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Numerical study of quintic NLS equation with defect

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Abstract

In this work, we numerically investigate how a defect can affect the behavior of traveling explosive solutions of quintic NLS equation in the one-dimensional case. Our numerical method is based on a Crank-Nicolson scheme in the time, finite difference method in space including a Perfectly Matched Layer (PML) treatment for the boundary conditions. It is observed that the defect splits the incident wave in one reflected part and one transmitted part; hence the dynamics of the solution may be changed and the blow-up may be prevented depending on the values of the defect amplitude Z. Moreover, it is numerically found that the defect can be considered as a barrier for large Z.

Keywords: Quintic NLS equation, delta-function, explosive traveling solution, blow-up.

MSC: 35Q53, 65M06, 65M70, 35G25, 76B15.

1 Introduction

Nonlinear Schrödinger equation (NLS) plays an important role in the understanding of many physical phenomena such as wave propagation in nonlinear media, quantum mechanics or plasma physics. During the last decade, an intensive effort has been paid on the study of the influence of a single defect on the behavior of the solutions that can be physically interpreted as an impurity in the domain.
In this paper, we study the one-dimensional NLS equation with a quintic nonlinearity and a defect represented by a delta-function:

$$\begin{cases} iu_t + u_{xx} + Zu\delta_0 + |u|^4 u = 0, & x \in \mathbb{R}, \quad t > 0, \\ u(0,x) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{1}$$

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where $u_t = \frac{\partial u}{\partial t}$ and $u_{xx} = \frac{\partial^2 u}{\partial x^2}$. Here, Z stands for the amplitude of the defect and $u = u(t,x) \in \mathbb{C}$. The exponent involved in the nonlinearity is known as the *critical* exponent, for which blow-up may occur at finite time.

Schrödinger equations involving delta functions have been recently studied in the literature. For example, in a serie of papers, Holmer, Marzuela and Zworski analyzed the splitting of a soliton in presence of the defect, using the scattering properties in the cubic one-dimensional integrable case (see Holmer, Marzuola, and Zworski 2007a, Holmer, Marzuola, and Zworski 2007b) for which the Cauchy problem is globally well-posed in $H^1(\mathbb{R})$. Asymptotic rates for the transmission coefficients of solitons have been obtained and numerically illustrated. The stability question of standing waves solutions for this perturbed model has been adressed in Le Coz et al. 2008. In the defocusing case, the H^1 asymptotic completeness for the scattering operator has been proved in Banica and Visciglia 2016. The Gross-Pitaevskii equation with non-zero boundary conditions at infinity has also been investigated in Ianni, Le Coz, and Royer 2017.

The aim of this work is to study the influence of the defect on the behavior of the well-known solutions in the absence of defect in the quintic critical case, especially traveling standing wave solutions and blowing-up solutions that may be encountered in this case. Since this equation is not integrable, the inverse scattering method is not available which makes the numerical investigation crucial in order to have a good qualitative understanding of the solution dynamics. The paper is organized as follows: in Section 2, some theoretical results are given for the mathematical analysis of equation (1). In Section 3, the numerical method that will be used for simulations is presented. Finally, numerical results are discussed in Section 4.

2 Main theorical results

In this section, we recall the characteristics and the theoretical results of the NLS equation with a point defect. This ensures a good understanding of numerical approaches used afterwards. The following theorem concerns the well-posedness of equation (1) in $H^1(\mathbb{R})$ (see Theorem 3.7.1 in Cazenave 2003):

Theorem 1 – *For any $u_0 \in H^1(\mathbb{R})$, there exists $T > 0$ and a unique $u \in \mathcal{C}([0,T), H^1(\mathbb{R})) \cap \mathcal{C}([0,T), H^{-1}(\mathbb{R}))$ solving (1) such that either $T = +\infty$ or $T < +\infty$ and $\|u_x\|_{L^2} \to \infty$ as $t \to T$. Moreover, u satisfies the conservation of mass $M(u(t)) = M(u_0)$ and conservation of energy $E_Z(u(t)) = E_Z(u_0)$ for $t \in [0,T)$, where M and E_Z are formally defined for a given function $v = v(x)$ as*

$$M(v) = \|v\|_{L^2}^2 \quad \textit{and} \quad E_Z(v) = \|v_x\|_{L^2}^2 - Z|v(0)|^2 - \frac{1}{3}\|v\|_{L^6}^6.$$

We now recall some elementary properties of the solutions of (1), proved in Fukuizumi, Ohta, and Ozawa 2008 (and in the references therein) for smooth solutions.

Proposition 1 – *Assume that the initial data u_0 is smooth (say $\mathcal{C}^\infty$) and has compact support in $(-\infty, 0)$. Let $u \in \mathcal{C}([0,T]; H^1(\mathbb{R}))$ solution of* (1). *Then for each t, we have $u(t) \in H^2(\mathbb{R}^*) \cap H^1(\mathbb{R})$ and satisfies both $iu_t + u_{xx} + |u|^4 u = 0$ for $x \in \mathbb{R}^*$, $t > 0$ as well as the boundary condition*

$$u_x(t, 0^+) - u_x(t, 0^-) = -Zu(t, 0). \tag{2}$$

This result comes from the initial formulation of (1) set in a distributional sense. Indeed, the linear part acting on a test-function $\varphi \in \mathcal{C}_0^\infty$ writes

$$< u_{xx} + Z\delta_0 u, \varphi >= - < u_x, \varphi_x > + Zu(t,0)\varphi(0).$$

Assuming that u belongs to H^1, u is continuous at $x = 0$. Moreover, if the first spatial derivative of u coincides with a $\mathcal{C}^1$ fonction in the two half-lines with a finite jump at $x = 0$, this product reduces to

$$< u_{xx} + Z\delta_0 u, \varphi >= \int_{-\infty}^{+\infty} u_{xx}\varphi \, dx + [u_x(t, 0^+) - u_x(t, 0^-) + Zu(t, 0)]\varphi(0)$$

using two distinct integrations by parts performed on $(-\infty, 0)$ and $(0, +\infty)$. By choosing φ adequately, we finally obtain (2) and the NLS equation for $x \neq 0$.

From the mathematical point of view, the solution belongs to $C([0, +\infty); D(A))$ where A is the unbounded operator $-\Delta$ whose domain is $D(A) = \{u \in H^2(\mathbb{R}^*) \cap H^1(\mathbb{R})$; the condition (2) is valid$\}$. The condition (2) can be seen as a jump condition at the defect location. Note that for $Z = 0$, this reduces to the continuity of the first derivative at zero. For a general nonlinearity $|u|^{p-1}u$ where $p \in [1, +\infty)$, Fukuizumi, Ohta and Ozawa in Fukuizumi, Ohta, and Ozawa 2008 proved the existence and uniqueness of a local solution in time with initial values u_0 in $H^1(\mathbb{R})$. They also showed that the Cauchy problem is globally well-posed in $H^1(\mathbb{R})$ for $1 < p < 5$.

