Numerical study of fractional nonlinear Schrödinger equations

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Using a Fourier spectral method, we provide a detailed numerical investigation of dispersive Schrödinger-type equations involving a fractional Laplacian in an one-dimensional case. By an appropriate choice of the dispersive exponent, both mass and energy sub- and supercritical regimes can be identified. This allows us to study the possibility of finite time blow-up versus global existence, the nature of the blow-up, the stability and instability of nonlinear ground states and the long-time dynamics of solutions. The latter is also studied in a semiclassical setting. Moreover, we numerically construct ground state solutions of the fractional nonlinear Schrödinger equation.

1. Introduction

(a) Background and motivation

This work is concerned with a numerical study for non-local dispersive equations of nonlinear fractional Schrödinger type (fNLS). More specifically, we consider equations of the form

\[ i \partial_t \psi = \frac{1}{2} (-\Delta)^s \psi + \gamma |\psi|^{2p} \psi, \quad \psi(0, x) = \psi_0(x), \]  

(1.1)

for \((t, x) \in \mathbb{R} \times \mathbb{R}^d\) and \(p > 0\). In addition, \(\gamma = \pm 1\) distinguishes between focusing (repulsive) \(\gamma = -1\) and defocusing (attractive) \(\gamma = +1\) nonlinearities. Finally, the
parameter $0 < s \leq 1$ describes the fractional dispersive nature of the equation. The fractional Laplacian $(-\Delta)^s$ is thereby defined via

$$(-\Delta)^s f(x) := \mathcal{F}^{-1}(\mathcal{F}[|k|^{2s} \mathcal{F}f]) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |k|^{2s} \hat{f}(k) e^{i k \cdot x} \, dk,$$

where $\hat{f} \equiv \mathcal{F}f$ denotes the Fourier transform of $f$. Clearly, for $s = 1$ this is the usual Laplacian, whereas for $s < 1$ the equation is indeed non-local. (The factor $\frac{1}{2}$ in front of the fractional Laplacian is kept for historic reasons but could be safely scaled away by replacing $x \mapsto \sqrt{2} x$.)

Equation (1.1) generalizes the classical nonlinear Schrödinger equation (where $s = 1$), which is a canonical model for weakly nonlinear wave propagation in dispersive media (cf. [1]). In the context of quantum mechanics, the case $s = \frac{1}{2}$ can be seen as a toy model for the description of particles with a relativistic dispersion relation $\omega(k) = \sqrt{|k|^2 + m^2}$. This has been recently used in the mathematical description of Boson-stars [2,3]. Fractional NLS also arise in the continuum limit of discrete models with long range interaction [4], in some models of water wave dynamics [5,6] and by generalizing the Feynman path integral to also include Lévy processes [7].

From the mathematical point of view, fNLS equations have recently drawn quite a lot of interest from various authors. For example, the question of local and/or global well-posedness of the initial value problem (1.1) has been studied in [8,9]. In addition to that, finite time blow-up of solutions of fNLS (with Hartree-type nonlinearities) has been established in [3,10]. Moreover, the existence, uniqueness and stability properties of the associated \textit{standing wave solutions} of solutions of fNLS have been investigated in [11–13]. To this end, we recall that (non-trivial) standing waves are obtained by setting $\psi(t,x) = \varphi(x)e^{-i \omega t}$, $\omega \in \mathbb{R}$, which leads to the study of the following nonlinear elliptic equation:

$$\frac{1}{2}(-\Delta)^s \psi - |\psi|^{2p} \psi = \omega \varphi, \quad (1.2)$$

see §2b for more details.

\textbf{(b) Basic mathematical properties of fractional nonlinear Schrödinger}

In this work, we are mainly interested in the interaction between the (non-local) dispersion and the nonlinearity in the time evolution of (1.1). To this end, we shall take on the point of view that $p > 0$ is fixed and $0 < s \leq 1$ is allowed to vary. Intuitively, we expect the model to be better behaved the stronger the dispersion, i.e. the larger $s > 0$. To obtain more insight, we first note that the following quantities are conserved by the time evolution of (1.1):

\textbf{Mass: } $M(t) = \int_{\mathbb{R}^d} |\varphi(t,x)|^2 \, dx = M(0)$ \hspace{1cm} (1.3)

\textbf{Energy: } $E(t) = \int_{\mathbb{R}^d} \left( \frac{1}{2} |\nabla^s \varphi(t,x)|^2 + \frac{\gamma}{p+1} |\varphi(t,x)|^{2p+2} \right) \, dx = E(0)$, \hspace{1cm} (1.4)

where $\nabla^s \varphi = \mathcal{F}^{-1}((-i|k|)^s \hat{\varphi})$. Note that in the defocusing (repulsive) case $\gamma = +1$, the energy is the sum of two non-negative terms (the kinetic and nonlinear potential energy). This, together with the conservation of mass, allows inference of an \textit{a priori} bound on the $H^s(\mathbb{R}^d)$ Sobolev norm of $\varphi$, as well as its $L^{2p+2}(\mathbb{R}^d)$ norm, provided that, either $\gamma = +1$ (repulsive case) or, for $\gamma = -1$ (attractive case) the embedding $H^s(\mathbb{R}^d) \hookrightarrow L^{2p+2}(\mathbb{R}^d)$ holds. The latter is true for $0 < p < p_*(s, d)$, where

$$p_*(s, d) = \begin{cases} \frac{2s}{d - 2s}, & 0 < s \leq \frac{d}{2}, \\ +\infty, & s \geq \frac{d}{2}. \end{cases} \hspace{1cm} (1.5)$$

