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Spectral splitting method for nonlinear Schrödinger equations with singular potential

Andrea Sacchetti

Dipartimento di Matematica Pura ed Applicata, Universitá di Modena e Reggio Emilia, Via Campi 213/B, Modena 41100, Italy

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Abstract

We consider the time-dependent one-dimensional nonlinear Schrödinger equation with pointwise singular potential. By means of spectral splitting methods we prove that the evolution operator is approximated by the Lie evolution operator, where the kernel of the Lie evolution operator is explicitly written. This result yields a numerical procedure which is much less computationally expensive than multi-grid methods previously used. Furthermore, we apply the Lie approximation in order to make some numerical experiments concerning the splitting of a soliton, interaction among solitons and blow-up phenomenon.

Keywords: Nonlinear Schrödinger equations; Spectral splitting

1. Introduction

In this paper we study the one-dimensional time-dependent nonlinear Schrödinger equation (hereafter NLS) with a spatially localized point defect represented by means of a Dirac's delta. Such a basic model has recently attracted an increasing interest, from both theoretical [2,10,12,20] and numerical [11,14–16] points of view; in fact, scattering of solitons by point defects is a natural model extensively studied in physics (see, e.g., [9]).

Previous numerical experiments performed by Goodman et al. [14] are mainly based on finite difference approximation schemes where the Dirac's delta function is approximated either as a single point discontinuity, or by a smoother function with small support; a slightly different procedure with a nonuniform two-dimensional grid has been adopted by Holmer et al. [15,16] where they choose a finer grid centered at the origin (where the Dirac's delta is supported) in order to better study the effects of the interaction with the point defect. In these models a linear system has to be solved at each step.

In the first part of this paper we develop a different numerical procedure based on spectral splitting techniques for Schrödinger equations (see, e.g., the contributions given by [6,17,19]), that is we approximate the

E-mail address: Sacchetti@unimore.it

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evolution operator of the NLS with point defect by means of the Lie evolution operator. These techniques, applied by Besse et al. [7] for NLS without potential, are adapted here to the case of point defect. In particular, in Theorem 1 we prove that the solution $\psi_t(x) = \psi(x,t)$ (hereafter, index t denotes the dependence on time of the solution) of the NLS equation with point defect

$$\begin{cases} i\frac{\partial\psi_t}{\partial t} = -\frac{\partial^2\psi_t}{\partial x^2} + \gamma\delta\psi_t + \epsilon|\psi_t|^{2\mu}\psi_t, \\ \psi_t(x)|_{t=0} = \psi_0(x) \in L^2(\mathbb{R}) \end{cases} \tag{1}$$

is approximated by means of the Lie evolution operator in the following sense: for any fixed $T \geqslant 0$, for any $N > 0$ large enough and for any $\beta < \frac{1}{4}$ there exists a positive constant C which depends on β and on $\max_{t\in[0,T]}\|\psi_t\|_{L^\infty}$, but independent on $h = T/N$, such that

$$\|\psi_T - [X^hY^h]^N\psi_0\|_{L^2} \leqslant Ch^\beta, \quad h = T/N,$$

where Y^h simply acts as $Y^hw = e^{-i\epsilon h|w|^{2\mu}}w$ and where X^h is the evolution operator of the linear Hamiltonian with Dirac's delta. Here $\gamma \in \mathbb{R}$ is the strength of the Dirac's delta function, $\epsilon \in \mathbb{R}$ is the strength of the nonlinear term and $\mu > 0$. For $\gamma > 0$ (resp. $\gamma < 0$) then we speak of *repulsive* (resp. *attractive*) pointwise interaction; for $\epsilon > 0$ (resp. $\epsilon < 0$) we speak of *de-focusing* (resp. *self-focusing*) nonlinearity.

Since the evolution operator X^h of the exact linear problem is given by means of an integral operator which kernel is explicitly written (Lemma 1) then such a method simply consists of an iterative procedure where at each step the computation just consists of a numerical integration. Furthermore, we do not need to make any approximation of the Dirac's delta function. Therefore, the numerical scheme we have developed here seems to be much less computationally expensive and more robust than the previous ones.

In the second part of this paper we perform some numerical experiments.

The first experiment concerns the motion of solitons and the effect of the pointwise perturbation on such a motion. This kind of experiment concerning the motion of a single soliton is not new, see, e.g., [14–16], and the main effect is the splitting of the soliton when its *center of mass*, defined as

$$\langle x\rangle^t = \int_{\mathbb{R}} x|\psi_t(x)|^2\,dx,$$

hits the support of the pointwise perturbation. One part of the wave function will move according to the initial velocity while the other part will move in the opposite direction (see Fig. 1), and the motion of the center of mass will slow down (see Fig. 3) for both attractive and repulsive pointwise perturbation. We then consider a new experiment concerning the collision of two solitons, and we have different pictures depending on the sign of the strength of the Dirac's delta. In fact, in the case of repulsive pointwise interaction (i.e. $\gamma > 0$) then the motion of the center of mass will be accelerated when it passes through the support of the pointwise interaction; in contrast, in the case of attractive pointwise interaction (i.e. $\gamma < 0$) then the motion of the center of mass will be decelerated when it passes through the support of the pointwise interaction and, as in the case considered in Fig. 4, the motion of the center of mass inverts its direction.

The second experiment concerns the appearance of blow-up phenomena for increasing self-focusing nonlinearity and when the nonlinear power μ is hyper-critical (that is $\mu > 2$). This phenomenon has been previously studied by [1] for NLS equation with a pointwise interaction and a general criterion has been formulated for the appearance of blow-up. Here we consider a state that initially coincides with the stationary state of the linear Schrödinger equation (with attractive Dirac's delta): when the strength $|\epsilon|$ of the nonlinear term is smaller than a given value ϵ_1 then there is no blow-up, in contrast when the strength $|\epsilon|$ of the nonlinear term is larger than a given value ϵ_2 then there is blow-up in finite time. In an explicit example we numerically compute ϵ_1 and ϵ_2 and we perform some experiments for different values of ϵ. Our experiments fully agree with the theoretical analysis and also the transition from no-blow-up to blow-up condition appears (Fig. 5).

2. Spectral-splitting method

We consider the time-dependent nonlinear Schrödinger equation (hereafter NLS) with real-valued potential V

$$\begin{cases} \mathrm{i}\frac{\partial \psi_t}{\partial t} = -\frac{\partial^2 \psi_t}{\partial x^2} + V\psi_t + \epsilon|\psi_t|^{2\mu}\psi_t, \\ \psi_t(x)|_{t=0} = \psi_0(x) \in L^2(\mathbb{R}), \end{cases} \tag{2}$$

where $\mu > 0$ and $\epsilon \in \mathbb{R}$ are fixed parameters. Under some assumptions on V (see, e.g., [8]) then Eq. (2) admits an unique local solution

$$\psi_t = S^t\psi_0,$$

where

$$S^t : L^2(\mathbb{R}) \to L^2(\mathbb{R})$$

is a unitary evolution operator.

