\}} |u(x)|^2 \log |u(x)|^2 dx.$$

Besides, let us point out that the negative part of the energy is bounded for $u \in H^1(\mathbb{R})$ by Sobolev embeddings. It is then natural to seek a solution that belongs to

$$(8) \quad W = \{u \in H^1(\mathbb{R}) \text{ such as } |u|^2 \log(|u|) \in L^1(\mathbb{R})\}.$$

We recall from [11], [12], [18] that this space is a reflexive Orlicz Banach space. We now recall Theorem 3.3 in [18] (stated in the case $\nu(x) = 1$ but that works also in our case; we emphasize that in our case $\nu(x) \geq \min(\nu_-, \nu_+) > 0$.)

Theorem 2.1. *For every $u_0 \in W$ an initial data, then it exists a unique solution $u \in C(\mathbb{R}, W) \cap C^1(\mathbb{R}, W^*)$ for the problem (1), such that the following properties hold true*

(i) *we have the conservation of the mass and energy, i.e. for every $t \in \mathbb{R}$, the following identities are valid*

$$(9) \quad \|u(t)\|_{L^2(\mathbb{R})} = \|u_0\|_{L^2(\mathbb{R})} \text{ and } E(u(t)) = E(u_0).$$

(ii) *The flow map $S(t) : u_0 \mapsto S(t)u_0 = u(t)$ is continuous in W , i.e. that if u_0^m converges towards u_0 in W , then the corresponding solution $u^m(t) = S(t)u_0^m$ converge towards $u(t) = S(t)u_0$ uniformly on bounded intervals.*

We refer to [18] for a proof that uses a regularization of the nonlinearity at a neighborhood of zero and a limiting argument. An alternate route following the maximal operator theory ([6],[7], [8]) can be found in [1], as in [11] for the case $\nu(x) = 1$. In both proofs it is instrumental to use the following inequality that is valid for a pair of complex numbers

$$(10) \quad \left| \operatorname{Im} \int_{\mathbb{R}} \overline{z - z'} (z \log |z|^2 - z' \log |z'|^2) \right| \leq 2|z - z'|^2,$$

that leads to the estimate

$$\|S(t)u_0 - S(t)v_0\|_{L^2(\mathbb{R})} \leq e^{2t} \|u_0 - v_0\|_{L^2(\mathbb{R})}.$$

2.3. Introducing a regularized equation. In order to avoid numerical round-off errors, we introduce a regularized nonlinearity that reads for a given $\varepsilon > 0$,

$$u \log(|u|^2 + \varepsilon^2) = u f_{\varepsilon}(|u|^2).$$

The new equation reads

$$(11) \quad u_t - i\partial_x(\nu(x)\partial_x)u - iu \log(|u|^2 + \varepsilon^2) = 0.$$

This regularized nonlinearity is similar but differs from $2u \log(|u| + \varepsilon)$ that is used in [4], [5]. The regularization above was used in [10] in the defocusing case. For the regularized equation, the classical theory developed in [12] for $\nu = 1$ (see a sketch of the proof below the statement of the theorem) applies and we have

Theorem 2.2. *For every $u_0 \in H^1(\mathbb{R})$ an initial data, then it exist a unique solution $u \in C(\mathbb{R}, H^1(\mathbb{R})) \cap C^1(\mathbb{R}; H^{-1}(\mathbb{R}))$ for the problem (11), such that the following properties hold:*

- (i) *we have the conservation of the mass (9) and energy, indeed for every $t \in \mathbb{R}$, we have*

$$(12) \quad E(u) = \|A^{\frac{1}{2}}u\|_{L^2(\mathbb{R})}^2 - \int_{\mathbb{R}} F_{\varepsilon}(|u|^2)dx,$$

where

$$F_{\varepsilon}(s) = s \log(s + \varepsilon^2) - s + \varepsilon^2 \log\left(1 + \frac{s}{\varepsilon^2}\right).$$

- (ii) *The flow map $S_{\varepsilon}(t) : u_0 \mapsto S_{\varepsilon}(t)u_0 = u(t)$ is continuous in $H^1(\mathbb{R})$, i.e. that if u_0^m converges towards u_0 in $H^1(\mathbb{R})$, then the corresponding solution $u^m(t) = S_{\varepsilon}(t)u_0^m$ converge towards $u(t) = S_{\varepsilon}(t)u_0$ uniformly on bounded intervals.*

Let us sketch why this theorem holds true. Using as in [10] the change of unknown $v(t, x) = \varepsilon \exp(-2it \log \varepsilon) u(t, x)$ solving (11) amounts to solve the equation

$$v_t - i\partial_x(\nu(x)\partial_x)v - iv \log(1 + |v|^2) = 0$$

in $H^1(\mathbb{R})$. Introduce the linear operator defined as $\exp(-itA)u_0 = v$ if and only if

$$v_t + iAv = 0, \quad v(0) = v_0.$$

This linear operator is an isometry in $L^2(\mathbb{R})$ or in $H^1(\mathbb{R})$ (for the modified norm $\|u\|_{L^2}^2 + (Au, u)$ according to (5)). Since the nonlinear term $v \mapsto v \log(1 + |v|^2)$ is locally Lipschitz in the Banach algebra $H^1(\mathbb{R})$, it is standard to construct a mild solution of the equation on a bounded interval of time $[-T, T]$. Following [13],

since this nonlinearity is smooth, we can prove that this mild solution is a weak solution in $C(-T, T; H^1(\mathbb{R}))$ of (11). Moreover since $\xi^2 \log(1 + \xi^2) \leq \xi^4$ we are in the subcritical $H^1(\mathbb{R})$ case. Then the conservation of the mass and of the energy imply that the solution exists for all times.

3. THE CRANK-NICOLSON NUMERICAL SCHEME

We are interested in a conservative scheme (see [15], [16]) that reads for the regularized equation

$$(13) \quad \frac{u^{n+1} - u^n}{\tau} + iA\left(\frac{u^{n+1} + u^n}{2}\right) - if_\varepsilon\left(\left|\frac{u^{n+1} + u^n}{2}\right|^2\right)\frac{u^{n+1} + u^n}{2} = 0.$$

Here we have kept the space variable x continuous. Then the analysis will work for suitable discretization in space of the operator. For smooth nonlinearities, this scheme is of order 2. The drawbacks of the Crank-Nicolson scheme is that we have to solve a fixed point at each time step, since this scheme is an implicit scheme.