We remark that the embedding is used for proving a local in-time existence theorem in the repulsive case.
In addition to the conservation laws above, the fNLS equation preserves the radial symmetry and is also invariant under the scaling transformation
\[
\psi(t, x) \mapsto \psi_\lambda(t, x) := \lambda^{s/p} \psi(\lambda^{2s} t, \lambda x),
\] (1.6)
for any \( \lambda > 0 \). In other words, if \( \psi \) solves (1.1) then so does \( \psi_\lambda \). With this in mind, one can check that under the scaling transformation (1.6), the homogeneous \( H^\sigma(\mathbb{R}^d) \) Sobolev norm of \( \psi_\lambda \) behaves like
\[
\| \psi_\lambda \|_{H^\sigma} = \| \nabla^\sigma \psi_\lambda \|_{L^2} = \lambda^{d/2-\sigma-s/p} \| \psi \|_{H^\sigma}.
\] (1.7)
The equation is called \( H^\sigma \) critical whenever this scaling leaves the \( H^\sigma \) norm invariant, i.e. whenever
\[
\frac{d}{2} - \frac{s}{p} = \sigma.
\] (1.8)
For \( \sigma = 0 \), we therefore obtain the \( L^2 \) critical, or mass critical case whenever the dispersion rate is \( s = s^*(p, d) = pd/2 \), or, equivalently, whenever \( p = 2s/d \). The equation is called mass subcritical if \( s > s^* \) and mass supercritical for \( s < s^* \) (and vice versa for \( p \)). This should be compared to the situation for the usual NLS in which \( s = 1 \) is fixed. The corresponding mass critical case is found for \( p = 2/d \), particular examples being the cubic NLS in \( d = 2 \), or the quintic NLS in \( d = 1 \). It is well known (cf. [1,14]) that in the mass subcritical case \( p < 2/d \) the classical NLS is globally well-posed (regardless of the sign of \( \gamma \)). On the other hand, finite time blow-up of solutions in the \( H^1(\mathbb{R}^d) \) norm can occur in the focusing case \( \gamma = -1 \) as soon as \( p \geq 2/d \). This means that there exists a finite time \( 0 < t^* < +\infty \), depending on the initial data \( u_0 \), such that
\[
\lim_{t \to t^*} \| \nabla \psi(t, \cdot) \|_{L^2} = +\infty.
\]
Moreover, it is known that for mass critical NLS, the threshold for finite time blow-up is given by the mass of the corresponding ground state, i.e. the unique positive radial solution \( Q(\omega) = \varphi(\|x\|) \) of the nonlinear elliptic equation (1.2), with \( \omega = 1 \). In other words, if \( p = 2/d \) and \( M(u_0) < M(Q) \), global existence still holds, whereas blow-up occurs as soon as \( M(u_0) \geq M(Q) \). For the fractional NLS, an analogous dichotomy appears and has been rigorously studied, for example, in [3].

As we have seen there is a second conserved quantity, namely the energy. We, therefore, can introduce a corresponding second notion of criticality. More precisely, the energy critical case is obtained for \( s = s_\gamma \), in which case the kinetic energy of the solution is indeed a scale invariant quantity of the time evolution. This yields another critical index \( s_\gamma(p, d) = pd/(2 + 2p) \), which is equivalent to \( p = p_\gamma(s, d) \) as defined in (1.5). Clearly, the energy critical index is always smaller than the mass critical one, i.e. \( s_\gamma < s^* \). For classical NLS with \( s = 1 \) fixed, the energy critical case is given by \( p = 2/(d - 2) \) and hence only appears in dimensions \( d \geq 3 \). The latter is no longer true for fractional NLS with \( s < 1 \). In the attractive energy critical and supercritical case, the quantity \( E(t) \) can no longer be used in order to obtain \( a \) priori estimates on the solution. Furthermore, the classical well-posedness theory for semilinear dispersive partial differential equations breaks down as the time of existence of local solutions in general may depend on the profile \( \psi_0 \), not only its \( H^\sigma \) norm. For classical NLS \( (s = 1) \), partial results on the existence and long-time behaviour of solutions in the energy critical case are still available [15–18], but a complete picture is not found so far. The corresponding situation for energy critical fNLS has been recently studied in [9].

(c) Structure of the present work

All of the above considerations paint a picture in which the theory for fNLS seems to follow closely the usual NLS results. While this is certainly true for basic questions such as existence and uniqueness versus finite time blow-up, the non-local nature of (1.1) with \( s < 1 \) is expected to have a considerable influence on more qualitative properties of the solution. In this paper, numerical simulations are performed in order to study the influence of a non-local dispersion term on different mathematical questions, including: the particular type of finite time blow-up (e.g. self-similar or not), qualitative features of the associated ground states solutions (including
their stability) and the possibility of well-posedness in the energy supercritical regime. The fact that we can vary the dispersion coefficient $0 < s < 1$, allows us to perform our simulations for both sub- and supercritical regimes in $d = 1$ spatial dimension, which is a big advantage. (In contrast to that, numerical simulations for energy supercritical NLS require at least $d = 3$ [19].) For our numerical simulations, we will thus fix the nonlinearity to be cubic, i.e. $p = 1$, in which case (1.1) becomes

\[ i \partial_t \psi = \frac{1}{2} \left(-\Delta^s\right) \psi + \gamma |\psi|^2 \psi, \quad \psi(0, x) = \psi_0(x), \quad x \in \mathbb{R}. \]  

(1.9)

This equation in $d = 1$ is mass critical for $s^* = \frac{1}{2}$ and energy critical for $s_\ast = \frac{1}{4}$. We consequently have global well-posedness for $\gamma = +1$ (defocusing case) and $s > \frac{1}{4}$. In the focusing case $\gamma = -1$, we can expect finite time blow-up of solutions whenever $\frac{1}{2} \geq s > \frac{1}{4}$. Finally, the energy supercritical regime corresponds to $s < \frac{1}{4}$ where, in principle, a different type of blow-up (than in the mass supercritical regime) might happen. The numerical simulations conducted are based on a Fourier spectral methods, to be explained in more detail in the following section.