2.1 Global solutions

In the case $Z = 0$, Weinstein proved in Weinstein 1983 that the Cauchy problem for the quintic NLS equation is globally well-posed in $H^1(\mathbb{R})$ for sufficiently small initial-value u_0. This reads as

Theorem 2 – *Given $Z = 0$ and $u_0 \in H^1(\mathbb{R})$, a sufficient condition for global existence in the initial-value problem* (1) *is*

$$\|u_0\|_{L^2} < \|R\|_{L^2}, \tag{3}$$

where R is the positive solution of the equation $-\phi + \phi_{xx} + \phi^5 = 0$, of minimal L^2 norm, often referred as the ground state.

This result shows that $\|R\|_{L^2}$ appears as the critical mass for the formation of singularity for the solutions of NLS equation

$$iu_t + u_{xx} + |u|^4 u = 0, \quad x \in \mathbb{R}, \quad t > 0. \tag{4}$$

One may wonder if there exists a similar but different result for solutions of (1). We know (see Le Coz et al. 2008) that for some values of Z, there exists ground states that are different of the usual ground state without defect. Actually, the condition (3) comes from a precise formulation of the Gagliardo-Nirenberg inequality that reads (see Genoud, Malomed, and Weishauupl 2016)

$$\|u\|_{L_6}^6 \leq 3\Big(\frac{\|u\|_{L_2}}{\|R\|_{L_2}}\Big)^4 \|u_x\|_{L_2}^2. \tag{5}$$

One may wonder for instance in the case $Z < 0$ what is the best constant in the modified Gagliardo-Nirenberg inequality that reads

$$\|u\|_{L_6}^6 \leq C_Z \|u\|_{L_2}^4 (\|u_x\|_{L_2}^2 - Z|u(0)|^2), \tag{6}$$

for any u in $H^1(\mathbb{R})$, where $\|u_x\|_{L^2}^2 - Z|u(0)|^2 = (Au, u)$. We have straightforwardly $C_Z \leq C_0 = \frac{3}{\|R\|_{L_2}^4}$.

Conversely, taking $u(x) = R(x - \mu)$ and letting $\mu \to +\infty$, we have that in fact $C_Z = C_0$. It transpires from this simple computations that of course the defect does not play any role for solutions whose location is very far from 0. We will see numerically in the sequel that the point defect does play a role for solutions that encounter its location.

Actually, an analogous result of theorem 2 holds true if $Z \neq 0$.

Proposition 2 – *A sufficient condition for global existence in the initial value problem* (1) *for* $Z \neq 0$ *and* $u_0 \in H^1(\mathbb{R})$ *is*

$$\|u_0\|_{L^2} < \|R\|_{L^2}.$$

Proof. We prove that under this smallness assumption, the L^2 norm of the gradient remains uniformly bounded. Due to the conservation of energy, we have that

$$Z|u^Z(t,0)|^2 = \|u_x^Z\|_{L^2}^2 - \frac{1}{3}\|u^Z\|_{L^6}^6 - E_Z(u_0) \geq \|u_x^Z\|_{L^2}^2 \left(1 - \Big(\frac{\|u\|_{L^2}}{\|R\|_{L^2}}\Big)^4\right) - E_Z(u_0) \tag{7}$$

due to Gagliardo-Nirenberg inequality (5). We now claim that for any $\varepsilon > 0$, we have

$$|Z||u^Z(t,0)|^2 \leq |Z|\|u^Z\|_{L^2}\|u_x^Z\|_{L^2} \leq \frac{Z^2}{2\varepsilon}\|u^Z\|_{L^2}^2 + \frac{\varepsilon}{2}\|u_x^Z\|_{L^2}^2. \tag{8}$$

using Agmon inequality and Young inequality. Combining (7) and (8), we then find that

$$\|u_x^Z\|_{L^2}^2 \left(1 - \left(\frac{\|u_0\|_{L^2}}{\|R\|_{L^2}}\right)^4 - \frac{\varepsilon}{2}\right) \leq E_Z(u_0) + \frac{Z^2}{2\varepsilon}\|u_0\|_{L^2}^2$$

since the mass conservation holds. Choosing then ε sufficiently small such that each term is strictly positive, which is possible since $\|u_0\|_{L^2} < \|R\|_{L^2}$, we conclude that $\|u_x^Z\|_{L^2}$ is bounded which implies that the solution u^Z is global in H^1. This concludes the proof. □

2.2 Blow-up solutions and the virial identity

For sufficiently large initial data, Glassey Glassey 1977 produced the necessary conditions for blow-up for solutions of (4) introducing the momentum and virial of a given function u as respectively

$$q(u) = \int_{\mathbb{R}} x^2|u|^2\,dx \quad \text{and} \quad V(u) = \mathrm{Imm}\left(\int_{\mathbb{R}} x u_x \overline{u}\,dx\right).$$

Set $E(u) = E_0(u)$ for the energy in the case $Z = 0$. We recall from Genoud, Malomed, and Weishauupl 2016; Glassey 1977

Theorem 3 – *Let u be a solution of* (4) *such that $q(u_0) < +\infty$. Assume that either $E(u_0) < 0$ or $E(u_0) = 0$ and $V(u_0) < 0$. Then there exists a finite blow-up time T^* such that*

$$\lim_{t\to T^*} \|u_x\|_{L^2} = +\infty \quad \textit{and} \quad \lim_{t\to T^*} \|u\|_{L^\infty} = +\infty.$$

The key argument in the proof is that $q(u)$ cannot exist for any positive time t. Actually, we may address the same strategy in the case $Z \neq 0$ and we have (see Le Coz et al. 2008):

Theorem 4 – *Let $u_0 \in H^1(\mathbb{R})$ such that $xu_0 \in L^2(\mathbb{R})$ and let u solves* (1). *Setting $q(t) := q(u(t))$ and $V(t) := V(u(t))$, we have for $t \in (0,T)$*

$$q'(t) = 4V(t) \tag{9}$$

and

$$V'(t) = 2E_Z(u_0) + Z|u(t,0)|^2. \tag{10}$$

The calculations we present in the following are formal. A rigorous proof of the virial theorem is given in Le Coz et al. 2008.