Remark 3.1. *One may wonder why to regularize the nonlinearity for the Crank-Nicolson scheme. On the one hand, the theoretical results in Section 3.1 and 3.2 are valid if $\varepsilon = 0$. On the other hand to implement the scheme requires to solve a nonlinear fixed point by an iterative scheme. The non-regularized nonlinearity is not differentiable at 0.*

3.1. Well-posedness of the scheme. We plan to prove that the map $u^n \mapsto u^{n+1}$ is well-posed. Set $v = \frac{u^{n+1} + u^n}{2}$. Solving (13) amounts to solve

$$(14) \quad \frac{v - u^n}{\frac{\tau}{2}} + iAv - if_\varepsilon(|v|^2)v = 0,$$

and then to write $u^{n+1} = 2v - u^n$. To solve (14) we rely on (see [11], [12])

Lemma 3.2. *Consider the nonlinear operator $M_\varepsilon v = iAv - if_\varepsilon(|v|^2)v$ whose domain is $D(A)$. Then for $\lambda > 2\pi$, the operator $M_\varepsilon + \lambda Id$ is maximal monotone in $L^2(\mathbb{R})$.*

Proof. We just check the monotonicity that we will use in the sequel. Consider v, w in $D(A)$. Then

$$(15) \quad |(M_\varepsilon v - M_\varepsilon w, v - w)| = 2|\operatorname{Im} \int_{\mathbb{R}} v\bar{w} \log\left(\frac{\varepsilon^2 + |v|^2}{\varepsilon^2 + |w|^2}\right)|.$$

We have, since $f_\varepsilon(y) - f_\varepsilon(x) = (\int_0^1 f'_\varepsilon(x + s(y-x))ds)(y-x)$,

$$|\log\left(\frac{\varepsilon^2 + |v|^2}{\varepsilon^2 + |w|^2}\right)| \leq |v - w| \int_0^1 \frac{|v| + |w|}{\varepsilon^2 + s|v|^2 + (1-s)|w|^2} ds.$$

Since

$$|\operatorname{Im}v\bar{w}|(|v| + |w|) = |\operatorname{Im}(v-w)\bar{w}||v| + |\operatorname{Im}(\bar{w}-\bar{v})v||w| \leq 2|v||w||v-w|,$$

we have

$$|2\operatorname{Im}(\bar{v}w) \log\left(\frac{\varepsilon^2 + |v|^2}{\varepsilon^2 + |w|^2}\right)| \leq |v-w|^2 \int_0^1 \frac{4|v||w|}{s|v|^2 + (1-s)|w|^2} ds.$$

We then have, using $2\sqrt{s(1-s)}|v|w \leq s|v|^2 + (1-s)|w|^2$,

$$(16) \quad \left| \int_{\mathbb{R}} 2\text{Im}(\bar{v}w) \log\left(\frac{\varepsilon^2 + |v|^2}{\varepsilon^2 + |w|^2}\right) \right| \leq \left(\int_0^1 \frac{2ds}{\sqrt{s}\sqrt{1-s}} \right) \|v - w\|_{L^2(\mathbb{R})}^2.$$

This concludes the proof of the Lemma since $\int_0^1 \frac{2ds}{\sqrt{s}\sqrt{1-s}} = 2\pi$. \square

Corollary 3.3. *For $\frac{1}{\tau} > \pi$, the map $u^n \mapsto v$ defined in (14) is well posed.*

3.2. Stability and error estimate. Consider $\tilde{u}^n = u(n\tau)$ the interpolation of the solution of the continuous equation (11). Then \tilde{u}^n solves the equation (13) up to a consistency error denoted by $\varepsilon^{n+\frac{1}{2}}$. Set $w^n = \tilde{u}^n - u^n$. We then have

$$(17) \quad \frac{w^{n+1} - w^n}{\tau} + iM_\varepsilon \frac{\tilde{u}^{n+1} + \tilde{u}^n}{2} - iM_\varepsilon \frac{u^{n+1} + u^n}{2} = \varepsilon^{n+\frac{1}{2}}.$$

Considering the scalar product of this equation with $w^n + w^{n+1}$ we obtain, using Lemma 3.2 above

$$(18) \quad \frac{\|w^{n+1}\|_{L^2(\mathbb{R})}^2 - \|w^n\|_{L^2(\mathbb{R})}^2}{\tau} \leq 4\pi \left\| \frac{w^n + w^{n+1}}{2} \right\|_{L^2(\mathbb{R})}^2 + \|\varepsilon^{n+\frac{1}{2}}\|_{L^2(\mathbb{R})} \|w^n + w^{n+1}\|_{L^2(\mathbb{R})},$$

that leads to

$$(19) \quad (1 - \tau\pi) \|w^{n+1}\|_{L^2(\mathbb{R})} \leq (1 + \tau\pi) \|w^n\|_{L^2(\mathbb{R})} + \tau \|\varepsilon^{n+\frac{1}{2}}\|_{L^2(\mathbb{R})}.$$

For τ small enough, we use $1 + \tau\pi \leq (1 - \tau\pi)(1 + 3\tau\pi)$ and $1 \leq 2(1 - \tau\pi)$. Starting from $w^0 = 0$ we then have by the discrete Gronwall lemma

$$(20) \quad \|w^n\|_{L^2(\mathbb{R})} \leq 2\tau \sum_{k \leq n} (1 + 3\tau\pi)^{n-k} \|\varepsilon^{k+\frac{1}{2}}\|_{L^2(\mathbb{R})} \leq \frac{1}{\pi} \sup_k \|\varepsilon^{k+\frac{1}{2}}\|_{L^2(\mathbb{R})}.$$

3.3. Consistency. We now compute the consistency error, i.e. the estimate on $\varepsilon^{n+\frac{1}{2}}$. We assume that the initial data u_0 belongs to $D(A^m)$ for m large enough.