Indeed, the paper is organized as follows: In § 2, we describe in more detail the numerical methods used to handle the time evolution, as well as the steady-state problem for fNLS. In § 3, we present numerical and analytical methods used for the study of the blow-up phenomenon. In § 4, we study the possibility of finite time blow-up for mass critical and super-critical fNLS, by comparing the situation with the one occurring for the quintic and septic NLS. In § 5, the time evolution of focusing and defocusing energy (super)critical fNLS simulated numerically. The possibility of blow-up is studied and we also study the long-time behaviour of the scaling invariant $H^s(\mathbb{R})$ norm in the defocusing case. Finally, in § 6, we study the time evolution of (1.9) within a semiclassical scaling regime. In addition, we have conducted several numerical experiments on the stability of fractional ground states, which are summarized in appendix A.

2. Numerical methods

In the following, we will discuss the numerical methods used to compute the time evolution of the solution and its corresponding ground states.

(a) Numerical methods for the time evolution

For the numerical integration of (1.1), we use a Fourier spectral method in $x$. The reason for this choice is that the fractional derivatives are most naturally computed in frequency space which is approximated via a discrete Fourier transform computed through a fast Fourier transform (FFT). The excellent approximation properties of a Fourier spectral method for smooth functions are also extremely useful. This is especially important in the context of dispersive equations since spectral methods are known for a minimal numerical dissipation which (in principle) could overwhelm dispersive effects within our model.

**Remark 2.1.** For the same reasons, a recent numerical study using the same numerical methods has been conducted for fractional Korteweg–de Vries (KdV) and Benjamin–Bona–Mahony (BBM) type equations [20].

The discretization in Fourier space leads to a system of (stiff) ordinary differential equations for the Fourier coefficients of $\psi$ of the form

\[ \partial_t \hat{\psi} = \mathcal{L} \hat{\psi} + \mathcal{N}(\psi), \]  

(2.1)

where $\mathcal{L} = -i|k|^{2s}/2$ and where $\mathcal{N}(\psi) = iy|\hat{\psi}|^2 \hat{\psi}$ denotes the nonlinearity. It is an advantage of Fourier methods that the $x$-derivatives are most naturally computed in frequency space which is approximated via a discrete Fourier transform computed through a fast Fourier transform (FFT). The excellent approximation properties of a Fourier spectral method for smooth functions are also extremely useful. This is especially important in the context of dispersive equations since spectral methods are known for a minimal numerical dissipation which (in principle) could overwhelm dispersive effects within our model.

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time-splitting scheme as in [22,23] was the most efficient, whereas in the focusing case a composite Runge–Kutta method [24] is preferable. The two codes are also used to test each other and were found to agree within the indicated numerical precision. We shall therefore use these two approaches also in this paper.

In order to test the numerical methods, we take $\psi_0(x) = Q(x)$, i.e. the ground state solution whose numerical construction is explained in the next subsection. In this case, the time-dependence of the exact solution of (1.1) is simply given by $\psi(t, x) = Q(x)e^{it}$. A comparison of the numerical solution of the fNLS with initial data $\psi_0 = Q$ therefore tests both $Q$ and the time evolution. In figure 1, we take $p = 1$ (cubic nonlinearity), $s = 0.6$ and show the difference between the numerical solution and $Q(x)e^{it}$ for $N = 2^{16}$ and $N_t = 20000$ time steps for $t \leq 6$. It can be seen that the ground state is reproduced up to errors of order $10^{-12}$, i.e. essentially with machine precision (which is approx. $10^{-14}$ in our case).

In our numerical computations, we also ensure that the computed relative energy of the solution, i.e.

$$\Delta E = \left| \frac{E(t)}{E(0)} - 1 \right|$$

remains small up to the threshold $\Delta E < 10^{-3}$. For example, in figure 1, the quantity $\Delta E$ is of the order of machine precision in accordance with expectations. Generally, this quantity is smaller than $10^{-10}$ in our computations unless otherwise noted.

(b) Numerical construction of fractional ground states

Recall that standing wave solutions of (1.1) are obtained in the focusing case $\gamma = -1$ by setting $\psi(t, x) = \varphi(x)e^{-i\omega t}$ for some $\omega \in \mathbb{R}$. By rescaling

$$\varphi_\omega = \omega^{1/(2p)} \varphi_1(x\omega^{1/(2s)})$$

we can assume without restriction of generality that $\omega = 1$ and hence $\varphi \equiv \varphi_1$ solves

$$\frac{1}{2}(-\Delta)^s \varphi + \varphi = |\varphi|^{2p} \varphi.$$  

Solutions $\varphi \in H^s(\mathbb{R}^d) \cap L^{2p+2}(\mathbb{R}^d)$ of this equation exist for admissible $0 < p < p^*$, where $p^* = p^*(s, d)$ is given by (1.5). Indeed, by invoking Pohozaev-type identities, it can be shown that equation (2.4) does not admit any non-trivial solution in $H^s(\mathbb{R}^d) \cap L^{2p+2}(\mathbb{R}^d)$, when $p \geq p^*$. Of special interest are solutions with minimal energy, the so-called ground states, which are known to
be real and radially symmetric and thus satisfy

\[ \frac{1}{2}(-\Delta)^s Q + Q = Q^{2p+1}. \] (2.5)

For \( s \neq 1 \), ground state solutions \( Q \) decay like \( |x|^{-(d+2s)} \) as \( |x| \to \infty \), i.e. only algebraically fast [12]. This is in contrast to the case of the usual NLS ground states obtained for \( s = 1 \), which are known to decay exponentially fast (e.g. [14]). Indeed, for \( s = d = 1 \), one has the well-known explicit solution of the so-called bright solitary wave (at time \( t = 0 \)):

\[ Q(x) = \left( \frac{p + 1}{\cosh^2(\sqrt{2}px)} \right)^{1/(2p)}, \quad 0 < p < p^*. \] (2.6)

For fNLS, with \( s < 1 \), no explicit solutions of (2.5) are known.