2.1. Lie approximation

We consider, separately, the linear Cauchy problem

$$\begin{cases} \mathrm{i}\frac{\partial v_t}{\partial t} = -\frac{\partial^2 v_t}{\partial x^2} + Vv_t, \\ v_t(x)|_{t=0} = v_0(x) \in L^2(\mathbb{R}) \end{cases} \tag{3}$$

and the nonlinear Cauchy problem

$$\begin{cases} \mathrm{i}\frac{\partial w_t}{\partial t} = \epsilon|w_t|^{2\mu}w_t, \\ w_t(x)|_{t=0} = w_0(x) \in L^2(\mathbb{R}) \end{cases} \tag{4}$$

and we denote by X^t and Y^t, respectively, the evolution operator associated with (3) and (4):

$$v_t = X^t v_0 \quad \text{and} \quad w_t = Y^t w_0.$$

The evolution operator X^t will depend on the potential V; in contrast, the evolution operator Y^t is simply given by:

$$w_t = Y^t w_0 = w_0 \exp[-\mathrm{i}\epsilon t|w_0|^{2\mu}]. \tag{5}$$

We recall that (2) and (4) have the mild representation (Duhamel formula)

$$\psi_t = S^t\psi_0 = X^t\psi_0 + \mathrm{i}\epsilon\int_0^t X^{t-s}|\psi_s|^{2\mu}\psi_s\,\mathrm{d}s \tag{6}$$

and

$$w_t = Y^t w_0 = w_0 + \mathrm{i}\epsilon\int_0^t |w_s|^{2\mu}w_s\,\mathrm{d}s. \tag{7}$$

Let us introduce the Lie evolution operator

$$Z^t := Z^t_L = X^t Y^t. \tag{8}$$

In the case of the free one-dimensional problem it has been proved [7] that such an evolution operator represents a good approximation of the evolution operator S^t in the following sense:

$$S^t \approx [Z^{t/N}]^N \tag{9}$$

for N large enough and t fixed.

Here, we consider the Lie approximation 8 for the one-dimensional NLS (1) with singular potential V given by a pointwise Dirac's δ interaction, where γ is a real parameter.

It is well known [4] that the linear operator

$$H_\gamma = -\frac{\partial^2}{\partial x^2} + \gamma\delta$$

is self-adjoint on the domain $H^2(\mathbb{R}\setminus\{0\})$ with boundary conditions

$$\psi(0+0)=\psi(0-0) \tag{10}$$

and

$$\psi'(x+0)-\psi'(x-0)=\gamma\psi(0+0). \tag{11}$$

Namely

$$D(H_\gamma)=\{\psi\in H^2(\mathbb{R}\setminus\{0\}):\psi \quad \text{satisfies} \quad (10) \quad \text{and} \quad (11)\}.$$

Notice that, due to (10), the function $\psi\in D(H_\gamma)$ is continuous at $x=0$ and therefore $D(H_\gamma)$ is a subspace of $H^1(\mathbb{R})$. Thus, in the following we denote by $\psi(0)$ the limit (10).

We recall also that (Theorem 1 in [2]) if the initial data ψ_0 belongs to $H^1(\mathbb{R})$ then Eq. (1) admits a unique local solution

$$\psi_t=S^t\psi_0\in H^1 \quad \text{for any } t\in(-T_-,T_+) \tag{12}$$

for some $T_\pm=T_\pm(\psi_0)>0$. Furthermore, the following conservation laws hold:

– *Conservation of the norm*: S^t is a unitary evolution operator:

$$\|\psi_t\|_{L^2}=\|S^t\psi_0\|_{L^2}=\|\psi_0\|_{L^2}.$$

– *Conservation of the energy*: let us introduce the following functional, named *energy*:

$$\mathcal{E}[\psi]=\left\|\frac{\partial\psi}{\partial x}\right\|^2_{L^2}+\gamma|\psi(0)|^2+\frac{\epsilon}{\mu+1}\|\psi\|^{2(\mu+1)}_{L^{2(\mu+1)}(\mathbb{R})}. \tag{13}$$

Then

$$\mathcal{E}[\psi_t]=\mathcal{E}[S^t\psi_0]=\mathcal{E}[\psi_0].$$

We state now our main theorem.

Theorem 1. *Let $\psi_0\in H^1$ and let Z^t be the Lie evolution operator*

$$Z^t=X^tY^t,$$

where $X^t=e^{-iH_\gamma t}$ is the evolution operator of the linear problem with singular potential and where Y^t is the evolution operator (5). Let S^t be the evolution operator associated with the NLS (1) for $t\in[0,T]$ where $0<T<T_+$ is fixed. Let $N\in\mathbb{N}$ and $0<h\ll 1$ such that $T=Nh$, where h is small enough in order to have $hm^{2\mu}\leqslant 1$ where

$$m:=m_T=\max\left[\max_{t\in[0,T]}\|\psi_t\|_{L^\infty},\max_{t\in[0,T-h]}\|Z^h\psi_t\|_{L^\infty}\right], \tag{14}$$

$$m_1:=\max_{t\in[0,T]}\|\psi_t\|_{H^1}. \tag{15}$$

Then, for any $\beta<\frac{1}{4}$

$$\|(Z^h)^N(\psi_0)-S^{Nh}(\psi_0)\|_{L^2}\leqslant[e^{2|\epsilon|\mu m^{2\mu-1}T}-1]\cdot e^{|\epsilon|Cm^{2\mu}h}|\epsilon|Cm^{4\mu}[\sqrt{h}m_1+|\gamma|h^\beta] \tag{16}$$

some positive constant $C>0$ independent of ψ_0,h and T.

Remark 1. Estimate (16) holds in the limit of small h, $T=Nh$ fixed and with m and m_1 bounded for any time $t\leqslant T$. When we apply this result in a proximity of the blow-up (that is T close to T_+) then m becomes larger and larger and, in such a case, it seems better to make use of a numerical adaptive scheme in order control the remainder term (16).

Remark 2. In the case of $\epsilon=0$, that is we have only the linear problem, then (16) agrees with the trivial result $Z=S$. When $\gamma=0$, that is we have the free potential, then (16) agrees with the results given by [7].

Remark 3. Here, for the sake of definiteness, we consider the Lie evolution operator of the form $Z_L^t = X^t Y^t$; however, it is possible to treat in a similar way the cases where

$$Z_L^t = Y^t X^t$$

and where Z^t is one of the Strang evolution operators

$$Z_S^t = X^{\frac{1}{2}t} Y^t X^{\frac{1}{2}t} \quad \text{and} \quad Z_S^t = Y^{\frac{1}{2}t} X^t Y^{\frac{1}{2}t}.$$

2.2. Properties of the linear problem

Let us recall some basic properties of the spectrum of H_γ. For details see [3,4,18].

The essential spectrum of H_γ is purely absolutely continuous and coincides with the positive real axis:

$$\sigma_{\text{ess}}(H_\gamma) = \sigma_{\text{ac}}(H_\gamma) = [0, +\infty).$$

Moreover,

– If $\gamma \geqslant 0$ then the discrete spectrum of H_γ is empty.
– If $\gamma < 0$ then the discrete spectrum of H_γ is given by just one simple eigenvalue

$$\lambda = -\frac{1}{4}\gamma^2$$

with associated normalized eigenvector

$$\phi_\gamma(x) = \sqrt{\frac{|\gamma|}{2}} \mathrm{e}^{-|\gamma| \cdot |x|/2}. \tag{17}$$

Besides, we shall make use of the explicit expression of the time evolution generated by H_γ, that is an integral operator

$$[X^t v](x) = \int_{\mathbb{R}} U_\gamma^t(x, y) v(y) \, \mathrm{d}y \tag{18}$$

whose kernel reads [3,18]

$$U_\gamma^t(x, y) = U_0^t(x - y) + \gamma R_\gamma^t(x, y),$$

where

$$R_\gamma^t(x, y) = \begin{cases} -\frac{1}{2} \int_0^{+\infty} \mathrm{d}u \mathrm{e}^{-\frac{1}{2}\gamma u} U_0^t(u + |x| + |y|), & \text{if } \gamma > 0, \\ 0, & \text{if} \gamma = 0, \\ \frac{1}{\gamma} \mathrm{e}^{\mathrm{i}\frac{\gamma^2}{4}t} \phi_\gamma(x)\phi_\gamma(y) + \frac{1}{2} \int_0^{+\infty} \mathrm{d}u \, \mathrm{e}^{\frac{1}{2}\gamma u} U_0^t(u - |x| - |y|), & \text{if } \gamma < 0 \end{cases} \tag{19}$$

and where

$$U_0^t(\zeta) = \frac{1}{\sqrt{4\pi \mathrm{i} t}} \exp\left(-\frac{|\zeta|^2}{4\mathrm{i}t}\right)$$

is the integral kernel associated to the free Laplacian.