Theorem 3.4. *There exists a constant C that depends on the initial data u_0 and on T , but that is independent of ε and of τ such that for $k\tau \leq T$ we have $\|\varepsilon^{k+\frac{1}{2}}\|_{L^2(\mathbb{R})} \leq C\tau^2\varepsilon^{-\frac{8}{3}}$*

Remark 3.5. *Combining this with estimate (20) provides the error estimate for the Crank-Nicolson scheme. We can compare this estimates with those obtained in [4], [5] where an order 2 semi-implicit scheme is used. As long as $L^2(\mathbb{R})$ error estimates are considered our result is better, i.e. with respect to the dependence in ε^{-1} for the constant. Besides, it is worth to point out that in [4], [5] the author consider also a discretization in space. For numerical implementations the semi-implicit scheme used is [4], [5] is more convenient, since it does not requires to solve a fixed point problem for the nonlinear term that is explicit.*

Proof. Throughout the computations, various norms of u and its derivatives are computed and depend on ε . We have aggregated these results in Section 5 below. To begin with, integrating in time the continuous equation (11), we have, setting $\tilde{u}^n = u(n\tau)$

$$(21) \quad \begin{aligned} \frac{\tilde{u}^{n+1} - \tilde{u}^n}{\tau} + \frac{i}{\tau} \int_{n\tau}^{(n+1)\tau} Au(s) ds = \\ \frac{i}{\tau} \int_{n\tau}^{(n+1)\tau} u(s) f_\varepsilon(|u(s)|^2) ds. \end{aligned}$$

To have an upper bound on the consistency estimate in L^2 requires to have an upper bound on

$$I_1 = \|A(\frac{\tilde{u}^{n+1} + \tilde{u}^n}{2}) - \frac{1}{\tau} \int_{n\tau}^{(n+1)\tau} Au(s) ds\|_{L^2(\mathbb{R})},$$

and on

$$I_2 = \|\frac{1}{\tau} \int_{n\tau}^{(n+1)\tau} u(s) f_\varepsilon(|u(s)|^2) ds - f_\varepsilon(|\frac{\tilde{u}^{n+1} + \tilde{u}^n}{2}|^2) \frac{\tilde{u}^{n+1} + \tilde{u}^n}{2}\|_{L^2(\mathbb{R})}.$$

For this we use the following trapezoidal formula

Lemma 3.6. *Consider E a Banach space. There exists $C > 0$ such that for any g in $C^2(\mathbb{R}; E)$*

$$\|\int_a^b g(s) ds - \frac{b-a}{2}(g(b) + g(a))\|_E \leq C(b-a)^3 \sup_t \|g''\|_E.$$

This implies that in one hand due to Corollary 5.6 below

$$(22) \quad I_1 \leq C\tau^2 \sup_t \|Au_{tt}\|_{L^2(\mathbb{R})} \leq \tilde{C}\tau^2 \varepsilon^{-\frac{8}{3}}.$$

We now tackle I_2 by the two following estimates. On the one hand due to Propositions 5.1, 5.3 and 5.4.

$$(23) \quad \begin{aligned} \|\frac{\tilde{u}^{n+1} f_\varepsilon(|\tilde{u}^{n+1}|^2) + \tilde{u}^n f_\varepsilon(|\tilde{u}^n|^2)}{2} - \frac{1}{\tau} \int_{n\tau}^{(n+1)\tau} u(s) f_\varepsilon(|u(s)|^2) ds\|_{L^2(\mathbb{R})} \\ \leq C\tau^2 \sup_t \|(u f_\varepsilon(|u|^2))_{tt}\|_{L^2(\mathbb{R})} \leq C\tau^2 \frac{|\log \varepsilon|}{\varepsilon^{\frac{4}{3}}}, \end{aligned}$$

since by mere computations

$$\|(u f_\varepsilon(|u|^2))_{tt}\|_{L^2(\mathbb{R})} \leq c(|\log \varepsilon| \|u_{tt}\|_{L^2(\mathbb{R})} + \varepsilon^{-1} \|u_t\|_{L^4(\mathbb{R})}^2).$$

On the other hand, for C that depends on the L^∞ bound for u , due to Propositions 5.1, 5.3 and 5.4.

$$\begin{aligned}
(24) \quad & \left\| \frac{\tilde{u}^{n+1} f_\varepsilon(|\tilde{u}^{n+1}|^2) + \tilde{u}^n f_\varepsilon(|\tilde{u}^n|^2)}{2} - \frac{\tilde{u}^{n+1} + \tilde{u}^n}{2} f_\varepsilon(|\tilde{u}^{n+\frac{1}{2}}|^2) \right\|_{L^2(\mathbb{R})} \\
& \leq \sup_t \|u(t)\|_{L^\infty} \sup_n \|f_\varepsilon(|\tilde{u}^n|^2) - f_\varepsilon(|\tilde{u}^{n+\frac{1}{2}}|^2)\|_{L^2(\mathbb{R})} \\
& \leq C\tau^2 \sup_t \|(f_\varepsilon(|u|^2))_{tt}\|_{L^2(\mathbb{R})} \leq C\tau^2 \varepsilon^{-\frac{7}{3}}
\end{aligned}$$

since by mere computations $\|(f_\varepsilon(|u|^2))_{tt}\|_{L^2(\mathbb{R})} \leq C(\varepsilon^{-1}\|u_{tt}\|_{L^2(\mathbb{R})} + \varepsilon^{-2}\|u_t\|_{L^4(\mathbb{R})}^2)$. This completes the proof of the Proposition. \square

4. NUMERICAL EXPERIMENTS

In this section, we describe the numerical experiments for the Crank-Nicolson scheme applied to the regularized equation (11). As pointed above, for $\varepsilon = 0$ the code may have problem; then we focus on the regularized equation. We perform the computations for x in a finite box $[-L, L]$ with L large enough and homogeneous Dirichlet boundary conditions; since in the sequel we run the code with test solutions that are numerically zero outside a compact set this does not introduce any spurious reflection waves at the boundary. We complete the Crank-Nicolson scheme in time with a finite difference approximation in space that we describe now. Let $N \in \mathbb{N} - \{0\}$ and set $\delta x = \frac{2L}{N+1}$. We mesh $[-L, L]$ with nodes $x_j = j\delta x$ for $|j| \leq N+1$.