To solve equation (2.5) numerically, we use the same approach as in [20] to which we refer the reader for more details. The basic idea is to expand \( Q \) on a finite interval \( x \in D[-\pi, \pi], D > 0 \), in a discrete Fourier series, computed via FFT. In Fourier space, equation (2.5) takes the form

\[ F(Q) := (\frac{1}{2}|k|^{2s} + 1)\hat{Q} - \hat{Q}^{2p+1} = 0, \] (2.7)

subject to periodic boundary conditions. Owing to the slow algebraic decay of \( Q \) for \( s < 1 \), the constant \( D \) thereby has to be chosen sufficiently large in order to reduce the discontinuity of the derivatives of \( Q \) at the boundaries of the computational domain. It is well known that such discontinuities imply an algebraic decrease in the Fourier coefficients with the wavenumber \( k \) and thus a slow convergence of the numerical approximation with the number \( N \) of Fourier modes. We choose here \( D = 100 \) and \( N = 2^{16} \) Fourier modes. Numerically, \( \hat{Q} \) is approximated by a discrete Fourier transform, i.e. by a finite vector, which implies that a system of \( N \gg 1 \) nonlinear equations has to be solved. To this end, we invoke an iterative Newton method in order to find the (non-trivial) zeroes of the function \( F(Q) \). This means that we iterate

\[ \hat{Q}_{n+1} = \hat{Q}_n - J^{-1}(F(\hat{Q}_n)), \]

where \( J \) is the Jacobian of \( F \). However, for \( N = 2^{16} \), the dimension of the Jacobian is very high in order to be efficiently implemented, and we therefore apply a Newton–Krylov method. This means that the inverse of the Jacobian is computed via GMRES [25], iteratively. By doing so only the action of the Jacobian on a vector has to be computed, whereas the full Jacobian is never explicitly stored.

An additional obstruction is given by the fact that (2.5), or equivalently (2.7), always has the trivial solution \( \hat{Q} = 0 \). Thus, a fixed point iteration, in general, will converge to the latter. To circumvent this problem, we have to make sure to start sufficiently close to the exact non-trivial solution \( Q \). For \( s = 1 \), the latter is given explicitly by (2.6) and thus, we use a continuation method, i.e. we start with values of \( s \) close to 1, say \( s = 0.9 \), and an initial iterate given by (2.6). Then we use the solution for \( s = 0.9 \) as the starting point for the iteration for \( s = 0.8 \) and so on. The results can be found in figure 2 where we have chosen \( p = 1 \), i.e. a cubic nonlinearity. We see that the smaller \( s < 1 \), the more the ground state solution becomes peaked, and the slower its spatial decay as \( |x| \to \infty \) in accordance with the theoretical predictions.

Remark 2.2. The slow decay of \( Q \) also affects the convergence of the iteration, and hence we have to decrease \( s \) in smaller and smaller increments in order to assure convergence. In each case, the iteration is stopped whenever equation (2.7) is satisfied to be better than \( 10^{-12} \). This implies that the solutions are well resolved in Fourier space for larger \( s > 0.5 \). It is shown in figure 3 that the modulus of the Fourier coefficients decreases to machine precision for the high wavenumbers, whereas they only decrease to \( 10^{-4} \) for \( s = 0.4 \).

Finally, the total energy and the mass of the ground solutions \( Q \) are depicted in dependence of \( s \) in figure 4. It can be seen that the energy is monotonically decreasing with \( s \) while the mass is increasing. Note that the energy vanishes with numerical precision (\( \approx 10^{-5} \)) in the \( L^2 \) critical case, where \( p = 1 \) and \( s = 0.5 \).
Figure 2. Ground state solutions $Q(x)$ of (1.9) for different values of $s$, depicted close to the origin. (Online version in colour.)

Figure 3. (a) The asymptotic behaviour for large $x$ of the ground state solutions $Q$ for different values of $s$. (b) The modulus of the Fourier coefficients for two of the ground states shown in figure 2, the more rapidly decreasing for $s = 0.9$, the other for $s = 0.4$. (Online version in colour.)

Figure 4. The $s$ dependence of the total energy (a) and mass (b) of the ground state solutions $Q(x)$ to (1.9). (Online version in colour.)
Figure 5. Time dependence of the modulus squared of the solution of the focusing fNLS equation (1.9) with $s = 0.9$ and initial data $\psi_0(x) = e^{ix}Q(x)$ (a). The behaviour in time of the corresponding $L^\infty$ norm is given in (b). (Online version in colour.)