Furthermore, we have the following result.

Lemma 1. *Let $t > 0$, then the kernel R_γ^t can be written as*

$$R_\gamma^t(x, y) = -\frac{1}{4} \mathrm{e}^{\frac{\mathrm{i}}{4}\gamma^2 t + \frac{1}{2}(|x| + |y|)\gamma} \mathrm{erfc}\left[\frac{t\gamma - \mathrm{i}(|x| + |y|)}{2\sqrt{-\mathrm{i}t}}\right] \tag{20}$$

for any $\gamma \in \mathbb{R} - \{0\}$. Furthermore, for any fixed $0 < \beta < \frac{1}{4}$ and any $t^\star > 0$ small enough there exists $C = C_{\beta,t^\star} > 0$ such that for all $w \in H^1$ then

$$\|X^t w - w\|_{L^2} \leqslant C\left[\sqrt{t}\|w\|_{H^1} + |\gamma| t^\beta \|w\|_{L^2}\right], \quad \forall t \in [0, t^\star]. \tag{21}$$

Remark 4. It is immediate to note that

$$R_\gamma^{-|t|}(x,y) = \overline{R_\gamma^{|t|}(x,y)}$$

and

$$U_\gamma^{-|t|}(x,y) = \overline{U_\gamma^{|t|}(x,y)}.$$

Furthermore, for $t < 0$ it follows that:

$$R_\gamma^t(x,y) = -\frac{1}{4} e^{\frac{i}{4}\gamma^2 t + \frac{1}{2}(|x|+|y|)\gamma} \left\{ 2 - \operatorname{erfc}\left[\frac{t\gamma - i(|x|+|y|)}{2\sqrt{-it}} \right] \right\}.$$

Proof. At first, we consider the case $\gamma > 0$ where (20) will follow by direct computation. Indeed, for $\gamma > 0$ we have that:

$$\begin{aligned}
R_\gamma^t(x,y) &= -\frac{1}{2\sqrt{4\pi i t}} \int_0^{+\infty} \exp\left[-\frac{1}{2}\gamma u - \frac{(u+|x|+|y|)^2}{4it} \right] du \\
&= -\frac{1}{2\sqrt{\pi}} e^{\frac{1}{4} i t \gamma^2 + \frac{1}{2}\gamma(|x|+|y|)} \int_0^{+\infty} \exp\left[-\left(\frac{u}{\sqrt{4it}} + \frac{it\gamma + |x| + |y|}{\sqrt{4it}} \right)^2 \right] \frac{du}{\sqrt{4it}} \\
&= -\frac{1}{2\sqrt{\pi}} e^{\frac{1}{4} i t \gamma^2 + \frac{1}{2}\gamma(|x|+|y|)} \int_{i[t\gamma - i(|x|+|y|)]/\sqrt{4it}}^{e^{-i\pi/4}\infty} e^{-z^2} dz = -\frac{1}{4} e^{\frac{1}{4} i t \gamma^2 + \frac{1}{2}\gamma(|x|+|y|)} \operatorname{erfc}\left(\frac{i[t\gamma - i(|x|+|y|)]}{\sqrt{4it}} \right)
\end{aligned}$$

proving (20) for $t > 0$ and $\gamma > 0$. The case $\gamma < 0$ similarly follows.

Then, (21) will follow by means of a stationary phase argument and standard argument applied to the free evolution operator. To this end, let us write:

$$X^t = X_0^t + \gamma X_\gamma^t,$$

where X_0^t is the free evolution operator with kernel U_0^t and X_γ^t is the integral operator with kernel R_γ^t. Hence,

$$\|X^t w - w\|_{L^2} \leqslant \|X_0^t w - w\|_{L^2} + |\gamma| \cdot \|X_\gamma^t w\|_{L^2},$$

where

$$(X_0^t w)(x) = \frac{1}{\sqrt{4\pi i t}} \int_{\mathbb{R}} e^{-(x-y)^2/4it} w(y)\, dy = w(x) + O(w'\sqrt{t}), \quad \text{as } t \to 0^+,$$

then

$$\|X_0^t w - w\|_{L^2} \leqslant C\sqrt{t} \|w\|_{H^1} \tag{22}$$

for some $C > 0$ (see also Lemma 2.2 by [7]). In order to estimate the second term we remark that

$$\|X_\gamma^t w\|_{L^2}^2 = \int_{\mathbb{R}} \left| \int_{\mathbb{R}} R_\gamma^t(x,y) w(y)\, dy \right|^2 dx = \int_{B_t} \left| \int_{\mathbb{R}} R_\gamma^t(x,y) w(y)\, dy \right|^2 dx + \int_{B_t^\star} \left| \int_{\mathbb{R}} R_\gamma^t(x,y) w(y)\, dy \right|^2 dx,$$

where

$$B_t = \{ x \in \mathbb{R} : |x| \leqslant t^{2\beta} \}, \quad \beta < \frac{1}{4}, \quad \text{and } B_t^\star = \mathbb{R} - B_t.$$

We remark that

$$\int_{B_t} \left| \int_{\mathbb{R}} R_\gamma^t(x,y) w(y)\, dy \right|^2 dx \leqslant \|w\|_{L^2}^2 \int_{B_t} \int_{\mathbb{R}} |R_\gamma^t(x,y)|^2\, dx\, dy \leqslant C t^{2\beta} \|w\|_{L^2}^2$$

since

$$\mathrm{erfc}(z) = 1 + \mathrm{O}(z) \quad \text{as } z \to 0$$

and

$$\mathrm{erfc}(z) \sim \frac{\mathrm{e}^{-z^2}}{z\sqrt{\pi}}[1 + \mathrm{O}(z^{-2})] \quad \text{as } z \to \infty, \quad |\arg z| \leqslant \frac{3}{4}\pi. \tag{23}$$

In order to estimate the integral over $B_t^\star$ we make use of (23) obtaining that

$$\int_{B_t^\star} \left| \int_{\mathbb{R}} R_\gamma^t(x,y)w(y)\,\mathrm{d}y \right|^2 \mathrm{d}x \leqslant \frac{t}{4\pi} \int_{\mathbb{R}} \mathrm{d}x \left| \int_{\mathbb{R}} \frac{w(y)}{1+|x|+|y|} \mathrm{e}^{-\mathrm{i}(1+|x|+|y|)^2/(2t)}\,\mathrm{d}y \right|^2 \leqslant Ct^3[\|w\|_{L^2}^2 + \|w'\|_{L^2}^2]$$

by integrating by parts. □

Remark 5. We have that

$$Y^t : H^1 \to H^1 \quad \text{and} \quad \|Y^t w\|_{H^1} \leqslant C[1 + \|w\|_{L^\infty}^{2\mu} \epsilon t]\|w\|_{H^1} \tag{24}$$

for some constant C independent of w, ϵ and t. This fact immediately follows from the definition of Y^t. Furthermore, we have also that (see [1])

$$S^t, X^t : H^1 \to H^1.$$

2.3. *Proof of Theorem 1*

The proof of Theorem 1 is split in several Lemmas, and follows some ideas by [7] adapted to our model. In the following let:

$$p = 2\mu.$$

Lemma 2. *Let* $w, w_1, w_2 \in L^2 \cap L^\infty$, *let*

$$M = \max[\|w_1\|_{L^\infty}, \|w_2\|_{L^\infty}].$$

The evolution operator Y^t *satisfies to the Lipschitz condition*

$$\|Y^t w_1 - Y^t w_2\|_{L^2} \leqslant [1 + p|\epsilon|tM^{p-1}] \cdot \|w_1 - w_2\|_{L^2}. \tag{25}$$