To approximate Au we use standard finite difference scheme. We define a discrete differential operator \tilde{A} as, for any vector U defined on the grid, setting respectively $\nu(x_j) = \nu_+$ if j positive and respectively ν_- if j negative

$$\begin{aligned}
(25) \quad & (\tilde{A}U)_j = \nu(x_j) \frac{2U_j - U_{j+1} - U_{j-1}}{\delta x^2} \text{ if } j \neq 0, \\
& (\tilde{A}U)_0 = \frac{(\nu_+ + \nu_-)U_0 - \nu_+U_1 - \nu_-U_{-1}}{\delta x^2}.
\end{aligned}$$

Therefore the numerical scheme reads, setting $U_j^n \simeq u(n\delta t, x_j)$ for $n \geq 0$ and $|j| \leq N$

$$(26) \quad \frac{U_j^{n+1} - U_j^n}{\tau} + i(\tilde{A} \frac{U^n + U^{n+1}}{2})_j - if_\varepsilon(|\frac{U_j^{n+1} + U_j^n}{2}|^2) \frac{U_j^{n+1} + U_j^n}{2} = 0.$$

This scheme is supplemented with boundary conditions $U_{N+1}^n = U_{-N-1}^n = 0$ and initial condition U^0 . Let us point out that solving (26) requires to solve at each time step a fixed point procedure.

It is standard to prove that this Crank-Nicolson scheme preserves the mass $\|U^n\|_{L^2}$ where here the subscript L^2 stands for the discrete finite-difference L^2 norm and the discrete energy $E_n = \|\tilde{A}^{\frac{1}{2}}U^{n+1}\|_{L^2(\mathbb{R})}^2 - \|f_\varepsilon(|U^{n+1}|^2)|U^{n+1}|^2\|_{L^1}$.

4.1. Test solutions. We begin with a true solution for equation (1). Recalling $\nu(x) = \nu_+ > 0$ if $x > 0$ and $\nu_- > 0$ if $x < 0$ we consider the following Standing Wave Solution (SWS)

$$(27) \quad u_s(t, x) = \exp\left(-it - \frac{|x|^2}{2\nu(x)}\right).$$

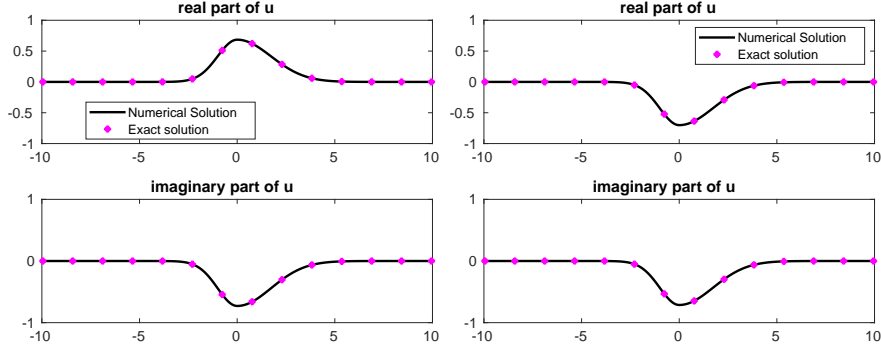


FIGURE 1. SWS: The real and imaginary parts of the exact and numerical solution at $t = 15 \times \tau$ (left) and at $t = 45 \times \tau$ (right).

Remark 4.1. As observed in [10] if u_s is solution then $qu_s(t, x) \exp(2it \log q)$ is also a solution. We then chose to normalize $q = 1$.

This SWS allows us to make numerical tests for a discontinuous viscosity. The drawbacks of this true solution is that its modulus does not depend on time and then we actually solve a linear equation.

Besides, to build the second test solution we introduce

$$(28) \quad u_-(t, x) = u_s(t, x + 20 - 2vt) \exp\left(\frac{ivx}{\nu_-}\right) \exp\left(\frac{-iv^2t}{\nu_-}\right),$$

with $v > 0$ the constant speed.

Indeed this is a solution to the equation when the viscosity is constant on the line: $\nu(x) = \nu_-$ for any x in \mathbb{R} . It is then not a true solution for (1) because here $\nu(x) \neq \nu_-$ in \mathbb{R}^+ . We refer as Gausson Solution (GS) the solution obtained solving our equation with $u_0(x) = u_-(0, x)$ and $v = 3$.

The solution u_- starts from a position $x_1 < 0$, moves to the right, then reaches the hyperplane $x = 0$ at time $t = t_1$ where a wave reflection occurs. We expect that u_- will be an approximate solution of our equation for $t < t_1$.

It is worth to point out that GS defines a test solution with a time-dependent L^2 norm. Here the difficulty is that we do not have an explicit expression of a solution which is defined for all position x and all time t . To overcome this we compute an approximate solution in $[-L, L] \times [0, T]$ with a much thinner mesh and consider it as the reference solution.

4.2. Numerical Tests. Throughout this section we will take $\varepsilon = 10^{-6}$ and $\nu_- = 1$ and $\nu_+ = 3$.

We first start with an accuracy test, we plot in Figure 1 the SWS and the numerical solution when $L = 10$ and the time and space steps are $\tau = \delta x = \frac{2 \times 10}{392} \simeq 0.0510204$. We can see that the both solutions are matching.

We now move to the test with the Gausson solution. We consider the initial data given by (28) with $t = 0$ and $v = 3$. The spatial domain is $[-25, 25]$ and the time and space steps are $\delta x = \frac{2 \times 25}{51200} \simeq 9.765625 \cdot 10^{-4}$. This GS (28) allows us to test the accuracy of the schema for $t < t_1$ and to visualize the behavior of the numerical approximated wave after crossing the hyperplane $x = 0$. The Figure 2

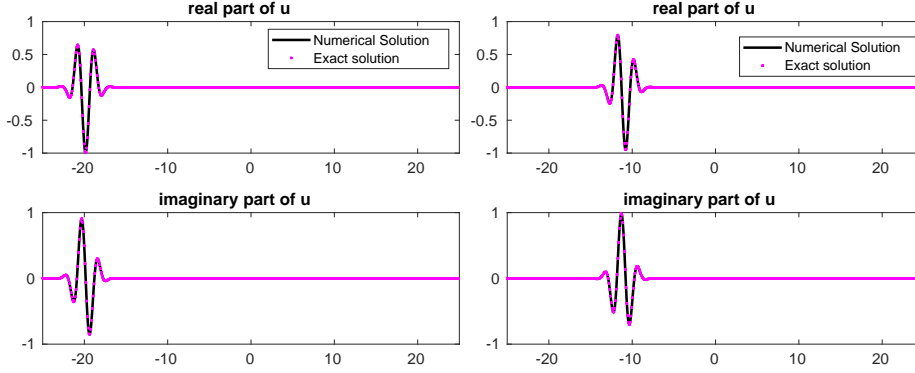


FIGURE 2. GS: The real and imaginary parts of the numerical solution and of u_- at $t = 15\tau$ (left) and at $t = 1510\tau$ (right).