As a last numerical test within this section, we first recall that the classical NLS equation ($s = 1$) is Galilei invariant. This means, that if $\psi(t, x)$ is a solution, then so is

$$\tilde{\psi}(t, x) = \psi(t, x - ct)e^{i|c|^2/2},$$

(2.8)

with $c \in \mathbb{R}^d$ some finite speed. In particular, if initially we choose $\psi(0, x) = Q(x)$, then we obtain the so-called solitary wave solution for NLS. For $s \neq 1$, the Galilei symmetry of the model is broken, and hence we cannot expect an exact formula of the same type as in (2.8). Thus, it is not obvious how an initial data of the form $\psi_0(x) = Q(x)e^{ix}$ (we set $c = 1$ for simplicity) will evolve. However, it is shown in figure 5 that the initial hump still propagates essentially with constant velocity $\tilde{c} \approx 1$, similar to a solitary wave. The corresponding amplitude $|\psi(t, x)|$ oscillates around an asymptotically constant $L^\infty$ norm, similar to the situation depicted in appendix A. The latter is even more visible from the $L^\infty$ norm of the solution shown also in figure 5. In other words, we find that initial data of the form $Q(x)e^{ix}$ give rise to a solution which can be seen as an approximate solitary wave, the amplitude of which converges as $t \to +\infty$ to some, yet unknown, asymptotic profile.

3. Methods for the numerical study of blow-up

In this section, we briefly present the methods used for the numerical study of finite time blow-up. Firstly, we use a dynamic rescaling which allows, in principle, an adaptive mesh refinement near blow-up. Secondly, we explain how to numerically identify singularities on the real axis by tracing singularities of the solution in the complex plane via the asymptotic behaviour of the Fourier coefficients.

(a) Dynamical rescaling

In the numerical study of blow-up in NLS equations, dynamically rescaled codes have proved to provide an interesting approach (see [1, ch. 6] and references therein). In the case of radially symmetric solutions $\psi(t, r) \equiv \psi(t, |x|)$, one thereby introduces the change of variables

$$y = \frac{r}{L(t)}, \quad \frac{\mathrm{d} \tau}{\mathrm{d} t} = \frac{1}{L^{2s}(t)} \quad \text{and} \quad \psi(t, r) = L(t)^{-s/p} \Psi(\tau, y).$$

(3.1)

Using this for the focusing ($\gamma = -1$) fNLS, we find a rescaled equation for $\Psi$ in the form

$$i\partial_\tau \Psi = i\alpha(\tau) \left( s \frac{\partial}{\partial y} \Psi + y \partial_y \Psi \right) + \frac{1}{2} (-\Delta)^{s/p} \Psi - |\Psi|^{2p} \Psi,$$

(3.2)
where \((-\Delta)^s \psi(x) := \mathcal{F}^{-1}(|k|^{2s} \hat{\psi}(k))\), for \(k \in \mathbb{R}\), and
\[
a = L^{2s-1} \frac{dL}{dt} = \frac{d \ln L}{d\tau}.
\] (3.3)

Under this rescaling, the mass and energy behave like
\[
M = \frac{|\mathcal{S}^{d-1}|}{L(\tau)^{d-2s/p}} \int_0^\infty |\psi(\tau, y)|^2 y^{d-1} dy
\] (3.4)
and
\[
E = \frac{|\mathcal{S}^{d-1}|}{L(\tau)^{d-2s-2s/p}} \int_0^\infty \left( \frac{1}{2} |\partial_y^s \psi(\tau, y)|^2 - \frac{1}{p+1} |\psi(\tau, y)|^{2p+2} \right) y^{d-1} dy,
\] (3.5)
where \(\partial_y^s f(x) := \mathcal{F}^{-1}((-ik)^s \hat{f}(k))\). The scaling function \(L\) should be chosen in such a way that \(L(\tau) \to 0\), sufficiently fast, as \(\tau \to +\infty\). It is then expected that, as \(\tau \to +\infty\), both \(a \to a^\infty\) and \(\psi \to \psi^\infty\) become \(\tau\)-independent (in the mass supercritical case). The profile \(\psi^\infty\), consequently solves
\[
0 = \frac{\partial_t \psi^\infty}{\partial_y^s \psi^\infty} + (\Delta)^s \psi^\infty - |\psi|^{2p} \psi = 0, \quad y \in \mathbb{R}_+.
\] (3.6)

In \(d = 1\), this is a fractional ordinary differential equation. It is not known whether this equation has localized solutions, and if yes, whether these are unique. If such a unique solution exists, it will give the blow-up profile of the self-similar blow-up. It is beyond the scope of this article to address the related problems.

Remark 3.1. If \(a^\infty = 0\), this equation corresponds to the standing wave equation (1.2) with \(\omega = 0\). The associated stationary solution \(\psi = W(x)\), which is often called the Rubin–Talenti solution, plays a similar role for energy critical NLS, as does the ground state solution \(\psi = Q(x)\) for mass critical NLS (see [16] for more details).

There are different ways of constructing \(L(t)\) [1]. One of them involves the use of an integral norm of \(\psi\) which goes to infinity at the blow-up. This is preferable from the numerical point of view and hence, we shall choose a scaling which keeps \(\|\partial_y \psi(t, \cdot)\|_{L^2}\) constant. This leads to
\[
L(t)^{1-d/2+s/p} = \left( \frac{\|\partial_y \psi_0\|_{L^2}}{\|\partial_y \psi(t, \cdot)\|_{L^2}} \right),
\] (3.7)
where the constant \(\|\partial_y \psi_0\|_{L^2}\) is chosen to be \(\|\partial_y \psi_0\|_{L^2}\). For given \(\|\partial_y \psi(t, \cdot)\|_{L^2}\), we can read off the time dependence of \(L\) from (3.7). Alternatively to obtain an equation for \(a\) from (3.7), we differentiate \(\|\partial_y \psi_0\|_{L^2}\) knowing the resulting expression vanishes by assumption. Then we use (3.2) to eliminate the \(\tau\)-derivative of \(\psi\) which leads to an equation involving \(a\). After some partial integrations, we end up with
\[
a(\tau) = \frac{2|\mathcal{S}^{d-1}|}{(2s/p + 1)\|\partial_y \psi\|_{L^2}^2} \int_0^\infty |\psi|^{2p} \text{Im} (\bar{\psi} \partial_y^s \psi) y^{d-1} dy.
\] (3.8)