Proof. Indeed,

$$Y^t w_1 - Y^t w_2 = w_1 \exp[-\mathrm{i}\epsilon t|w_1|^p] - w_2 \exp[-\mathrm{i}\epsilon t|w_2|^p] = (w_1 - w_2)\exp[-\mathrm{i}\epsilon t|w_1|^p] + w_2[\mathrm{e}^{-\mathrm{i}\epsilon t|w_1|^p} - \mathrm{e}^{-\mathrm{i}\epsilon t|w_2|^p}].$$

Hence

$$\|Y^t w_1 - Y^t w_2\|_{L^2} \leqslant \|w_1 - w_2\|_{L^2} + \|w_2\|_{L^\infty} \|1 - \mathrm{e}^{-\mathrm{i}\epsilon t(|w_2|^p - |w_1|^p)}\|_{L^2},$$

where

$$\|1 - \mathrm{e}^{-\mathrm{i}\epsilon t(|w_2|^p - |w_1|^p)}\|_{L^2} \leqslant p|\epsilon t| \cdot \|w_2 - w_1\|_{L^2} M^{p-1}$$

since $|1 - \mathrm{e}^{\mathrm{i}z}| \leqslant |z|$, for any $z \in \mathbb{R}$, and $|y|^p - |x|^p \leqslant p|y-x||y|^{p-1}$ for any $p \geqslant 1$ and for $|x| \leqslant |y|$. □

Lemma 3. *Let* $w_1, w_2 \in L^2 \cap L^\infty$. *The evolution operator* Z^t *satisfies to the Lipschitz condition*:

$$\|Z^t w_1 - Z^t w_2\|_{L^2} \leqslant [1 + p|\epsilon|tM^{p-1}] \cdot \|w_1 - w_2\|_{L^2}, \quad M = \max[\|w_1\|_{L^\infty}, \|w_2\|_{L^\infty}]. \tag{26}$$

Proof. Indeed, it directly comes from the previous estimate and from the fact that evolution operator X^t is linear and unitary:

$$\|Z^t w_1 - Z^t w_2\|_{L^2} = \|X^t[Y^t w_1 - Y^t w_2]\|_{L^2} = \|Y^t w_1 - Y^t w_2\|_{L^2}. \qquad \square$$

Let us denote

$$F(u) = |u|^p u.$$

Lemma 4

$$\|F(u) - F(v)\|_{L^2} \leqslant (p+1)M^p\|u - v\|_{L^2}, \quad M = \max[\|u\|_{L^\infty}, \|v\|_{L^\infty}].$$

Proof. A simple computation yields

$$\begin{aligned}\|F(u) - F(v)\|_{L^2} &= \|u|u|^p - v|v|^p\|_{L^2} \leqslant \|u\|^p_{L^\infty}\|u - v\|_{L^2} + \|v\|_{L^\infty}\||u|^p - |v|^p\|_{L^2} \\ &\leqslant \|u\|^p_{L^\infty}\|u - v\|_{L^2} + \|v\|_{L^\infty}\|u - v\|_{L^2}[p\max[\|u\|_{L^\infty}, \quad \|v\|_{L^\infty}]^{p-1}] \leqslant K\|u - v\|_{L^2}, \\ K &= (p+1)M^p, \quad M = \max[\|u\|_{L^\infty}, \quad \|v\|_{L^\infty}]. \qquad \square\end{aligned}$$

We compare now the mild representation of equations (1)

$$\psi_t = S^t\psi_0 = X^t\psi_0 + \mathrm{i}\epsilon\int_0^t X^{t-s}|\psi_s|^p\psi_s\,\mathrm{d}s = X^t\psi_0 + \mathrm{i}\epsilon\int_0^t X^{t-s}F[S^s(\psi_0)]\,\mathrm{d}s$$

with the evolution $Z^t\psi_0 = X^tY^t\psi_0$, where

$$Y^t\psi_0 = \psi_0 + \mathrm{i}\epsilon\int_0^t F[Y^s(\psi_0)]\,\mathrm{d}s.$$

Then

$$\begin{aligned} S^t\psi_0 - Z^t\psi_0 &= S^t\psi_0 - X^tY^t\psi_0 && (27)\\ &= X^t\psi_0 + \mathrm{i}\epsilon\int_0^t X^{t-s}F[S^s(\psi_0)]\,\mathrm{d}s - X^t[\psi_0 + \mathrm{i}\epsilon\int_0^t [Y^s(\psi_0)]\,\mathrm{d}s] \\ &= +\mathrm{i}\epsilon\left[\int_0^t X^{t-s}F[S^s(\psi_0)]\,\mathrm{d}s - \int_0^t X^tF[Y^s(\psi_0)]\,\mathrm{d}s\right] \\ &= +\mathrm{i}\epsilon\int_0^t X^{t-s}\{F[S^s(\psi_0)] - F[Z^s(\psi_0)]\}\,\mathrm{d}s + \mathcal{R}(t,\psi_0), && (28)\end{aligned}$$

where

$$\mathcal{R}(t,\psi_0) = +\mathrm{i}\epsilon\left[\int_0^t X^{t-s}F[Z^s(\psi_0)]\,\mathrm{d}s - \int_0^t X^tF[Y^s(\psi_0)]\,\mathrm{d}s\right].$$

We are going now to estimate the remainder term $\mathcal{R}$.

Lemma 5. *Let $0 < \beta < \frac{1}{4}$, let $t > 0$ fixed, let $u \in H^2 \cap L^2$ and let*

$$K = C\max_{s\in[0,t]}[\|X^sY^s(u)\|^p_{L^\infty}, \|Y^s(u)\|^p_{L^\infty}],$$

where C is a positive constant independent onu, but depending on β. We assume that t is such that $tK \leqslant 1$. Then

$$\|\mathcal{R}(t,u)\|_{L^2} \leqslant |\epsilon|K^2[t^{3/2}\|u\|_{H^1} + C|\gamma|t^{\beta+1}\|u\|_{L^2}]. \tag{29}$$

Proof. We set

$$\mathcal{R}(t,u) = \mathrm{i}\epsilon\int_0^t X^{t-s}\mathcal{R}_1(s,u)\,\mathrm{d}s,$$

where

$$\mathcal{R}_1(s,u) = F[Z_1^s(u)] - X^s F[Y^s(u)] = I + II$$

with

$$I = F[X^s Y^s(u)] - F[Y^s(u)] \quad \text{and} \quad II = X^s F[Y^s(u)] - F[Y^s(u)].$$