Proof. We first calculate $q'(t)$. We formally have

$$q'(t) = 2\,\mathfrak{Re}\left(\int_{\mathbb{R}} x^2 u_t \overline{u}\, dx\right).$$

Recalling that $u_t = iu_{xx} + i|u|^4 u$ and that $u_x(t,0^+) - u_x(t,0^-) = -Zu(t,0)$ for each $t \in (0,T)$, we deduce with integrations by parts performed on $(-\infty,0)$ and $(0,+\infty)$ that

$$\begin{aligned} q'(t) = -2\,\mathfrak{Im}\left(\int_{\mathbb{R}} x^2 u_{xx}\overline{u}\, dx\right) &= 2\,\mathfrak{Im}\left(\int_{\mathbb{R}} u_x (x^2\overline{u})_x\, dx\right) - 2\,\mathfrak{Im}\left([x^2 u_x \overline{u}]_{0^-}^{0^+}\right) \\ &= 4\int_{\mathbb{R}} x\, u_x \overline{u}\, dx = 4V(t). \end{aligned}$$

We also have

$$V'(t) = -2\,\mathfrak{Im}\left(\int_{\mathbb{R}} x\, u_t u_x\, dx\right) + \mathfrak{Im}\left(\int_{\mathbb{R}} x (u_t\overline{u})_x\, dx\right).$$

On one hand,

$$\begin{aligned} \mathfrak{Im}\left(\int_{\mathbb{R}} x\,(u_t\overline{u})_x\, dx\right) &= -\mathfrak{Im}\left(\int_{\mathbb{R}} u_t\overline{u} dx + [x\, u_t\overline{u}]_{0^+}^{0^-}\right) \\ &= -\mathfrak{Im}\left(\int_{\mathbb{R}} (iu_x x + i|u|^4 u)\, \overline{u}\, dx\right) \\ &= \|u_x\|_{L^2}^2 - \|u\|_{L^6}^6 - [u_x\overline{u}]_{0^+}^{0^-}. \end{aligned}$$

Using the transmission condition in zero, the first integral rewrites

$$\mathfrak{Im}\left(\int_{\mathbb{R}} x (u_t\overline{u})_x\, dx\right) = \|u_x\|_{L^2}^2 - \|u\|_{L^6}^6 - Z|u(t,0)|^2.$$

On the other hand,

$$\begin{aligned} 2\,\mathfrak{Im}\left(\int_{\mathbb{R}} x\, u_t u_x\, dx\right) &= -2\,\mathfrak{Re}\left(\int_{\mathbb{R}} x\,(u_{xx} + |u|^4 u)\overline{u}_x\, dx\right) \\ &= -2\,\mathfrak{Re}\left(\int_{\mathbb{R}} x\, u_{xx}\overline{u}_x\, dx\right) - 2\,\mathfrak{Re}\left(\int_{\mathbb{R}} x\, |u|^4 u\overline{u}_x\, dx\right) \\ &= \|u_x\|_{L^2}^2 + \frac{1}{3}\|u\|_{L^6}^6. \end{aligned}$$

It follows that $V'(t) = 2\|u_x\|_{L^2}^2 - Z|u(t,0)|^2 - \frac{2}{3}\|u\|_{L^6}^6$ which finally leads to $V'(t) = 2E_Z(u_0) + Z|u(t,0)|^2$. □

A sufficient condition for blow-up is the following:

Proposition 3 – *Let $Z < 0$ and let u solves* (1) *with finite momentum. If $E_Z(u_0) < 0$, then there exists a finite time T^* such that*

$$\lim_{t\to T^*} \|u_x\|_{L^2} = +\infty.$$

Proof. If $Z < 0$ and $E_Z(u_0) < 0$, the energy conservation and virial equality (10) shows that $V(t)$ is a decreasing function, that implies

$$0 \le q(t) \le q(0) + 4V(u_0)t + 4E_Z(u_0)t^2. \tag{11}$$

Hence, the solution cannot last forever since $t \to +\infty$ leads to a contradiction if $E_Z(u_0) < 0$. □

Once again, at a first glance, Z does not play a role for *all* blow-up solutions. We will discuss numerically in the sequel that in fact it does.

2.3 The wall effect while $|Z| \to +\infty$

We now focus on the case $|Z| \to +\infty$. In this case, Z can be seen as a penalization term in transmission condition (2). This means that when $|Z|$ is large, this condition formally reduces to Dirichlet condition $u(t,0) = 0$. We intend here to derive a rigorous asymptotic.

We then give the following statement

Theorem 5 – *Let the initial data $u_0 \in H^1(\mathbb{R})$ of the problem* (1) *be such that $supp(u_0) \subset (-\infty, 0)$ and that*

$$\|u_0\|_{L^2}^2 < \|R\|_{L^2}^2 \tag{12}$$

where $\|R\|_{L^2}^2$ is related to the best constant involved in the one-dimensional Gagliardo-Nirenberg inequality (5)*. Then, when Z converges to $-\infty$, the solution $u = u^Z$ of the problem* (1) *converges to u^∞ solution of the limit problem*

$$\begin{cases} iv_t + v_{xx} + |v|^4 v = 0, & x \in (-\infty, 0), \quad t > 0, \\ v(0,x) = u_0(x), & x \in (-\infty, 0), \\ v(t,0) = 0, & t > 0. \end{cases} \tag{13}$$

Proof. Using the energy conservation and since $\mathrm{supp}(u_0) \subset (-\infty, 0)$ we obtain

$$\|u_x^Z\|_{L^2}^2 - Z|u^Z(t,0)|^2 - \frac{1}{3}\|u^Z\|_{L^6}^6 = \|(u_0)_x\|_{L^2}^2 - \frac{1}{3}\|u_0\|_{L^6}^6 = E_0(u_0). \tag{14}$$

Using assumption (12), the Gagliardo-Nirenberg inequality implies that $E_0(u_0)$ is a positive constant, since

$$\|(u_0)_x\|_{L^2}^2 - \frac{1}{3}\|u_0\|_{L^6}^6 \ge \|(u_0)_x\|_{L^2}^2 \left(1 - \left(\frac{\|u_0\|_{L_2}}{\|R\|_{L_2}}\right)^4\right).$$

Furthermore, in the case $Z < 0$, (14) implies

$$E_0(u_0) \geq \|u_x^Z\|_{L^2}^2 - \frac{1}{3}\|u^Z\|_{L^6}^6 \geq \|u_x^Z\|_{L^2}^2 \left(1 - \left(\frac{\|u_0\|_{L_2}}{\|R\|_{L_2}}\right)^4\right).$$

Consequently the H^1 norm of the solution is uniformly bounded in time: indeed, we have

$$\|u^Z\|_{H^1}^2 = \|u^Z\|_{L^2}^2 + \|u_x^Z\|_{L^2}^2 = \|u_0\|_{L^2}^2 + \|u_x^Z\|_{L^2}^2 \leq \|u_0\|_{L^2}^2 + \frac{E_0(u_0)}{1 - \left(\frac{\|u_0\|_2}{\|R\|_2}\right)^4}.$$

From this, we conclude that the solution u^Z is global in $H^1(\mathbb{R})$. The estimate (14) also leads us to

$$-Z|u^Z(t,0)|^2 \leq E_0(u_0)$$

and passing to the limit $Z \to -\infty$, we finally have

$$\lim_{Z \to -\infty} |u^Z(t,0)| = 0.$$

Hence, we can extract a subsequence that converge weakly-star in $L^\infty(0,T;H^1(\mathbb{R}))$ towards u^∞. We denote by u^Z this subsequence. We have $u^\infty(t,0) = 0$ if it makes sense.