This allows us, in principle, to study the type of the blow-up for fNLS in a similar way as it has been done for generalized KdV equations in [26]. However, it was shown numerically in [26] that generic rapidly decreasing hump-like initial data lead to a tail of dispersive oscillations as \(|x| \to \infty\) with slowly decreasing amplitude. Owing to the imposed periodicity (in our numerical domain), these oscillations reappear after some time on the opposing side of the computational domain and lead to numerical instabilities in the dynamically rescaled equation. The source of these problems is the term \(y\psi_y\) in (3.2) since \(y\) is large at the boundaries of the computational domain. Therefore, this term is very sensitive to numerical errors. For generalized KdV, this can be addressed by using high resolution in time and large computational domains. It turns out that for fractional KdV equations [20] and for fNLS, the dispersive oscillations have an amplitude that decreases very slowly towards infinity which is also reflected by the slow decrease of the solitons. The consequence of this is that we cannot compute long enough with the dynamically rescaled code to get conclusive results. Instead, we integrate fNLS directly, as described above, and then
we use post-processing to characterize the type of blow-up via the above rescaling. For instance, we read off the time evolution of the quantity $L$ from (3.7).

Under the hypothesis that $L(\tau) \sim \exp(-\kappa \tau)$ with $\kappa > 0$ some positive constant, (3.1) yields a connection between $t$ and $\tau$. Namely,

$$L(t) \propto (t^* - t)^{1/2s},$$

(3.9)

where $t^* > 0$ is the blow-up time, corresponding to $\tau = +\infty$. With (3.7) and (3.1), this implies

$$\|\partial_x \psi(t, \cdot)\|^2 \propto (t^* - t)^{-(1/p + 1/(2s))}, \quad \|\psi(t, \cdot)\| \propto (t^* - t)^{-1/(2p)}.$$  

(3.10)

In particular, for $s = 1$ we have $L \propto \sqrt{t^* - t}$, which is the expected blow-up rate for NLS in the mass supercritical regime. In the mass critical case $p = 2$, one finds a correction to (3.7) in the form

$$L(t) \propto \sqrt{\frac{t^* - t}{\ln \ln(t^* - t)}},$$

(3.11)

i.e. one has $\tau \propto \ln(t^* - t)(1 - \ln \ln(t^* - t))$ instead of $\tau \propto \ln(t^* - t)$. This so-called log–log-scaling regime for mass critical NLS has been rigorously proved in [27]. We will test whether such scalings can be observed in the numerical experiments for fNLS, but it cannot be expected that the logarithmic corrections can be seen numerically.

(b) Singularity tracing in the complex plane

In the case of a finite time blow-up, we observe essentially two types of behaviour of the numerical solution. Either the $L^\infty$ norm of the solution becomes so large that the computation of the nonlinear terms in the fNLS equation leads to an overflow error. In this case, the code breaks down by producing NaN results. The other possibility is that the code runs out of resolution in Fourier space which is indicated by a deterioration of the Fourier coefficients. The latter allows for an identification of an appearing singularity as follows (see also [28–30]): the function $\psi$ to be studied on the real axis, i.e. where the real solution becomes singular, as it was shown that the quantity $\delta$ can be reliably identified from a fitting of the Fourier coefficients. Unfortunately, this is not true for $\mu$, for which the numerical inaccuracy is very large. In the case of focusing NLS, it was shown in [29] that the best results are obtained when the code is stopped once the singularity is closer to the real axis than the minimal resolved distance via Fourier methods, i.e.

$$m := 2\pi \frac{D}{N},$$

(3.13)

with $N \in \mathbb{N}$ being the number of Fourier modes and $2\pi D$ the length of the computational domain in physical space. All values of $\delta < m$ cannot be distinguished numerically from 0.

Note that the time at which the code is stopped because of the criterion above is not the same as the blow-up time itself. Rather, it is only the time where the code stops to be reliable. As mentioned above, we will always provide sufficient resolution in time so that only the lack of resolution in Fourier space makes the code stop. The blow-up time will then be determined from the numerical data by fitting to the scalings given in the previous subsection. We generally choose the time step in blow-up scenarios such that the accuracy is limited by the resolution in Fourier space, i.e. that a further reduction of the time step for a given number of Fourier modes does not change the final result within numerical accuracy.
4. Numerical studies of finite time blow-up

In this section, we will study the appearance of finite time blow-up for solutions of the focusing cubic fNLS in $d = 1$ with rapidly decreasing initial data $\psi_0 \in S(\mathbb{R})$. The corresponding solution does not suffer from the same problems as the slowly decaying ground states, at least not on the studied timescales (at larger times, slow decrease might again appear due to the fractional Laplacian), and hence gives a more reliable picture of the blow-up phenomena. Our choice of initial data is

$$\psi_0(x) = \frac{\beta}{\cosh(x)} \equiv \beta \text{sech}(x), \quad \beta \in \mathbb{R},$$

(4.1)

which are motivated by the soliton for the cubic NLS at $t = 0$ (in particular, these type of initial data have exponential decay as $|x| \to \infty$ which is preferable for our numerical studies).

(a) Numerical reproduction of known results for nonlinear Schrödinger

Before we investigate the blow-up for fNLS, we will test our numerical methods via a study of the focusing quintic NLS $p = 2$ and septic NLS $p = 3$. For the blow-up computations in this section, we always use $N = 2^{17}$ Fourier modes for $x \in [0, \pi]$ and $N_t = 50,000$ time steps.