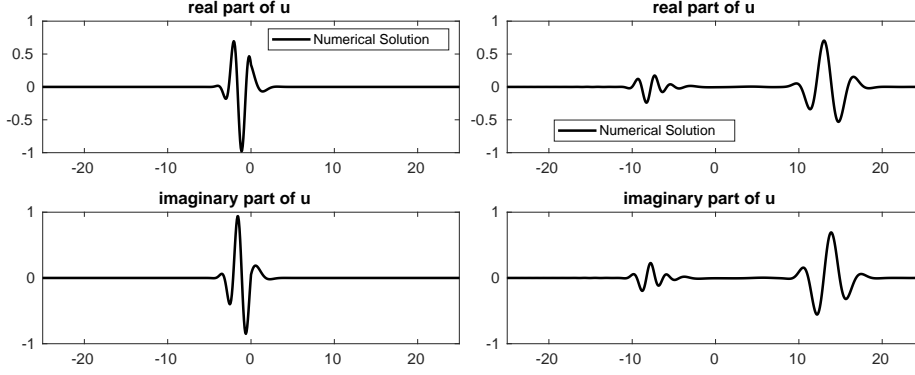


FIGURE 3. GS: The real and imaginary parts of the numerical solution at $t = 3200\tau$ (left) and at $t = 4800\tau$ (right).

shows u_- and the numerical solution for $x < 0$ and $t < t_1$ and the Figure 3 shows the numerical solution behavior during the reflection process.

We now give some numerical evidence that the Crank-Nicolson scheme is order 2 in time. We introduce the error function

$$(29) \quad e(t^n, \cdot) = U(t^n, \cdot) - U_{num}^n,$$

where U_{num}^n is the numerical solution at time $n\tau$ and U the reference solution (either the true solution or a numerical solution computed in a much thinner grid). In Figure 4 we can see $\|e\|_{L_{t,x}^\infty}$ as a function of τ for the two solutions. In the SWS case the numerical solution is compared to the exact solution while in the GS case the numerical solution is compared to a reference solution computed on the thin mesh $\delta x = \frac{2 \times 25}{51200} \simeq 9.765625 \cdot 10^{-4}$.

We finally give some numerical proofs of the conservation properties. We plot in figures 5 and 6 the variation of mass and the discret energy corresponding to (7) over time for the SWS solution and for the GS solution.

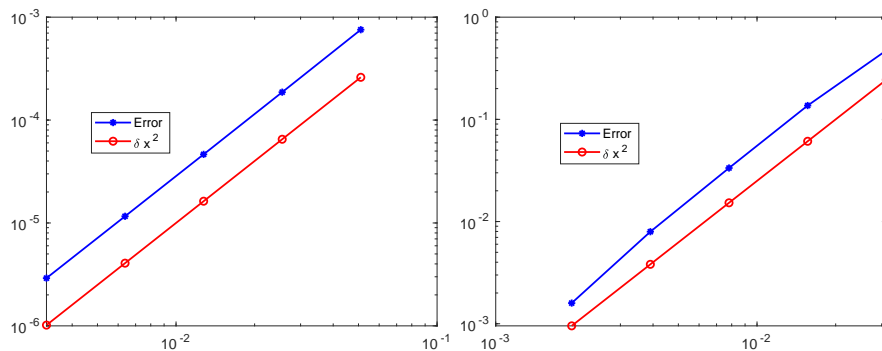


FIGURE 4. Errors $\|e\|_{L^{\infty}_{t,x}}$ as a function of τ on a logarithmic scale for the SWS (on left) and GS (on right) solutions.

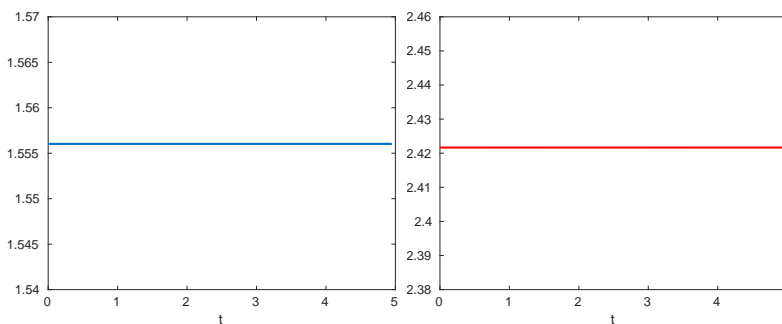


FIGURE 5. SWS: L^2 norms of u (left) and of the discrete energy (right) as a function of time.

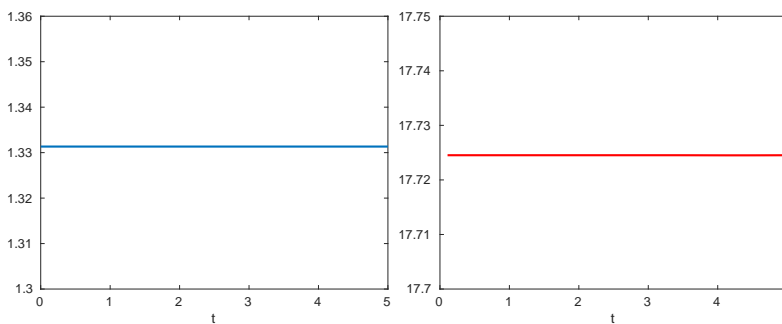


FIGURE 6. GS: L^2 norm of u (left) and of the discrete energy (right) as a function of time.