Let

$$M = \max[\|X^s Y^s(u)\|_{L^\infty}^p, \|Y^s(u)\|_{L^\infty}^p].$$

From Lemmas 1 and 4 it follows that:

$$\|I\|_{L^2} \leqslant (p+1)M\|X^s Y^s(u) - Y^s(u)\|_{L^2} \leqslant K[\sqrt{s}\|Y^s(u)\|_{H^1} + |\gamma|s^\beta\|Y^s(u)\|_{L^2}]$$

and

$$\|II\|_{L^2} \leqslant [\sqrt{s}\|F[Y^s(u)]\|_{H^1} + |\gamma|s^\beta\|F[Y^s(u)]\|_{L^2}] \leqslant K[\sqrt{s}\|Y^s(u)\|_{H^1} + |\gamma|s^\beta\|Y^s(u)\|_{L^2}]$$

since $\||u|^p u\|_{L^2} \leqslant \|u\|_{L^\infty}^p\|u\|_{L^2}$ and $\||u|^p u\|_{H^1} \leqslant C\|u\|_{L^\infty}^p\|u\|_{H^1}$ for some $C > 0$. From this fact and from Lemma 2 we can conclude that

$$\|\mathcal{R}_1(s,u)\|_{L^2} \leqslant K[\sqrt{s}\|Y^s(u)\|_{H^1} + |\gamma|s^\beta\|Y^s(u)\|_{L^2}] \leqslant K\{C[1 + \|u\|_{L^\infty}^p \epsilon s]\sqrt{s}\|u\|_{H^1} + K|\gamma|s^\beta\|u\|_{L^2}\}.$$

From this estimate then (29) immediately follows:

Now, from (28) and (29), it follows that:

$$\begin{aligned}\|S^t(\psi_0) - Z^t(\psi_0)\|_{L^2} &\leqslant |\epsilon|\int_0^t \|X^{t-s}\{F[S^s(\psi_0)] - F[Z^s(\psi_0)]\}\|_{L^2}\,\mathrm{d}s + \|\mathcal{R}(t,\psi_0)\|_{L^2} \\ &\leqslant |\epsilon|K\int_0^t \|S^s(\psi_0) - Z^s(\psi_0)\|_{L^2}\,\mathrm{d}s + |\epsilon|K^2[t^{3/2}\|\psi_0\|_{H^1} + |\gamma|t^{\beta+1}\|\psi_0\|_{L^2}].\end{aligned}$$

From this fact and from the Gronwall's Lemma (see, e.g., Lemma 2.1 in [7]) then for any $h > 0$ fixed we have the following uniform estimate:

$$\|S^t(\psi_0) - Z^t(\psi_0)\|_{L^2} \leqslant \mathrm{e}^{|\epsilon|Kh}|\epsilon|K^2[t^{3/2}\|\psi_0\|_{H^1} + |\gamma|t^{\beta+1}\|\psi_0\|_{L^2}], \quad \forall t \in [0,h]. \tag{30}$$

In particular, for $t = h$, it takes the form

$$\|S^h(\psi_0) - Z^h(\psi_0)\|_{L^2} \leqslant \mathrm{e}^{|\epsilon|Kh}|\epsilon|K^2[h^{3/2}\|\psi_0\|_{H^1} + |\gamma|h^{\beta+1}\|\psi_0\|_{L^2}]. \tag{31}$$

Now, let $h > 0$ and $N \in \mathbb{N}$ fixed, let $T = Nh$ and m and m_1 defined, respectively, by (14) and (15). The triangle inequality yields

$$\begin{aligned}&\|(Z^h)^N(\psi_0) - S^{Nh}(\psi_0)\|_{L^2} && (32)\\ &\leqslant \sum_{j=0}^{N-1}\|(Z^h)^{N-j-1}Z^h S^{jh}(\psi_0) - (Z^h)^{N-j-1}S^{(j+1)h}(\psi_0)\|_{L^2} \\ &\leqslant \sum_{j=0}^{N-1}(1 + |\epsilon|phm^{p-1})^{N-j-1}\|[Z^h - S^h]S^{jh}(\psi_0)\|_{L^2} \\ &\leqslant \sum_{j=0}^{N-1}(1 + |\epsilon|phm^{p-1})^{N-j-1}\mathrm{e}^{|\epsilon|Cm^p h}|\epsilon|Cm^{2p}[h^{3/2}\|S^{jh}\psi_0\|_{H^1} + |\gamma|h^{\beta+1}\|S^{jh}\psi_0\|_{L^2}] \\ &\leqslant \left[\sum_{j=0}^{N-1}(1 + |\epsilon|phm^{p-1})^j\right]\cdot \mathrm{e}^{|\epsilon|Cm^p h}|\epsilon|Cm^{2p}[h^{3/2}m_1 + |\gamma|h^{\beta+1}\|\psi_0\|_{L^2}] \\ &\leqslant \frac{(1 + |\epsilon|phm^{p-1})^N - 1}{|\epsilon|phm^{p-1}}\cdot \mathrm{e}^{|\epsilon|Cm^p h}|\epsilon|Cm^{2p}[h^{3/2}m_1 + |\gamma|h^{\beta+1}\|\psi_0\|_{L^2}] && (33)\\ &\leqslant [\mathrm{e}^{|\epsilon|pm^{p-1}T} - 1]\cdot \mathrm{e}^{|\epsilon|Cm^p h}|\epsilon|Cm^{2p}[h^{1/2}m_1 + |\gamma|h^\beta\|\psi_0\|_{L^2}] && (34)\end{aligned}$$

and the proof is completed. □

3. Numerical experiments

In this Section we implement the Lie approximation method in a Fortran program and then we perform some experiments concerning the interaction of solitons with pointwise perturbation and blow-up phenomenon.

3.1. The algorithm

Since we are able to give an explicit expression of the linear evolution operator $X^t = e^{-iH_\gamma t}$ by means of an integral operator (18) which kernel U^t_γ is explicitly written (Lemma 1) then the numerical procedure is quite simple and it is not particularly computationally expensive. The only problem we have to face consists in the fact that for small h this kernel becomes singular and we should take a larger grid. In order to avoid such a computationally expensive procedure we make use of a simple trick, we shall compute X^h for small h making use of the group property

$$X^h = X^{-t_0}X^{t_0+h},$$

where t_0 is fixed and much larger than h (for instance $t_0 = 1$) and where X^{-t_0} and X^{t_0+h} are computed numerically with a grid of just 8000 points. This trick, which consists in using one step backward and one (a little bit larger) step forward operator, has been also numerically validated comparing different simulations with small time step h on a very thin grid, with time steps $t_0 + h$ and $-t_0$ on the same thin grid and, finally, with time steps $t_0 + h$ and $-t_0$ on the relatively coarse grid; the results obtained fully agree.

The evolution operator X^t is an unitary operator and thus the norm of the vector $X^t\psi$ coincides with the norm of the vector ψ. However, the numerical evaluation of the action of the integral operator X^t is not *exactly* unitary because of the occurrence of numerical errors. We compensate these small errors by re-normalizing the vector $X^t\psi$ at each step. We could minimize these errors with, for instance, other procedures as increasing the size of the grid or making use of some adaptive scheme. As it appears in some numerical tests we did not see here any particular advantage in making use of these more computationally expensive procedures, then we adopt the faster re-normalization procedure.

Then, we compute N-times

$$Z^h = \mathcal{N} Y^h X^{-t_0} X^{t_0+h} \quad \text{for } h \ll 1 \text{ and } t_0 = 1,$$

where $\mathcal{N}$ normalizes the final output to the norm of the initial data.

This procedure is implemented by means of a simple Fortran program which:

– reads the parameters h, N, ϵ, γ, μ, the dimension $(x_{\min}, x_{\max})$ and the number of points $L + 1$ of the spatial grid;
– reads the initial data in a vector

$$y^0 = \{(x^0_j, y^0_j = \psi_0(x^0_j)),\ j = 1, 2, \ldots, M\}$$

of M elements;
– by means of a linear interpolation method the program adapts the initial data to the given grid of $L + 1$ elements

$$y^0 \to y = \{(x_j, y_j),\ j = 0, 1, \ldots, L\},$$

where $x_0 = x_{\min}$, $x_L = x_{\max}$ and $x_j - x_{j-1} = \frac{1}{L}(x_{\max} - x_{\min})$;
– compute the norm

$$c = \left[\frac{x_{\max} - x_{\min}}{L} \sum_{j=1}^{L} \frac{|y_{j-1}|^2 + |y_j|^2}{2}\right]^{1/2};$$

of the initial wave function;

– iterates N time the following cycle:
  + compute $y \to y^1 = X^{1+h}y$;
  + compute $y^1 \to y^2 = X^{-1}y^1$;
  + compute $y^2 \to y^3 = Y^h y^2$;
  + compute the norm $\tilde{c}$ of y^3 and define

$$y^3 \to y = \mathcal{N}y^3 = \{(x_j, y_j), j = 0, 1, \ldots, L\},$$

  where $y_j = \frac{c}{\tilde{c}} y_j^3$;
  + write the output y of the cycle on a file.