We first consider the initial data (4.1) with $\beta = 1$ for the focusing septic NLS equation, i.e. (1.9) with $s = 1$, $p = 3$ and $\gamma = -1$. This equation is mass supercritical (and energy subcritical). We find that the code breaks at $t \approx 1.4789$ due to an overflow error. The latter occurs in the computation of the nonlinearity $|\psi|^2 \psi$. At the last recorded time, the value of $\delta$ obtained by fitting the Fourier coefficients to the asymptotic formula (3.12) is $\delta \approx 2.4 \times 10^{-3}$ and thus more than an order of magnitude larger than the minimal resolved distance $m = 4.794 \times 10^{-4}$ in (3.13). In order to obtain the actual blow-up time, we use the optimization algorithm [32], which is accessible via Matlab as the command `fminsearch`. For $t \approx t^*$, we then fit for the $L^\infty$ and the $H^1$ norm (always normalized to 1 at $t = 0$ in this section) of $\psi(t, \cdot)$ to the expected asymptotic behaviour (3.10). The $L^\infty$ norm thereby catches the local behaviour of the solution close to the blow-up point, whereas the homogeneous Sobolev norm $H^1$ takes into account the solution on the whole computational domain. Thus, the consistency of the fitting results provides a test of the quality of the numerics. The results of the fitting are shown in figure 6. Fitting $\ln \| \nabla \psi(t, \cdot) \|_2^2$ to $\kappa_1 \ln(t^* - t) + \kappa_2$, we find $t^* = 1.4789$, $\kappa_1 = -0.8197 \approx -\frac{5}{6}$ and $\kappa_2 = -0.3644$. Similarly, we get for $\| \psi(t, \cdot) \|_\infty$ the values $t^* = 1.4789$, $\kappa_1 = -0.1634 \approx -\frac{1}{6}$ and $\kappa_2 = -0.0013$. Note the excellent agreement of the blow-up times which shows both the consistency of the fitting results and that the computation came very close to the blow-up. Note also the agreement with the predicted values $\frac{5}{6}$, respectively, $\frac{1}{6}$ for the values of the $\kappa_1$. These values are unchanged within numerical precision if only the last 100 computed time steps are used for the fitting.

The same initial data for the mass critical quintic NLS equation in $d = 1$ lead to a breaking of the code at $t \approx 4.971$, again due to an overflow error. At the last recorded time, the value of $\delta$ obtained by fitting the Fourier coefficients to the asymptotic formula (3.12) is $\delta \approx 4.8 \times 10^{-3}$ and thus roughly an order of magnitude larger than the minimal resolved distance $m = 4.794 \times 10^{-4}$. Fitting $\| \nabla \psi(t, \cdot) \|_2^2$ as in the supercritical case to $\kappa_1 \ln(t^* - t) + \kappa_2$, we get $t^* = 4.9711$, $\kappa_1 = -1.0077$ and $\kappa_2 = 1.3568$. Similarly, we obtain for $\| \psi(t, \cdot) \|_\infty$ the values $t^* = 4.9712$, $\kappa_1 = -0.2533$ and $\kappa_2 = 0.3426$. The agreement of the blow-up times shows again the consistency of the fitting results, and the agreement with the predicted values $1$, respectively, $\frac{1}{2}$ for the values of the $\kappa_1$, if the scaling (3.10) is assumed.

An important question is, whether the logarithmic corrections in (3.11) can also be seen within this approach. This is unlikely, since we do not use an adaptive rescaling here for the reasons explained before (that the periodic boundary conditions lead to numerical instabilities). To test what can be seen with the present code, we do the same fitting as above for the last 100 computed time steps since the logarithmic corrections will be mainly noticeable for $t \approx t^*$. In this case, we get with numerical precision the same values for $\kappa_1$ and $\kappa_2$. We denote the $L^2$ norm of the difference between the logarithm of the fitted norm and $\kappa_1 \ln(t^* - t) + \kappa_2$ as the fitting error $\Delta_2$. We find $\Delta_2 = $
1.88 × 10⁻² for the $L^2$ norm of $\psi_x$ and $\Delta_2 = 4.3 \times 10^{-3}$ for the $L^\infty$ norm of $\psi$. If we fit the same norms to $\tilde{\kappa}_1(\ln(t^* - t) - \ln \ln |\ln(t^* - t)|) + \tilde{\kappa}_2$, we get for the analogously defined fitting error $\Delta_2$ the values $3.72 \times 10^{-2}$, respectively, 0.014, i.e. higher values. Repeating the previous analysis for the last 10 computed points, the fitting errors become $\Delta_2 = 8.7 \times 10^{-3}$, respectively, $6.65 \times 10^{-2}$, and $\Delta_2 = 7.7 \times 10^{-4}$, respectively, $9.9 \times 10^{-3}$, i.e. a better agreement for the logarithm corrections. Thus, if there is an indication of the logarithmic corrections, they can only be expected very close to the time where the code is stopped for a lack of resolution.

(b) Finite time blow-up for fractional nonlinear Schrödinger

Having checked to which extent we are able to reproduce blow-up results for the usual NLS in $d = 1$, we turn now to the case of (1.9) with $s \leq \frac{1}{2}$ and initial data given by (4.1). By fitting the Fourier coefficients to the asymptotic formula (3.12), we find that a singularity is approaching the real axis in the complex plane for finite time, which indicates a blow-up. As discussed above, we stop the code once the value $\delta < m$ with $m$ given by (3.13). In contrast to the NLS examples with $p > 1$, no overflow error is observed in the present case, due to the smaller power of the (cubic) nonlinearity. The blow-up time is again determined via the fitting of certain norms of the solution to the expected formulae (3.10) and (3.11).