We know that u^Z is bounded in $L^\infty(0,T;H^1(\mathbb{R}))$. Now, we show that u_t^Z is bounded in an appropriate space. We have

$$u_t^Z = i(u_{xx}^Z + |u^Z|^4 u^Z + Z u^Z \delta_0).$$

It is easy to see that the map $u^Z \longmapsto u_{xx}^Z + u^Z\delta_0$ is continuous from $H^1(\mathbb{R})$ into $H^{-1}(\mathbb{R})$. Therefore u_t^Z remains in a bounded set of $L^\infty(0,T;H^{-1}(\mathbb{R}))$. We now use the following theorem (see Temam 1997)

Theorem 6 – *Consider $V \subset H$ a compact embedding between two Hilbert space. Consider $H \sim H'$ and then $H' \subset V'$. Consider $T > 0$ and a sequence v^n that is bounded in $L^2(0,T;V)$ and such that v_t^n is bounded in $L^2(0,T;V')$. Then there exists a subsequence $v^{n'}$ that converge strongly in $L^2(0,T;H)$.*

Here u^Z is bounded in $L^2(0,T;H^1(I))$ for any compact interval $I = [-L,L]$ of $\mathbb{R}$ and its time derivative is bounded in $L^2(0,T;H^{-1}(I))$. Then for any $I_n = [-n,n]$ we may extract a subsequence u_n^Z that converges strongly in $L^2(0,T;L^2(I_n))$. Using the Cantor diagonal process we may extract a subsequence still denoted by u^Z such that u^Z converges strongly towards u in $L^2(0,T;L^2(I))$, for *any* I. We set $L^2(0,T;L^2(\mathbb{R}_{loc}))$ for this convergence. Interpolating, we also have that this convergence holds in $L^2(0,T;\mathcal{C}(I))$ for any I.

We may now pass to the limit. Consider a test function $\varphi \in \mathcal{C}_0^\infty(I)$ for a given I. We have that

$$< u_t^Z - i(u_{xx}^Z + Zu^Z\delta_0), \varphi >_{H^{-1},H^1} = < i|u^Z|^4 u^Z, \varphi >_{H^{-1},H^1}, \tag{15}$$

where $< \cdot, \cdot >_{H^{-1},H^1}$ denotes the dual product. On the one hand, due to the weak convergence results stated above the left hand side of (15) pass to the limit. On the other hand, interpolating between $L^\infty(0,T;H^1(I))$ and $L^2(0,T;L^2(I))$ we now that u^Z converges strongly towards u in $L^6(0,T;L^6(I))$, and then we may pass to the limit in the right hand side of (15). Since the limit equation is valid for any I and any test function supported in I, then u is solution to the limit problem set in $\mathbb{R}$. We observe that since u belongs to $L^2(0,T;H^1(\mathbb{R}))$ and since its time derivative belongs to its dual space, then u is a continuous function in time with value in $L^2(\mathbb{R})$ (and by interpolation in $\mathcal{C}(\mathbb{R})$). Then the wall condition $u(t,0) = 0$ is valid and the initial condition $u(0,x) = u_0(x)$ holds true. This completes the proof of the theorem. □

In the following Sections, we investigate the ability for the defect to stop or slow down the blow-up mechanism.

3 The numerical method

3.1 Numerical method without defect

We start with the numerical method in the case $Z = 0$. Our discretization is based on a finite differences semi-implicit Crank-Nicolson scheme in time and space, that is well-known to be unconditionnally stable in L^2 and second-order both in time and space. In order to perform simulations in a bounded domain, one has to implement well-adapted boundary condition in order to avoid reflections due to the boundary. Among all possible choices known in the literature, we have chosen to use Perfectly Matched Layer approach (PML) Zheng 2007. This consists in solving a Schrödinger-like problem on a domain including absorbing layers that surround the numerical domain, where outgoing waves will be forced to vanish without propagation accross the domain under study. Let $\Omega = (x_L, x_R)$ be the computational domain and L be the width of PML band.

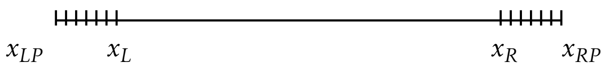

Figure 1 – Domain with PML.

The PML equation, defined in an enlarged interval $(x_{LP}, x_{RP}) = (x_L - L, x_R + L)$, is written

$$iu_t + \frac{1}{(1+R\sigma)^2}u_{xx} - \frac{R\sigma'}{(1+R\sigma)^3}u_x + |u|^4 u = 0, \quad x \in (x_{LP}, x_{RP}), \quad t > 0,$$

where $R \in \mathbb{C}$ and σ is the so-called absorption function

$$\sigma = \begin{cases} \sigma_0(x - x_L)^2, & x_{LP} < x < x_L, \\ 0, & x_L < x < x_R, \\ \sigma_0(x - x_R)^2, & x_R < x < x_{RP}, \end{cases}$$

with $\sigma_0 > 0$. A specific choice of parameters R, σ_0 and L (namely $R = e^{i\pi/4}$, $\sigma_0 = 1$ and $L = 2$) minimizes reflected waves at the boundary: indeed, the outgoing waves are anihilated when travelling inside the absorbing layer. At the two boundary points $\{x_{LP}, x_{RP}\}$ a zero Dirichlet boundary conditions is imposed. The strong formulation of the problem in the absence of defect is then given by

$$\begin{cases} iu_t + \dfrac{1}{(1+R\sigma)^2} u_{xx} - \dfrac{R\sigma'}{(1+R\sigma)^3} u_x + |u|^4 u = 0, & x \in (x_{LP}, x_{RP}), \quad t > 0, \\ u(0,x) = u_0(x), & x \in (x_{LP}, x_{RP}), \\ u(t, x_{LP}) = u(t, x_{LR}) = 0, & t > 0. \end{cases} \tag{16}$$

Following a finite difference strategy, we intend to compute the approximate value, say u_j^n, of the solution of (16) at time $t_n = n\Delta t$ and at spatial point $x_j = x_{LP} + j\Delta x$. Using Taylor expansions that enable us to compute approximations of the partial derivative operators, we get for each (j, n)

$$i\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{(1+R\sigma_j)^2} \frac{u_{j+1}^{n+1/2} - 2u_j^{n+1/2} + u_{j-1}^{n+1/2}}{\Delta x^2} \\ - \frac{R\sigma_j'}{(1+R\sigma_j)^3} \frac{u_{j+1}^{n+1/2} - u_{j-1}^{n+1/2}}{2\Delta x} + \frac{1}{2}\left(|u_j^{n+1}|^4 u_j^{n+1} + |u_j^n|^4 u_j^n\right) = 0, \tag{17}$$

where $u_j^{n+1/2} = (u_j^n + u_j^{n+1})/2$. This nonlinear system is solved using a fixed point method at each time step. It means that successive linear equations are solved until the nonlinear error that quantifies the size of two consecutive iterations becomes small enough.