3.2. Motion of solitons

A soliton is a solution of the free NLS which uniformly moves maintaining its initial shape. Here, we consider the effect of the singular perturbation on such a motion.

3.2.1. Splitting of a single soliton.

Let us a consider a single soliton-like wave function solution of the form

$$\psi_t(x) = \sqrt{\frac{2}{|\epsilon|}} \frac{1}{\cosh(x + 2v_1 t - x_1)} \mathrm{e}^{-\mathrm{i}(-t + v_1 x + v_1^2 t)},$$

where v_1 and x_1 are fixed real valued parameters. This function is the exact solution of the free Eq. (2) with $V \equiv 0$ with self-focusing cubic nonlinearity, that is $\mu = 1$ and $\epsilon < 0$ [1]; corresponding to the initial wave function

$$\psi_0(x) = \sqrt{\frac{2}{|\epsilon|}} \frac{1}{\cosh(x - x_1)} \mathrm{e}^{-\mathrm{i}v_1 x}. \tag{35}$$

As it is well known, such a wave function uniformly moves with "velocity" v_1 maintaining its initial shape.

If we introduce the singular potential then we see that the solution ψ_t of Eq. (1) with initial condition (35) splits in two different parts with soliton-like shape when the *center of mass* of the wave function defined as

$$\langle x \rangle^t = \int_{\mathbb{R}} x |\psi_t(x)|^2 \, \mathrm{d}x \tag{36}$$

hits the support of the Dirac's delta potential. One part of the solution still moves according to the initial velocity while the other part moves in the opposite direction; see, e.g., Fig. 1 where the wave function ψ_t hits a barrier given by means of a repulsive Dirac's delta with positive strength, that is $\gamma > 0$.

In fact, when the Dirac's delta perturbation is of attractive type, i.e. $\gamma < 0$, then a new term with cusp shape centered around the support of the singular perturbation appears (see Fig. 2). This term is the contribution due to the stationary solution $\varphi(x)$ of NLS of the form

$$\varphi(x) = A\,\mathrm{sech}[k(|x| - x_0)]$$

for some values of A, k and x_0. Indeed, Eq. (1) admits real-valued stationary solutions when the strength γ of the Dirac's delta potential is smaller than a critical value $\gamma_c(\mu)$ which depends on the nonlinearity power μ (see [20] for the cubic NLS, see also [10] for NLS with any power μ). In particular, for the numerical experiment discussed in Fig. 2 where $\mu = 1$, $\epsilon = -1$ and $\gamma = -3$ then $\gamma < \gamma_c$ since for $\mu = 1$ the critical value γ_c is given by

$$\gamma_c(1) = \begin{cases} \frac{1}{4} & \text{when } \epsilon = -1, \\ -\frac{1}{2} & \text{when } \epsilon = +1. \end{cases}$$

Finally, in Fig. 3 we compare the motion of the center of mass of the wave function for different cases and we can see that the effect of the singular perturbation on such a motion consists of a decreasing of the velocity.

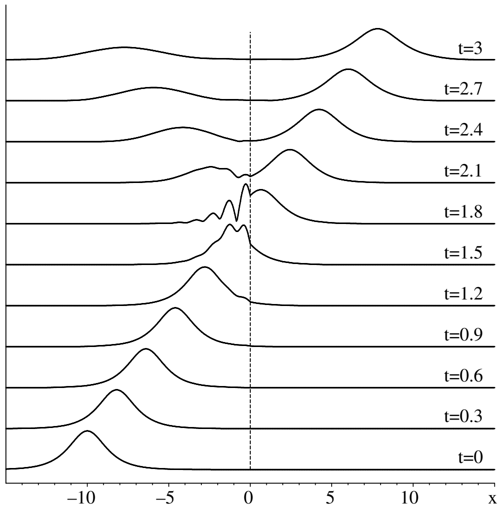

Fig. 1. Here we plot the graphics of the absolute value of the solution $\psi_t(x)$ of Eq. (1) for different values of t. Initially we have a soliton-like function (35) moving forward, i.e. $v_1 > 0$. When the center of mass of the wave function hits the barrier (broken line) given by means of a repulsive, that is $\gamma > 0$, Dirac's delta supported at $x = 0$ then the soliton splits in two parts with a soliton-like shape. One part of the wave function still moves forward with the same velocity while the other part moves backward. Here we choose the following values of the parameters: $\mu = 1$, $\epsilon = -1$, $x_1 = -10$, $v_1 = 3$ and $\gamma = 3$. The spatial grid consists of $L = 8000$ points, furthermore $N = 300$ and $h = 0.01$.

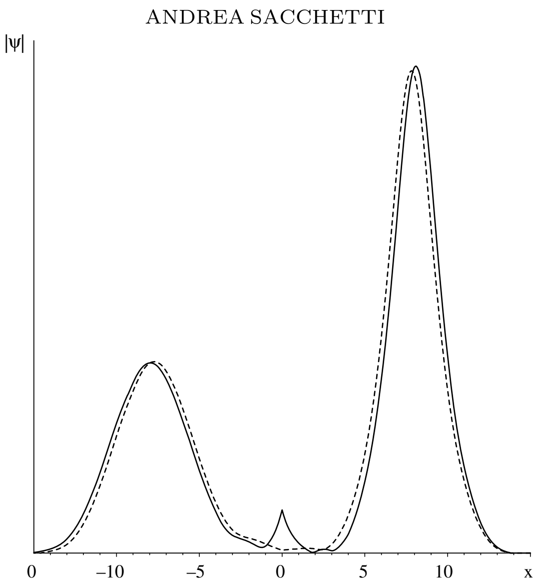

Fig. 2. Here we plot the graphics of the absolute value of the solutions $\psi_t(x)$ of Eq. (1) at $t = 3.0$ with initial condition (35) and with the choice of the parameters as in Fig. 1. Broken line represents the case of a repulsive Dirac's delta with $\gamma = 3$. Full line represents the case of an attractive Dirac's delta with $\gamma = -3$; in this case a cusp corresponding to a stationary state centered around the support of the singular perturbation appears.

Our results agree with the one obtained by [14–16]. We should emphasize that in [15] a two-dimensional (x, t) grid of size 15000×20000 has been chosen. Here, by taking advantage from the fact that the kernel of the integral operator is explicitly known, we only require of a spatial grid of 8000 points.