5. ANNEX

In this last section we quantify how various norms of the solution u of (11) and its derivative depend on ε . We begin with

Proposition 5.1. *Consider an initial data u_0 in $D(A)$. For any $T > 0$ there exists a constant C that may depend on u_0 and on T , but that is independent of ε in $(0, 1)$ such that for $t \in [0, T]$*

$$\|u_t(t)\|_{L^2(\mathbb{R})} + \|u(t)\|_{L^2(\mathbb{R})} + \|Au(t)\|_{L^2(\mathbb{R})} \leq C.$$

Proof. To begin with we have the conservation of mass that reads $\|u(t)\|_{L^2(\mathbb{R})} = \|u_0\|_{L^2(\mathbb{R})}$. We now consider the equation for $v = u_t$ that reads, differentiating (11),

$$(30) \quad v_t + iAv - ivf_\varepsilon(|u|^2) - 2iuf'_\varepsilon(|u|^2)\text{Re}\bar{u}v = 0.$$

Considering the scalar product of this equation with v in $L^2(\mathbb{R})$ we then have

$$(31) \quad \frac{1}{2} \frac{d}{dt} \|v\|_{L^2(\mathbb{R})}^2 \leq \left| \int_{\mathbb{R}} f'_\varepsilon(|u|^2) \text{Im}(\bar{u}^2 v^2) \right|.$$

Since $f'_\varepsilon(s) = \frac{1}{\varepsilon^2 + s}$ we then have $f'_\varepsilon(|u|^2) |\text{Im}(\bar{u}^2 v^2)| \leq |v|^2$. Therefore by Gronwall Lemma $\|v(t)\|_{L^2(\mathbb{R})}^2 \leq \exp(2t) \|v_0\|_{L^2(\mathbb{R})}^2$.

It remains to prove the estimate on Au . Due to the previous estimate we know that $Au - uf_\varepsilon(|u|^2) = iu_t$ remains in a bounded set of $L^2(\mathbb{R})$. We prove that both Au and $uf_\varepsilon(|u|^2)$ remain in a bounded set of $L^2(\mathbb{R})$. The Lemma 5.2 below completes the proof of Proposition 5.1. \square

Lemma 5.2. *Assume that u in $D(A)$ satisfies $Au - uf_\varepsilon(|u|^2) = g \in L^2(\mathbb{R})$. Then there exists C that depends on $\|g\|_{L^2(\mathbb{R})}$ and $\|u\|_{H^1(\mathbb{R})}$ such that $\|Au\|_{L^2(\mathbb{R})} + \|uf_\varepsilon(|u|^2)\|_{L^2(\mathbb{R})} \leq C$.*

Proof. Due to the identity

$$(32) \quad \|g\|_{L^2(\mathbb{R})}^2 = \|Au\|_{L^2(\mathbb{R})}^2 - 2(Au, uf_\varepsilon(|u|^2))_{L^2(\mathbb{R})} + \|uf_\varepsilon(|u|^2)\|_{L^2(\mathbb{R})}^2$$

we just have to bound by below the second term in the right hand side of (32). We set $X = -2(Au, uf_\varepsilon(|u|^2))_{L^2(\mathbb{R})}$. Integrating by parts we have

$$(33) \quad -X = 2 \int_{\mathbb{R}} \nu(x) |\nabla u(x)|^2 f_\varepsilon(|u|^2) dx + 4 \int_{\mathbb{R}} \nu(x) \frac{(\text{Re}\bar{u}u_x)^2}{\varepsilon^2 + |u|^2} dx.$$

The second term in the right hand side of (33) is bounded by above by $c\|A^{\frac{1}{2}}u\|_{L^2(\mathbb{R})}^2$. The positive part of the first term reads

$$2 \int_{\{\varepsilon^2 + |u|^2 > 1\}} \nu(x) |\nabla u(x)|^2 f_\varepsilon(|u|^2) dx.$$

Let us observe that since $\log(\varepsilon^2 + |u|^2) \leq |u|^2 + \varepsilon^2 - 1 \leq |u|^2$ then the function

$$\mathbb{1}_{\{\varepsilon^2 + |u|^2 > 1\}} \log(\{\varepsilon^2 + |u|^2 > 1\}) \leq |u|^2$$

remains bounded in $L^\infty(\mathbb{R})$ since $D(A^{\frac{1}{2}}) = H^1(\mathbb{R}) \subset L^\infty(\mathbb{R})$. The the second term is also bounded by above by $c\|A^{\frac{1}{2}}u\|_{L^2(\mathbb{R})}^2$. \square

We need also some L^∞ estimates.

Proposition 5.3. *Consider an initial data u_0 in $D(A^{\frac{3}{2}})$. For any $T > 0$ there exists a constant C that may depend on u_0 and on T , but that is independent of ε such that for $t \in [0, T]$*

$$\|u(t)\|_{L^\infty(\mathbb{R})} + \varepsilon^{\frac{1}{3}} (\|u_t(t)\|_{L^\infty(\mathbb{R})} + \|Au(t)\|_{L^\infty(\mathbb{R})}) \leq C.$$

Proof. The L^∞ bound for u comes from the bound in $D(A^{\frac{1}{2}})$ and the embedding $H^1(\mathbb{R}) \subset L^\infty(\mathbb{R})$. We now consider the scalar product of (30) with iv_t . This leads to, setting

$$(34) \quad \begin{aligned} J &= \int_{\mathbb{R}} \nu |v_x|^2 - \int_{\mathbb{R}} \frac{\operatorname{Re}(\bar{u}v)^2}{\varepsilon^2 + |u|^2} - \int_{\mathbb{R}} |v|^2 \log(\varepsilon^2 + |u|^2), \\ \frac{1}{2} \frac{d}{dt} J &= -2 \int_{\mathbb{R}} \frac{\operatorname{Re}(\bar{u}v)|v|^2}{\varepsilon^2 + |u|^2} + \int_{\mathbb{R}} \frac{\operatorname{Re}(\bar{u}v)^3}{(\varepsilon^2 + |u|^2)^2}. \end{aligned}$$

We first use

$$(35) \quad \frac{\operatorname{Re}(\bar{u}v)^2}{\varepsilon^2 + |u|^2} + |v|^2 \log(\varepsilon^2 + |u|^2) \leq |v|^2 (1 + (\varepsilon^2 - 1 + |u|^2)).$$