3.2 The delta-function approximation

We now focus on the discretization of the defect term at $x = 0$. As in the work of Le Coz and al. Le Coz et al. 2008, J. Holmer et C. Liu Holmer and Liu 2020 and also in Genoud, Malomed, and Weishauupl 2016, we do not consider the initial form of the problem but choose to take into account the transmission condition in zero. We thus consider the problem

$$\begin{cases} iu_t + \dfrac{1}{(1+R\sigma)^2} u_{xx} - \dfrac{R\sigma'}{(1+R\sigma)^3} u_x + |u|^4 u = 0, & x \neq 0, \quad t > 0, \\ u_x(t, 0^+) - u_x(t, 0^-) = -Zu(t, 0), & t > 0. \end{cases} \tag{18}$$

Discretization of the transmission condition is performed with a $\mathcal{O}(\Delta x^2)$ accuracy for the sake of consistency with the second order accuracy in space of the scheme. Starting from the approximation

$$u_x(t,0^+) = \frac{1}{\Delta x}\Big(-u(t,2\Delta x) + 4u(t,\Delta x) - 3u(t,0)\Big) + \mathcal{O}(\Delta x^2)$$

and the similar expression for $u_x(t,0^-)$, we get a second-order approximation of the transmission condition as

$$-u^n_{D+2} + 4u^n_{D+1} + 2(Z\Delta x - 3)u^n_D + 4u^n_{D-1} - u^n_{D-2} = 0$$

where integer D stands for the defect index (such that $x_{RL} + D\Delta x = 0$). This extra relation is added to the discretization (17) expressed for $j \neq D$.

3.3 Numerical evidence of blow-up

It is reported that for $Z = 0$ there are three ways of checking blow-up occurrence. Indeed, finite time blow-up can manifest itself as the divergence of the norms $\|u\|_{L^\infty}$ and $\|u_x\|_{L^2}$. Using Gagliardo-Nirenberg inequality (5), it leads us to the divergence of $\|u\|_{L^6}$. When dealing with numerical computations, one naturally wonders how blow-up can be numerically detected. In this condition, one can compute the three discrete norms and check the corresponding orders of magnitude.

Computing the L^∞ norm may seem the most intuitive way for the blow-up detection, because it is the most natural way of investigating how "big" the solution is. However, for conservative schemes for which the discrete l^2 norm $\|u^n\|_{l^2}$ is conserved, the maximal amplitude is attained at some index j_0 and it can be written that

$$\|u^n\|^2_{l^\infty} = |u^n_{j_0}|^2 \leq \|u^n\|^2_{l^2} = \sum_j |u^n_j|^2 = \sum_j |u^0_j|^2 \approx \frac{1}{\Delta x}\|u_0\|^2_{L^2}.$$

It means that the computed solution cannot go higher in amplitude than $\frac{C}{\sqrt{\Delta x}}$. Consequently, for a prescribed spatial mesh, the maximal amplitude is uniformly bounded and numerical detection of blow-up in terms of maximal amplitude requires to deal with well-adapted grid: approximate solutions of maximal magnitude M can only be computed for spatial mesh with size $\approx 1/\sqrt{M}$ which may be inappropriate if M is large.

Other way is to investigate the time evolution of the discrete versions of $\|u\|^6_{L^6}$ and $\|u_x\|^2_{L^2}$. Indeed, these two norms are involved in the energy; checking these quantities gives us information about the *energetic* divergence whereas the maximum amplitude depicts the *punctual* one.

In order to illustrate this, we plot in Figure 2 the temporal plot of these three discrete norms as well as the singular profile when computing a blowing-up solution

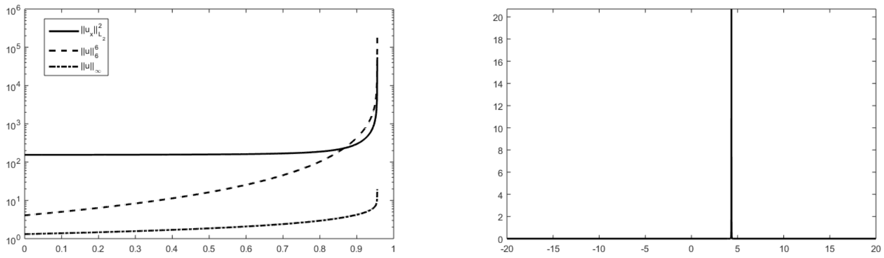

Figure 2 – Discrete versions of $\|u_x\|_{L^2}^2$, $\|u\|_{L^6}^6$ and $\|u\|_{L^\infty}$ versus time (left) and spatial singularity formation at $t = 0.9557$ (right).

that is initialized with initial data calculated from the self-similar solution that will be given in Section 4. It can be logically noticed that the orders of magnitude of $\|u\|_{L^6}^6$ and $\|u_x\|_{L^2}^2$ are much larger than the one found for $\|u\|_{L^\infty}$. This suggests us to detect the blow-up occurrence in terms of "energetic" norms instead of the maximal amplitude of the solution.

In all that follows, we will compute the discrete approximation of the quantity $\|u_x\|_{L^2}$ to state the occurrence of blow-up.

4 Numerical results

In this Section, we investigate the influence of the defect on the dynamics of solutions of the ideal case $Z = 0$. Several kinds of Cauchy data will be considered. We begin by travelling states.

4.1 Travelling solutions

We first perform simulations when considering travelling solutions built from the ground state C. Sulem and P. Sulem 1999, that explicitly express as

$$u(t,x) = R(x - vt - x_0)\ \exp\left(i\frac{v}{2}x\right)\ \exp\left(i\left(1 - \frac{v^2}{4}\right)t\right), \tag{19}$$

with $R(x) = 3^{1/4}/(\cosh(2x))^{\frac{1}{2}}$. This wave is located at x_0 that will be chosen far away for the defection location in order to be initially consistent with the transmission condition. As preliminary test, we numerically check the conservation of mass and energy with a defect of amplitude $Z = 10$. We have chosen discretization parameters $\Delta x = 5\times10^{-3}$ and $\Delta t = 2.5\times10^{-5}$ for a simulation performed until final time $T = 0.7$, starting for the initial standing wave centered at $x_0 = -5$ considered with $v = 30$. Let

M_n and E_n respectively stand for the discrete mass and energy at $t = t_n$. In Figures 3, we represent the order of magnitude of the relative errors made for M_n and E_n versus time. It is observed that the numerical scheme mimics the right preservation

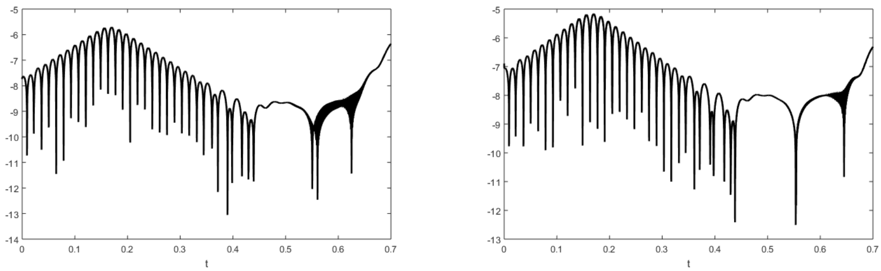

Figure 3 – Plot of $\ln \frac{M^{n+1}-M^n}{M^n}$ (left) and $\ln \frac{E^{n+1}-E^n}{E^n}$ (right) versus time.

of the invariants of the NLS equation at a discrete level, claiming that the relative error for these quantities is found smaller than 10^{-6}.