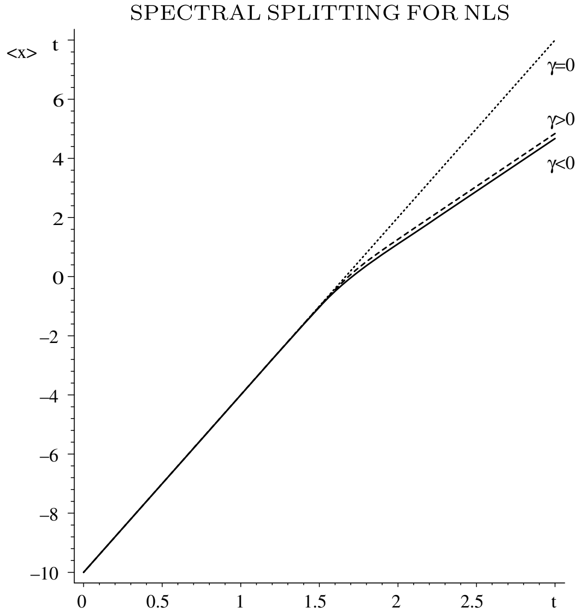

Fig. 3. For a free problem (dot line) the center of mass defined as (36) uniformly moves forward. The effect of a Dirac's delta at $x = 0$ produces the splitting of the wave function as seen in Figs. 1 and 2 and the velocity of the motion of the center of mass decreases. In the case of an attractive Dirac's delta the appearance of a stationary term produces a stronger decreasing effect of the velocity of the center of mass.

3.2.2. Collision of two solitons

We consider here the motion of a 2-soliton-like wave function $\psi_t(x)$ for an attractive cubic NLS (i.e. $\epsilon > 0$ and $p = 2$) with initial wave function of the form

$$\psi_0(x) = \sqrt{\frac{2}{\epsilon}} \frac{1}{\cosh(x - x_1)} e^{-iv_1 x} + \sqrt{\frac{2}{\epsilon}} \frac{1}{\cosh(x - x_2)} e^{-iv_2 x}$$

for some values of the real parameters $x_{1,2}$ and $v_{1,2}$. The two soliton-like terms move according to their velocity maintaining their initial shape till their supports remain disjoint. We consider now a numerical experiment where the two solitons move in opposite direction with different velocities and the collision point coincides with the support of the singular perturbation, that is $x_1 = -9$, $v_1 = 3$, $x_2 = 6$ and $v_2 = -2$.

In the case of the free problem, where $V \equiv 0$, then the two solitons cross at $x = 0$ and then still continue to move maintaining their velocities. In particular, *the center of mass* uniformly moves forward. In the presence of the Dirac's delta perturbation we observe a different picture: after the collision at $x = 0$ we observe four soliton-like different wave functions moving with different velocities. The global effect of such a motion is described by means of the motion of the center of mass. In particular, we can observe different behaviors of this motion for different type of singular perturbation. That is, in the case of an attractive Dirac's delta the center of mass is accelerated when it passes through the support of the Dirac's delta; while, in the case of a repulsive Dirac's delta then the center of mass is decelerated and, furthermore, it inverts its motion moving finally backwards (see Fig. 4).

3.3. Blow-up

The phenomenon of blow-up has been investigated extensively in the case of the free nonlinear Schrödinger equation (see, e.g., [5]) and recently new results have been obtained for NLS with Dirac's delta interaction [2]. In such a problem the definition of blow-up is the same as in the standard case: that is, let $\psi_t \in H^1(\mathbb{R})$ be the unique maximal solution of the Cauchy problem (1) with initial data $\psi_0 \in H^1(\mathbb{R})$. We call ψ_t a *blow-up solution* and say that ψ_t *blows up forward in finite time* if there exists a finite T_+ such that

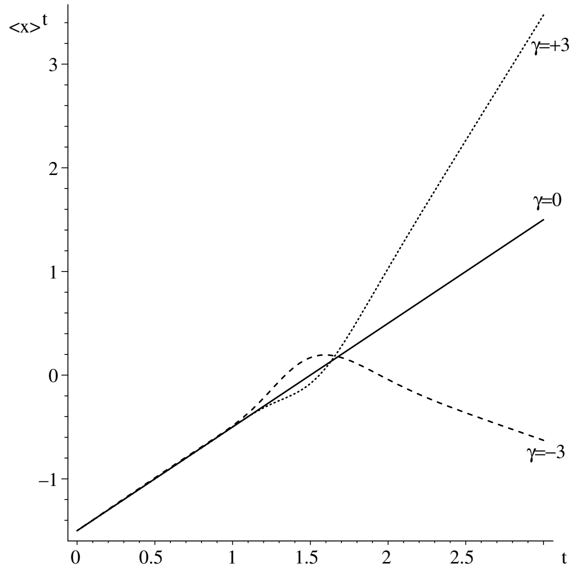

Fig. 4. We consider the case of the collision at $x = 0$, where the singular perturbation is supported, of oppositely moving soliton-like wave functions with different velocities. We plot the center of mass $\langle x\rangle^t$ in the cases of attractive Dirac's delta corresponding to $\gamma = -3$ (broken line), repulsive Dirac's delta corresponding to $\gamma = 3$ (dot line) and free potential corresponding to $\gamma = 0$ (full line). In the last case the center of mass moves uniformly forward. In the first two cases the final effect of the singular perturbation consists of an acceleration or deceleration of the center of mass when it hits the support of the singular perturbation; in particular in the case of an attracting singular perturbation the motion inverts its direction.

$$\lim_{t\to T_+ -0} \|\psi_t\|_{H^1} = +\infty.$$

As in the standard case, we have a blow-up alternative; namely, either the solution is global in time, or it blows up in finite time.

Usually, existence of global solution when $\epsilon < 0$ is proved by means of some *a priori* estimates on the norm of the gradient of ψ_t based on the energy conservation and on the Gagliardo–Niremberg inequality (see Appendix in [2]). In particular we have that

$$\begin{aligned}\mathcal{E}[\psi_t] &= \|\psi_t'\|_{L^2}^2 + \gamma|\psi_t(0)|^2 + \frac{\epsilon}{\mu+1}\|\psi_t\|_{L^{2(\mu+1)}}^{2(\mu+1)} \geqslant \|\psi_t'\|_{L^2}^2 - |\gamma|\cdot\|\psi_t'\|_{L^2} + \frac{\epsilon}{\mu+1}\|\psi_t\|_{L^{2(\mu+1)}}^{2(\mu+1)} \\ &\geqslant \|\psi_t'\|_{L^2}^2 - |\gamma|\cdot\|\psi_t'\|_{L^2} + \frac{4}{\pi^2}\frac{\epsilon}{\mu+1}\|\psi_t'\|_{L^2}^{\mu}.\end{aligned}$$

That is the quantity $z = \|\psi_t'\|_{L^2}$ has to satisfy the following inequality:

$$\mathcal{E}[\psi_0] \geqslant z^2 - |\gamma|z + \frac{4}{\pi^2}\frac{\epsilon}{\mu+1}z^{\mu}. \tag{37}$$

Let us denote by $\mathcal{S}$ the set of solutions of such inequality; if there exists a positive constant c such that $c \notin \mathcal{S}$ and $\|\psi_0'\|_{L^2} \leqslant c$ then $\|\psi_t'\|_{L^2} \leqslant c$ and the solution ψ_t exists globally in time.

On the other hand, the existence of blow-up is usually proved making use of the Virial method (also named Glassey's method [13]), based on the computation of the moment of inertia of the solution. To this end, let us define the set

$$\mathcal{K} = H^1(\mathbb{R}) \cap \{\psi \in L^2(\mathbb{R}) : x\psi \in L^2(\mathbb{R})\} \cap \{\psi \in L^2(\mathbb{R}) : \|\psi\|_{L^2} = 1\},$$

and let the initial data belonging to this set, that is $\psi_0 \in \mathcal{K}$. Then (see Theorem 2 in [2]) the solution ψ_t of NLS (1) belongs to $\mathcal{K}$ for any $t \in (T_-, T_+)$ and furthermore the variance $I(t)$ (also called moment of inertia) of the solution ψ_t, defined as follows:

$$I = I(t) = \int_{\mathbb{R}} x^2 |\psi_t(x)|^2 \, dx, \quad t \in (-T_-, T_+)$$

is such that $I \in C^2(-T_-, T_+)$ and

$$\ddot{I} = 8\mathcal{E}[\psi_t] + 4\epsilon \frac{\mu - 2}{\mu + 1} \|\psi_t\|^{2(\mu+1)}_{L^{2(\mu+1)}(\mathbb{R})} - 4\gamma |\psi_t(0)|^2. \tag{38}$$

The method of Glassey consists in proving an a *priori* estimate of the type $\ddot{I} \leqslant -C$, for some $C > 0$ independent of t, from which follows that $I(t^\star) = 0$ for some $t^\star > 0$; in such a case then blow-up will occur for some $T_+ \leqslant t^\star$.