Appealing Proposition 5.1 yields that there exists C that does not depend on ε such that $J \geq \int_{\mathbb{R}} \nu |v_x|^2 - C$. Besides, since $\frac{|\xi|}{\varepsilon^2 + \xi^2} \leq \frac{1}{2\varepsilon}$ the right hand side of (34) is bounded by above by $3(2\varepsilon)^{-1} \|v\|_{L^3(\mathbb{R})}^3$. Appealing the classical inequality

$$(36) \quad \|v\|_{L^\infty(\mathbb{R})} \leq \sqrt{2} \|v\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \|v_x\|_{L^2(\mathbb{R})}^{\frac{1}{2}}$$

and Proposition 5.1 we have that

$$\varepsilon^{-1} \|v\|_{L^3(\mathbb{R})}^3 \leq \sqrt{2} \varepsilon^{-1} \|v\|_{L^2(\mathbb{R})}^{\frac{5}{2}} \|v_x\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \leq C \varepsilon^{-1} \|v_x\|_{L^2(\mathbb{R})}^{\frac{1}{2}}.$$

Gathering these we have that

$$\frac{d}{dt} J \leq C \varepsilon^{-1} \|v_x\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \leq \tilde{C} \varepsilon^{-1} (J + C)^{\frac{1}{4}}.$$

Therefore $\|v_x\|_{L^2(\mathbb{R})}^{\frac{3}{2}} \leq cJ^{\frac{3}{4}} \leq C\varepsilon^{-1}$. Appealing inequality (36) gives the L^∞ bound for u_t . To complete the proof of Proposition 5.3, it remains to bound $\|Au\|_{L^\infty(\mathbb{R})}$. This comes from the identity (11) and from the previous estimates (observing that for $\varepsilon \leq 1$ and $|\xi| \leq C$ then $|\xi \log(\varepsilon^2 + \xi^2)| \leq \tilde{C}$). \square

We now iterate, differentiating in time

Proposition 5.4. *Consider an initial data u_0 in $D(A^2)$. For any $T > 0$ there exists a constant C that may depend on u_0 and on T , but that is independent of ε such that for $t \in [0, T]$*

$$\varepsilon^{\frac{4}{3}} (\|u_{tt}(t)\|_{L^2(\mathbb{R})} + \|Au_t(t)\|_{L^2(\mathbb{R})}) \leq C.$$

Proof. Differentiating (30) and setting $w = v_t = u_{tt}$ we have

$$(37) \quad \begin{aligned} w_t + iAw - iw f_\varepsilon(|u|^2) - 2iuf'_\varepsilon(|u|^2) \operatorname{Re} \bar{u} w - 2iuf'_\varepsilon(|u|^2) |v|^2 - \\ 4iv f'_\varepsilon(|u|^2) \operatorname{Re} \bar{u} v - 4iuf''_\varepsilon(|u|^2) (\operatorname{Re} \bar{u} v)^2 = 0. \end{aligned}$$

Considering the scalar product of this with w we have

$$(38) \quad \begin{aligned} \frac{1}{2} \frac{d}{dt} \|w\|_{L^2(\mathbb{R})}^2 &= 4\text{Im} \int_{\mathbb{R}} \bar{v} w f'_\varepsilon(|u|^2) \text{Re} \bar{u} v + 2\text{Im} \int_{\mathbb{R}} \bar{u} w f'_\varepsilon(|u|^2) |v|^2 + \\ &2\text{Im} \int_{\mathbb{R}} \bar{u} w f'_\varepsilon(|u|^2) \text{Re} \bar{u} v + 4\text{Im} \int_{\mathbb{R}} \bar{u} w f''_\varepsilon(|u|^2) (\text{Re} \bar{u} v)^2. \end{aligned}$$

Since $|s|^3 f''_\varepsilon(s^2) \leq \varepsilon^{-1}$ the last term in the right hand side of (37) is bounded by above by $4\varepsilon^{-1} \|w\|_{L^2(\mathbb{R})} \|v\|_{L^4(\mathbb{R})}^2$. The first and second terms in the right hand side of (37) have the same upper bound since $|s| f'_\varepsilon(s^2) \leq \varepsilon^{-1}$. The third term is bounded by above by $c \|w\|_{L^2(\mathbb{R})} \|v\|_{L^2(\mathbb{R})}$. We then have,

$$(39) \quad \frac{d}{dt} \|w\|_{L^2(\mathbb{R})} \leq c(\|v\|_{L^2(\mathbb{R})} + \varepsilon^{-1} \|v\|_{L^4(\mathbb{R})}^2) \leq c \|v\|_{L^2(\mathbb{R})} (1 + \varepsilon^{-1} \|v\|_{L^\infty(\mathbb{R})}).$$

Using Proposition 5.3 we then bound by above $\|w\|_{L^2(\mathbb{R})}$. Actually (30) yields

$$\|Au_t\|_{L^2(\mathbb{R})} \leq \|w\|_{L^2(\mathbb{R})} + (\|f_\varepsilon(|u|^2)\|_{L^\infty(\mathbb{R})} + 2) \|v\|_{L^2(\mathbb{R})}.$$

Since v remains bounded in $L^2(\mathbb{R})$ and $\|f_\varepsilon(|u|^2)\|_{L^\infty(\mathbb{R})} \leq C - 2 \log \varepsilon$ then we see that $\|Au_t\|_{L^2(\mathbb{R})}$ is of same order as $\|w\|_{L^2(\mathbb{R})}$. This completes the proof of the proposition. \square

We also have the $L^\infty(\mathbb{R})$ corresponding estimate

Proposition 5.5. *Consider an initial data u_0 in $D(A^{\frac{5}{2}})$. For any $T > 0$ there exists a constant C that may depend on u_0 and on T , but that is independent of ε such that for $t \in [0, T]$*

$$\varepsilon^{\frac{16}{9}} (\|u_{tt}(t)\|_{L^\infty(\mathbb{R})} + \|Au_t(t)\|_{L^\infty(\mathbb{R})}) \leq C.$$