We now investigate the influence of the defect on the propagation of the travelling wave solution for $Z = 10$, starting from an initial state that is located at the left-side of the defect (see Figure 4), inside the numerical domain $\Omega = (-20, 20)$. Following a phase of interaction with the defect that is observed in Figure 4, we see that the solution splits into two parts: a transmitted wave $u_\mathbf{t}$ and a reflected one $u_\mathbf{r}$. We note t_Z the interaction time such that for $t > t_Z$, we have $u = u_\mathbf{t} + u_\mathbf{r}$ where $u_\mathbf{t}$ turns to be the restriction of u on $(0, x_R)$, while $u_\mathbf{r}$ is the restriction of u on $(x_L, 0)$. In Figure 5, we point out that $u_\mathbf{t}$ travels to the right whereas the reflected wave $u_\mathbf{r}$ propagates to the left side of the domain.

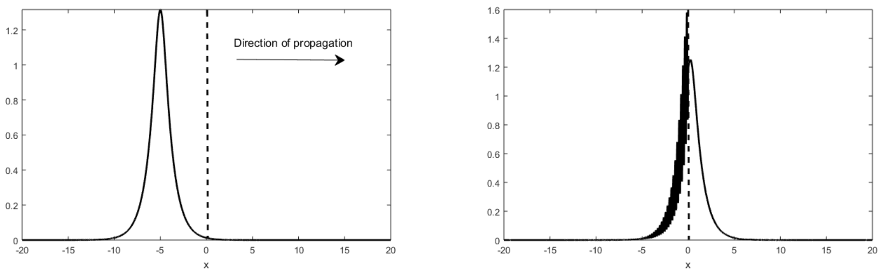

Figure 4 – Initial profile and solution profile when interacting with the defect for $Z = 10$ at $t = 0.174$.

In the following test, we calculate the transmitted mass for the same previous initial data and for different values of Z: $Z = 2$ and $Z = 10$. The plots viewed in Figure 5 show that large defect amplitude enhances the reflection of the incoming wave.

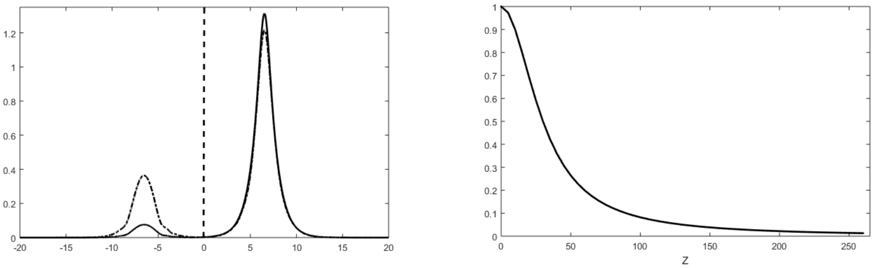

Figure 5 – Left: Solution profile after defect interaction for two values of Z (continuous line: $Z = 2$, dot-dashed line : $Z = 10$) at $t = 0.3846$. Right: plot of the transmitted mass ratio $\frac{M_Z^\infty}{\|u_0\|_{L^2}^2}$ as a function of Z.

To evaluate the transmitted mass, we compute M_Z^t as the portion of the mass located between the defect interface and the right boundary. We then set

$$M_Z^t = \int_{0.5}^{x_L} |u^Z(t,x)|^2 \, dx$$

for different Z. Our simulations have shown that as t is large enough, M_Z^t converges to a limit value M_Z^∞ that depends on Z. We have found in particular $M_2^\infty = 2.7091$, $M_5^\infty = 2.649$ and $M_{100}^\infty = 0.2261$. It is noticed that the bigger Z is, the smaller the transmitted part is. We also decide to plot the transmitted mass ratio $M_Z^\infty/\|u_0\|_{L^2}^2$ as a function of Z. The plot displayed in Figure 5 shows us that this ratio logically turns out to be a decreasing function of Z and tends to zero when Z tends to infinity. For large Z, no more mass is transmitted at the defect location and the point $x = 0$ behaves as a boundary point for which Dirichlet would have been prescribed. Thus, for large enough Z, the solution is totally reflected and the defect plays the role of a barrier. In Figure 6, we present the result obtained for $Z = -10000$ from a travelling data centered at $x_0 = -15$, that is far enough from the defect in order to avoid initial interactions. It can be clearly seen that the transmitted solution is nothing but the initial one that has been reflected by the defect.

In Figure 7, it is numerically checked that $|u^Z(t,0)|$ tends to zero when Z tends to $-\infty$, which is in good agreement with the theoretical results. Our simulations have shown that $-Z|u^Z(t,0)|^2$ is always bounded by $E_Z(u_0) = 612.567$ for all time, as shown in Section 2.

The question that now arises is what happens in the symmetric case $Z > 0$. In Figure 7, the convergence of $|u^Z(t,0)|$ to zero is observed when Z tends to $+\infty$. When

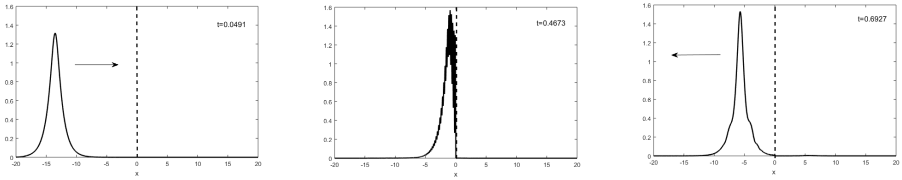

Figure 6 – Solution profile for $Z = -10000$ at different times.

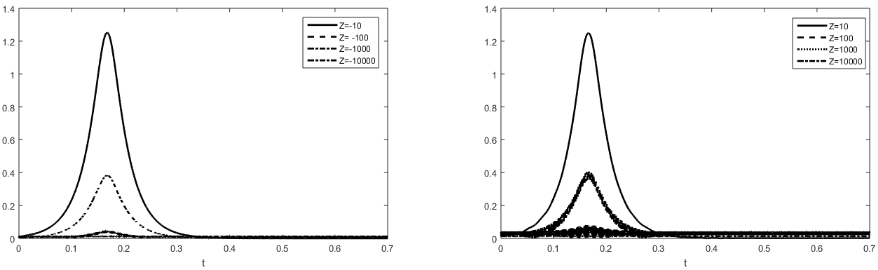

Figure 7 – Evolution of $|u(t,0)|$ versus time for $Z < 0$ (left) and $Z > 0$ (right).

$Z \to +\infty$, the defect behaves as a Dirichlet boundary condition (DBC) at $x = 0$. In Figure 8, we plot at the same final time $t = 0.777$ the solutions computed with $Z = -10000$ and $Z = 10000$ compared with the solution v calculated with DBC at $x = 0$. The superposition of the three curves is clearly observed. We then conclude that the defect always plays the role of a barrier when $|Z| \to \infty$. Note that the case $Z \to +\infty$ is not covered by Theorem 13 given in Section 2.