Now, we carry out the analysis of the blow-up for the NLS equation with singular potential (see Theorem 3 and its proof in [2]).

There is no blow-up and the solution ψ_t of Eq. (1) with initial data $\psi_0 \in \mathcal{K}$ exists globally in time if one of the following conditions is fulfilled:

(i) $\epsilon \geqslant 0$;
(ii) $\epsilon < 0$ and $\mu < 2$;
(iii) $0 > \epsilon > -\frac{3\pi^2}{4}$ and $\mu = 2$;
(iv) $0 > \epsilon > -\epsilon_1$, for some $\epsilon_1 > 0$ depending on ψ_0, and $\mu > 2$.
In contrast, the solution ψ_t of Eq. (1) with initial data $\psi_0 \in \mathcal{K}$ blows up in finite time if
(v) $\mu > 2$ and the energy (13) is such that

$$\mathcal{E}[\psi_0] < \begin{cases} 0 & \text{if } \gamma > 0, \\ -\frac{\gamma^2(\mu-1)^2}{4\mu(\mu-2)} & \text{if } \gamma < 0. \end{cases} \tag{39}$$

3.3.1. Blow-up analysis for a stationary state of the linear problem

Here we investigate in more detail the blow-up phenomenon when $\epsilon < 0$ and the initial data ψ_0 coincides with the ground state (17) for the Hamiltonian H_γ, where $\gamma < 0$. For the sake of definiteness we assume $\gamma = -1$ and $\mu = 3$. In such a case an explicit computation gives

$$\mathcal{E}[\psi] = \mathcal{E}[\psi_0] = \mathcal{E}[\phi_\gamma] = -\frac{1}{4}\gamma^2 + \epsilon \frac{|\gamma|^\mu}{2^\mu (\mu+1)^2} < 0.$$

In order to see when there is no blow-up then we have to consider inequality (37) which takes the form

$$-\frac{1}{4}\gamma^2 + \epsilon \frac{|\gamma|^\mu}{2^\mu(\mu+1)^2} \geqslant z^2 - |\gamma| z + \frac{4}{\pi^2} \frac{\epsilon}{\mu+1} z^\mu,$$

where $z = \|\psi_t'\|_{L^2}$ and where $\|\psi_0'\|_{L^2} = \frac{1}{2}$ for $\gamma = -1$. Such an inequality has, for $\mu = 3$ and $\gamma = -1$, the form

$$g(z) := -\frac{\epsilon}{\pi^2} z^3 - z^2 + z - \frac{1}{4} + \epsilon \frac{1}{128} \geqslant 0,$$

where the function $g(z)$ is such that

$$g(0) < 0, \quad g(\|\psi_0'\|_{L^2}) > 0 \quad \text{and} \quad \lim_{z \to +\infty} g(z) = +\infty.$$

In particular, when $|\epsilon| < \frac{1}{3}\pi^2$ this function has a minimum at

$$x_{\min} = \frac{2\pi^2}{6|\epsilon|} \left[1 - \sqrt{1 - \frac{3|\epsilon|}{\pi^2}} \right] > \|\psi_0'\|_{L^2} = \frac{1}{2}$$

given by

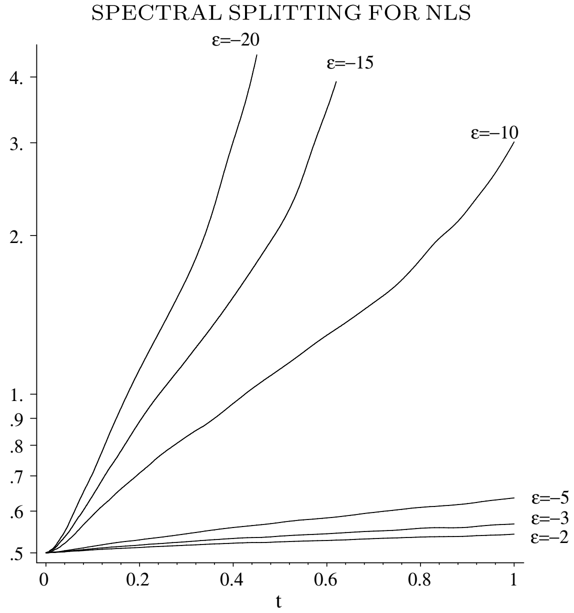

Fig. 5. Logarithmic plot of $\|\psi_t'\|_{L^2}$ for different values of the nonlinearity parameter $\epsilon < 0$. For $|\epsilon| = 2, 3, 5$ we do not see blow-up (as predicted when $|\epsilon| < \epsilon_1 \approx 2.998$). In contrast, for $|\epsilon| = 10, 15, 20$ the picture suggests the occurrence of blow-up (as predicted when $|\epsilon| > \epsilon_2 \approx 10.67$).

$$g(x_{\min}) = -\frac{[256\pi^4 + 256\pi^3\sqrt{\pi^2 - 3|\epsilon|} - 768\pi|\epsilon|\sqrt{\pi^2 - 3|\epsilon|} - 1152|\epsilon|\pi^2 + 864|\epsilon|^2 + 27|\epsilon|^3]}{3456|\epsilon|^2},$$

where $g(x_{\min}) < 0$ for any $|\epsilon| < \epsilon_1 \approx 2.998$. Therefore, in the case $\mu = 3$ and $\gamma = -1$ then we can conclude that the solution ψ_t with initial data $\psi_0 = \phi_\gamma$ there exists globally in time for any $\epsilon < \epsilon_1$.

In order to see when there exists blow-up then we make use of inequality (39), which implies that if the parameters $\mu > 1$ and $\epsilon < 0$ satisfy the following condition:

$$|\epsilon||\gamma|^{\mu-2} > f(\mu) := 2^\mu(\mu+1)^2\left[\frac{(\mu-1)^2}{4\mu(\mu-2)} - \frac{1}{4}\right],$$

then the solution ψ_t blows up in finite time. In particular, for $\mu = 3$ and $\gamma = -1$ then the linear stationary state $\phi(x) = \frac{1}{\sqrt{2}}e^{-\frac{1}{2}|x|}$ will blow-up in finite time for any $\epsilon < -\epsilon_2$ where $\epsilon_2 = f(3) = \frac{1}{3}32 \approx 10.67$. Therefore, we can conclude that our theoretical analysis will predict the following picture:

$$\mu = 3, \gamma = -1 \quad \text{and } \psi_0 = \phi_\gamma \quad \text{then } \begin{cases} |\epsilon| < \epsilon_1 \approx 2.998 & \text{no-blow-up,} \\ |\epsilon| > \epsilon_2 \approx 10.67 & \text{blow-up.} \end{cases}$$

In the range $|\epsilon| \in [\epsilon_1, \epsilon_2]$ the theoretical analysis does not work. A numerical experiment is described in Fig. 5 where we observe a transition from the no-blow-up regime, where $0 > \epsilon > -\epsilon_1$, to the blow-up regime where $\epsilon < -\epsilon_2$.

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