Proof. We consider the scalar product of (37) with iw_t to obtain $\frac{1}{2} \frac{d}{dt} H = G$ setting

$$(40) \quad \begin{aligned} H(w) &= \int_{\mathbb{R}} \nu |w_x|^2 - \int_{\mathbb{R}} (f_\varepsilon(|u|^2) |w|^2 + 2f'_\varepsilon(|u|^2) \text{Re}(\bar{u}w)^2) + \\ &- 8 \int_{\mathbb{R}} f'_\varepsilon(|u|^2) \text{Re}(\bar{v}w) \text{Re}(\bar{u}v) - 4 \int_{\mathbb{R}} f'_\varepsilon(|u|^2) \text{Re}(\bar{u}w) |v|^2 + \\ &- 8 \int_{\mathbb{R}} f''_\varepsilon(|u|^2) \text{Re}(\bar{u}v)^2 \text{Re}(\bar{u}w). \end{aligned}$$

and

$$(41) \quad \begin{aligned} G(w) &= -5 \int_{\mathbb{R}} f'_\varepsilon(|u|^2) |w|^2 \text{Re}(\bar{u}v) - 10 \int_{\mathbb{R}} f''_\varepsilon(|u|^2) \text{Re}(\bar{u}v) \text{Re}(\bar{u}w)^2 + \\ &- 10 \int_{\mathbb{R}} f'_\varepsilon(|u|^2) \text{Re}(\bar{u}w) \text{Re}(\bar{v}w) - 12 \int_{\mathbb{R}} f''_\varepsilon(|u|^2) \text{Re}(\bar{u}v)^2 \text{Re}(\bar{v}w) + \\ &- 8 \int_{\mathbb{R}} f'_\varepsilon(|u|^2) \text{Re}(\bar{v}w) |v|^2 - 12 \int_{\mathbb{R}} f''_\varepsilon(|u|^2) \text{Re}(\bar{u}v) \text{Re}(\bar{u}w) |v|^2 + \\ &- 8 \int_{\mathbb{R}} f'''_\varepsilon(|u|^2) \text{Re}(\bar{u}v)^3 \text{Re}(\bar{u}w). \end{aligned}$$

Due to (35) and Propositions 5.1 and 5.4 we first have

$$(42) \quad \int_{\mathbb{R}} (f_{\varepsilon}(|u|^2)|w|^2 + 2f'_{\varepsilon}(|u|^2)\operatorname{Re}(\bar{u}w)^2) \leq C\varepsilon^{-\frac{8}{3}}.$$

We now handle the first order terms in w in (40). The modulus of these three terms can be bounded by above by, using Propositions 5.4 and 5.3

$$C\varepsilon^{-1}\|v\|_{L^4(\mathbb{R})}^2\|w\|_{L^2(\mathbb{R})} \leq \tilde{C}\varepsilon^{-\frac{8}{3}}.$$

We now handle $G(w)$. The modulus of the quadratic terms in w can be bounded by above by, Propositions 5.4, 5.3 and (36)

$$C\varepsilon^{-1}\|v\|_{L^\infty(\mathbb{R})}\|w\|_{L^\infty(\mathbb{R})}\|w\|_{L^2(\mathbb{R})} \leq \tilde{C}\varepsilon^{-\frac{10}{3}}\|w_x\|_{L^2(\mathbb{R})}^{\frac{1}{2}}.$$

Analogously the modulus of the first order terms in w can be bounded by above by

$$C\varepsilon^{-2}\|v\|_{L^\infty(\mathbb{R})}\|v\|_{L^2(\mathbb{R})}^2\|w\|_{L^\infty(\mathbb{R})} \leq \tilde{C}\varepsilon^{-3}\|w_x\|_{L^2(\mathbb{R})}^{\frac{1}{2}}.$$

Gathering these inequalities yields that $H(w) \geq C(\|w_x\|_{L^2}^2 - \varepsilon^{-\frac{25}{12}})$ and that

$$\frac{d}{dt}H \leq C\varepsilon^{-\frac{10}{3}}(H + \varepsilon^{-\frac{8}{3}})^{\frac{1}{4}}.$$

Integrating in time leads to $H^{\frac{1}{4}} \leq C\varepsilon^{-\frac{10}{3}}$ and the bound on the L^∞ norm of w follows from inequality (36) and Proposition 5.4. Going back to (30) we see that $Au_t = iu_{tt}$ + lower order terms. This completes the proof of the proposition. \square

Proposition 5.6. *Consider an initial data u_0 in $D(A^3)$. For any $T > 0$ there exists a constant C that may depend on u_0 and on T , but that is independent of ε such that for $t \in [0, T]$*

$$\varepsilon^{\frac{8}{3}}\|Au_{tt}(t)\|_{L^2(\mathbb{R})} \leq C.$$

Proof. The proof is very similar to the proof of Proposition 5.4 and then omitted for the sake of conciseness. We first differentiate (37) with respect to t , to obtain setting $z = u_{tt}$

$$(43) \quad \begin{aligned} & z_t + iAz - izf_{\varepsilon}(|u|^2) - 2iuf'_{\varepsilon}(|u|^2)\operatorname{Re}\bar{u}z = \\ & 2ivf'_{\varepsilon}(|u|^2)\operatorname{Re}\bar{u}w + 2iuf'_{\varepsilon}(|u|^2)\operatorname{Re}\bar{v}w + 2iuf''_{\varepsilon}(|u|^2)\operatorname{Re}\bar{u}w\operatorname{Re}\bar{v}w + \\ & \frac{d}{dt}(2iuf'_{\varepsilon}(|u|^2)|v|^2 + 4ivf'_{\varepsilon}(|u|^2)\operatorname{Re}\bar{v}w + 4iuf''_{\varepsilon}(|u|^2)(\operatorname{Re}\bar{v}w)^2). \end{aligned}$$

We consider the scalar product of equation with z . We have the following upper bound for the fourth term in the left hand side of (43)

$$\int_{\mathbb{R}} |\operatorname{Im}u\bar{z}|^2 f'_{\varepsilon}(|u|^2) \leq \|z\|_{L^2(\mathbb{R})}^2.$$

Let us consider for instance the first term in the right of side of (43). Its contribution is, appealing Propositions 5.3 and 5.4

$$\left| \int_{\mathbb{R}} f'_{\varepsilon}(|u|^2)\operatorname{Re}\bar{u}w\operatorname{Im}\bar{v}z \right| \leq \varepsilon^{-1}\|w\|_{L^2(\mathbb{R})}\|v\|_{L^\infty(\mathbb{R})}\|z\|_{L^2(\mathbb{R})} \leq C\varepsilon^{-\frac{8}{3}}\|z\|_{L^2(\mathbb{R})}.$$

We carefully bound from above each term using the propositions above. We get the L^2 bound on z . Since u_{ttt} and Au_{tt} have the same order, the proof of the proposition is completed. \square

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