4.2 Blowing-up travelling solutions

We now study the influence of Z on the behavior of explosive solutions. We address here the question of blow-up prevention by the defect. It is well-know that a negative initial energy is a sufficient condition for blow-up occurrence. In this critical case, it is possible to compute explicit blowing-up solution with use of the pseudo-conformal invariance. We here consider the self-similar solution

$$\widetilde{u}(t,x) = \frac{1}{\sqrt{T-t}} \exp\left(\frac{-ix^2}{4(T-t)}\right) u\left(\frac{1}{T-t}, \frac{x}{T-t}\right),$$

where u is given by (19). What is remarkable with this solution is that it blows-up at prescribed time T. The simulation performed in the case $Z = 0$ (see Figure 2 in Section 3) has shown the formation of the singularity at $x \simeq 4.3$, that is at the right

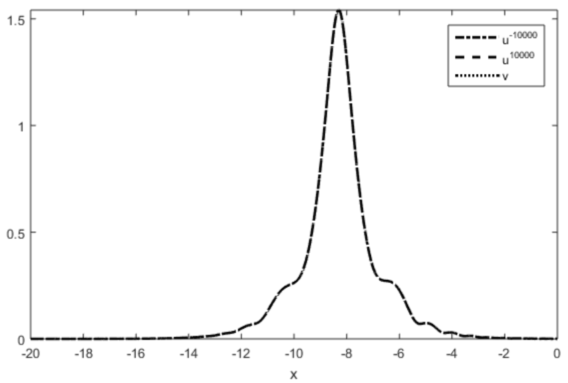

Figure 8 – Comparison between solution profile of NLS equation with DBC and the solutions obtained for $Z = -10000$ and $Z = 10000$ at $t = 0.777$.

side of the defect. This provides us to reference solution in order to investigate the defect influence on the explosive dynamics.

We first perform a simulation in the case $Z = 5$. We have considered the following parameters: $T = 1$, $v = 5$, $x_0 = -15$, $\Delta x = 2.5 \times 10^{-3}$ and $\Delta t/\Delta x^2 = 1$. Due to the shift term $v/(T-t)$ involved in the self-similar solution, the initial data is centered at $x_* = -10$. In this simulation, parameters have be chosen in such a way that the exact solution of the problem without defect blows-up at $x_* = 5$. As for the travelling stationary state, we now compute the mass of the transmitted wave as well as the norm $\|u_x\|_{L^2}^2$ versus time after the defect interaction.

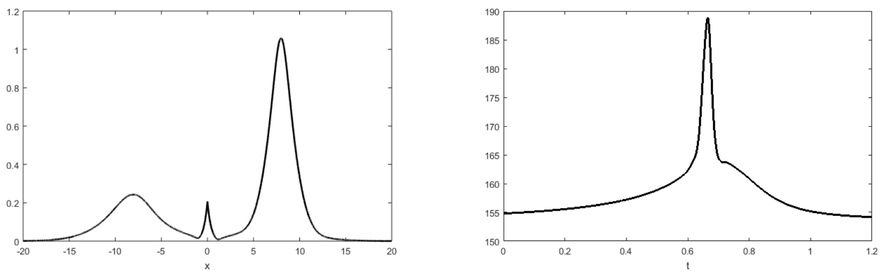

Figure 9 – Numerical solution after the defect interaction, $Z = 5$ (left) and evolution of $\|u_x\|_{L^2}^2$ versus time for $Z = 5$ (right).

In Figure 9 (left) is shown the temporal profile of the solution after it has crossed the defect. Once again, it consists in two parts and it can be observed that both the transmitted and reflected part have a mass that become strictly smaller than the initial one $\|u_0\|_{L^2} = \|R\|_{L^2}$. Note that the L^2 norm of u_x plotted in Figure 9 (right) is bounded, even if early stage mimics a divergent profile before the defect is reached by the solution. Consequently, this suggests that each of them gives a global solution: the splitting effect of the defect thus prevents blow-up. Of course, this is not rigorous since equation (1) is nonlinear. Nevertheless, if the support of the two waves are well-separated (meaning that $u_{\mathbf{t}} u_{\mathbf{r}} \simeq 0$ on the whole spatial domain), then $|u_{\mathbf{t}} + u_{\mathbf{r}}|^4 (u_{\mathbf{t}} + u_{\mathbf{r}}) \simeq |u_{\mathbf{t}}|^4 u_{\mathbf{t}} + |u_{\mathbf{r}}|^4 u_{\mathbf{r}}$ and the total solution u can be approximated by the sum $u \simeq u_{\mathbf{t}} + u_{\mathbf{r}}$, each of them solving (1). In our test case, we numerically have

$$\|u_{\mathbf{r}}\|_{L^2}^2 < \|u_{\mathbf{t}}\|_{L^2}^2 \simeq 2.441 < \|R\|_{L^2}^2 = 2.7207.$$

We have also performed simulations when considering the initial Gaussian data

$$u_0(x) = q \ \exp(ikx) \ \exp(-(x - x_0)^2). \tag{20}$$

Here, the global existence or finite time blow-up of the corresponding solution strongly depends on the choice of parameters q and k. First, the solution is global if $\|u_0\|_2 < \|R\|_2$, which implies $q < (\frac{3\pi}{2})^{\frac{1}{4}} := q_1^*$, this upper bound being independent of k. On the other hand, recalling that a sufficient condition of blow-up of the solution is $E(u_0) < 0$, we explicitly have

$$E(u) = E(u_0) = \frac{q^2}{2} \sqrt{\frac{\pi}{2}} \left((1 + k^2) - \frac{1}{3^{\frac{3}{2}}} q^4 \right).$$

Hence, $E(u_0) < 0$, if $q > 3^{\frac{3}{8}} (1 + k^2)^{\frac{1}{4}} := q_2^*(k)$. Consequently, for a prescribed k, the solution blows up for $q > q_2^*(k)$. Note that in this case, blow-up occurrence is very strong, which let the numerical investigation of the defect influence quite delicate since the solution cannot propagate on a long distance before blowing-up. Furthermore, one has to notice that the blow-up time is not explicitly know as opposed to the self-similar solution. Simulations made with $q \in (q_1^*, q_2^*(k))$ leading to blowing up solutions in the unperturbed case have shown that blow-up is prevented in presence of the defect. As an example, the values $k = 10$, $q = 1.55$ and $x_0 = -5$ for the Gaussian data (20) have given a global solution for the defect amplitude $Z = 20$. We conjecture that there exists a critical $Z_* = Z_*(q)$ for which the solution becomes global for $|Z| \geq Z_*(q)$.

4.3 The case of two defects

We finally study the influence of two defects with respective amplitudes Z_1 and Z_2 located at x_1 and x_2 on the explosive behavior of solutions. We have considered the discretization parameters $\Delta x = 2.5 \times 10^{-3}$ and $\Delta t / \Delta x^2 = 1$, starting from the initial data

$$u_0(x) = 2.18 \exp(60ix) \exp(-(x + 3)^2).$$

leading us to an explosive travelling solution. We first chose $Z_1 = 80$ and $Z_2 = 0$ (which means that only the first defect is present). In Figure 10 is shown the first splitting of the Gaussian data leading to blow-up. After crossing the first defect located at $x_1 = 0$, the solution divides itself into a reflected part and a transmitted one. After the interaction time t_{Z_1}, we thus have

$$u = u_{\mathbf{t}}^{Z_1} + u_{\mathbf{r}}^{Z_1},$$

where $u_{\mathbf{t}}^{Z_1}$ is the transmitted wave which is in our case the restriction of u on $(0,20)$, while $u_{\mathbf{r}}^{Z_1}$ stands for the reflected wave that can be seen as the restriction of u on $(-20,0)$. We observe that $u_{\mathbf{r}}^{Z_1}$ is a global solution, which can be numerically

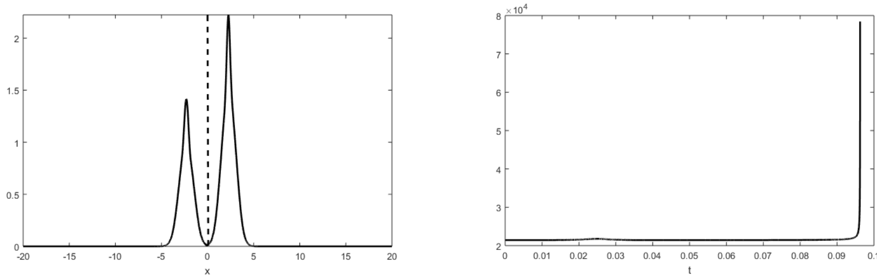

Figure 10 – Numerical solution after the first defect interaction ($Z_1 = 80$ and $Z_2 = 0$), $t = 0.0442$ (left) and plot of the norm $\|(u_{\mathbf{t}}^{Z_1})_x\|_{L^2}^2$ (right).

confirmed since $\|u_{\mathbf{r}}^{Z_1}\|_{L^2}^2 = 1.822 < \|R\|_2^2$. However, the transmitted part $u_{\mathbf{t}}^{Z_1}$ is an explosive solution: it can be explained by the fact that the defect did not extract a sufficient amount of mass to prevent blow-up. It implies that $\|u_{\mathbf{t}}^{Z_1}\|_{L^2}^2 > \|R\|_2^2$ and a singularity will develop for this transmitted part. The evolution of $\|(u_{\mathbf{t}}^{Z_1})_x\|_{L^2}^2$ plotted with respect to time in Figure 10 confirms this tendency.

We now introduce a second defect of amplitude $Z_2 = 120$ at $x = 5$, in order to investigate if the blow-up occurring after the first defect interaction can be prevented. The solution $u_{\mathbf{t}}^{Z_1}$ splits into two parts due to the second defect. Consequently, we write

$$u_{\mathbf{t}}^{Z_1} = u_{\mathbf{t}}^{Z_2} + u_{\mathbf{r}}^{Z_2},$$

where each part is now global since the computations show that $\|u_{\mathbf{t}}^{Z_2}\|_{L^2}^2 = 2.1003 < \|R\|_{L^2}^2$ and $\|u_{\mathbf{r}}^{Z_2}\|_{L^2}^2 = 2.0768 < \|R\|_{L^2}^2$.

We also note that the reflected solution encounters the first default and wave splitting phenomenon is repeated over time. Thus, the presence of two defects

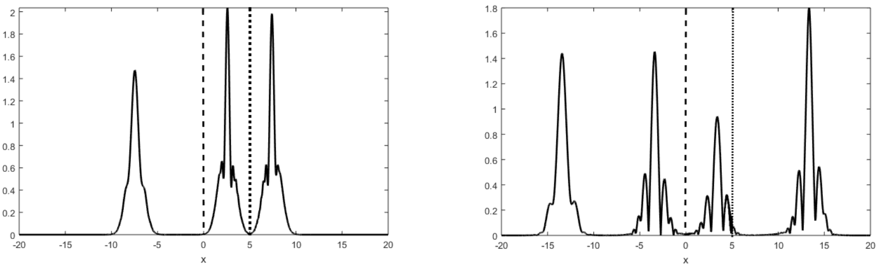

Figure 11 – Numerical solution after the second defect interaction, $t = 0.0873$ (left) and $t = 0.1371$ (right).

stopped the explosion. Of course, taking a larger amplitude for the initial data may change the qualitative property of the solution. Indeed, the blow-up may still occur for a larger total mass.

From these computations, it can be conjectured that a travelling blowing-up solution may become global in presence of a defect lattice formed with a family $(Z_k, x_k)_{k\geq 0}$ that could successively extract mass and generate interaction waves at each defect location.

5 Conclusion

In this work, we have theoretically and numerically investigated the influence of a defect on the dynamics of solutions of the quintic NLS equation in the one-dimensional case.

First, we showed that it is possible to obtain sufficient conditions for global well-posedness. Surprisingly, this condition is the same as in the absence of defect, involving the ground state of the NLS equation. Similarly, finite time blow-up is proved by means of virial identity for negative energy initial data. The asymptotics $Z \to -\infty$ has been studied, showing when $|Z|$ is large, the solution mimics on the negative half-line the one of the boundary NLS problem with homogeneous Dirichlet conditions set at $x = 0$. It means that large defect amplitude drives the point $x = 0$ to behave as a barrier. This can be interpreted as a consequence of the fact that Z acts as a penalty parameter in the transmission condition, meaning that if the jump of the spatial derivative of the solution at the origin is seeked bounded through time, then $Zu^Z(t, 0)$ is bounded and the solution tends to zero when $|Z|$ is large.

We then performed numerical simulations in order to observe the defect influence on two well-known classes of solutions: travelling standing waves and blowing-up self-similar solutions that can be explicitly computed in this one-dimensional critical case. The discretization of the transmission condition is performed and added to the classical Crank-Nicolson scheme. It is generally detected in our computations that the defect splits the incident wave in two parts: one reflected part and one transmitted one. The mass of each part depends on the value of Z and the mass transfer becomes more relevant as the defect amplitude is large.

What is remarkable is that even if a initial data localized far away from $x = 0$ may lead to blowing-up solution for $Z = 0$, the defect can prevent blow-up if each separate part has a remaining mass smaller than the one of the ground state. It means that at large distances, the time dynamics of each part is driven by the classical NLS without defect, as if both of them solved a separate NLS equation on each half-line. Of course, for a given initial mass, $|Z|$ has to be large enough in order to extract for the initial wave emitted and reflected parts that are "well-balanced" in such away that each mass is smaller than the critical one.

From all these computations, it turns out that the defect can be considered as a perturbation of the ideal NLS equation, meaning that for small Z, the classical travelling and blowing-up behaviors are recovered, with little influence of the singular contribution. However, large defect amplitude leads us to a breaking effect that drastically affects the well-known dynamics: in particular, blowing-up solutions in the case $Z = 0$ may become global after crossing the original. This could be somehow referred as a stabilization effect.

The same considerations could logically be addressed in higher spatial dimension, where the defect is located on a line or a curve. This should deserve a forthcoming paper.

Acknowledgments

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