In the mass critical case $s = \frac{1}{2}$, the code is stopped at $t = 2.9413$. Fitting, as before, the square of the $H^1$ norm of $\psi$ for the last 1000 recorded time steps to $\kappa_1 \ln(t^* - t) + \kappa_2$, we get $t^* = 2.9940$, $\kappa_1 = -2.0735$ and $\kappa_2 = 1.9783$. Similarly, we obtain for the $L^\infty$ norm of $\psi$ the values $t^* = 2.994$, $\kappa_1 = -0.5196$ and $\kappa_2 = 0.4003$. The agreement of the blow-up times provides again a check of the consistency of the fitting results. The obtained values for $\kappa_1$ also agree well with the predicted values $-2$, respectively, $-\frac{1}{2}$, if the scaling (3.10) is assumed. To see whether there is an indication of logarithmic corrections to this formula as in (3.11), we repeat this fitting for the last 10 recorded time steps, just like in the $L^2$ critical case for $s = 1$ above. We find a fitting error $\Delta_2 = 4.5 \times 10^{-3}$ for the $H^1$ norm and $\Delta_2 = 2.1 \times 10^{-3}$ for the $L^\infty$ norm of $\psi$. If we fit the same norms to $\tilde{\kappa}_1(\ln(t^* - t) - \ln \ln |\ln(t^* - t)|) + \tilde{\kappa}_2$, we get for the analogously defined fitting error $\Delta_2$ the values $4.8 \times 10^{-3}$ and $3.3 \times 10^{-5}$, respectively. In other words, we find essentially the same value for the $H^1$ norm, but a much better agreement of the logarithmic correction for the $L^\infty$ norm of $\psi$ close to the blow-up. It is possible, however, that we did not get close enough to the blow-up in order for this effect to be also seen within the $H^1$ norm, but it appears that the logarithmic correction is indeed visible locally near the blow-up.

The blow-up profile of the solution at the last recorded time is shown in figure 7a. In the same figure, we show the soliton rescaled according to (3.1). The scaling factor $L$ is simply fixed in a

Figure 6. Fitting the logarithms of the $H^1$ norm (a) and of the $L^\infty$ norm (b) of the solution of the septic NLS equation ($s = 1$) with initial data (4.1) close to the blow-up. The fitted $\kappa_1 \ln(t^* - t) + \kappa_2$ (see the description) is also given. (Online version in colour.)
Figure 7. Blow-up profiles of solutions of the fNLS equation for the initial data \( \psi_0(x) = \text{sech} \, x \) at the respective last recorded time: on (a) for the mass critical case \( s = 0.5 \) the modulus of the solution and the fitted soliton according to the scaling (3.1); on (b) for the energy supercritical case \( s = 0.2 \). (Online version in colour.)

way that the maxima of the solutions coincide. It can be seen that the agreement is qualitatively good and quantitatively convincing close to the maximum. Obviously, the asymptotic description is less satisfactory for a larger distance to the maximum due to the slow algebraic decrease of the soliton for \( |x| \to \infty \). It is to be expected that the asymptotic description would improve if times closer to blow-up could be reached.

In the mass supercritical case \( s = 0.4 \), we observe for the same initial data that the code is stopped at a larger time \( t = 3.1347 \) than in the case \( s = \frac{1}{2} \). Once again we fit the \( \dot{H}^1 \) norm of \( \psi \) for the last 1000 recorded time steps to \( \kappa_1 \ln(t^* - t) + \kappa_2 \) and obtain \( t^* = 3.1396, \kappa_1 = -2.3521 \) and \( \kappa_2 = 2.5182 \); similarly, we obtain for the \( L^\infty \) norm of \( \psi \) the values \( t^* = 3.1396, \kappa_1 = -0.5192 \) and \( \kappa_2 = 0.4441 \). There is again a good agreement of the fitted blow-up times and the values of the \( \kappa \) with the predicted values \(-2.25 \) and \(-\frac{1}{2} \), respectively, if the scaling (3.10) is assumed.

It is known (e.g. [14]) that multiplication of the initial data with a rapidly oscillating factor of the form \( e^{ib|x|^2} \) with \( b > 0 \) introduces a defocusing effect in the standard focusing NLS equation. Indeed, one can prove that for \( b > 0 \) sufficiently large, the solution of NLS exists for all \( t \geq 0 \), regardless of the sign of \( \gamma \) in (1.9). Again these analytical considerations do not directly carry over in the presence of fractional derivatives. But it is shown in Figure 8 that the fNLS solution for \( s = 0.4 \) and \( \psi(0, x) = e^{ix^2} \text{sech}(x) \) not only does not show blow-up as above, but also displays the behaviour of solutions to the defocusing fNLS equation to be studied in the sections below.

5. The energy critical and supercritical regime

Recall that there is no energy supercritical regime for the usual NLS in \( d = 1 \). However, we can reach this regime in the fractional NLS (1.9) as soon as \( s < \frac{1}{4} \). We shall study both, the focusing and the defocusing situations in more detail. For cases where no blow-up is observed, we also trace the \( \dot{H}^\sigma(\mathbb{R}) \) norm invariant under the rescaling (3.1). To this end, we consider here \( s = 0.2 \) for which the critical exponent is \( \sigma = 0.3 \), in view of (1.8). The initial data will be the same as in §4, i.e.

\[ \psi_0(x) = \beta \text{sech}(x), \quad \beta \in \mathbb{R}. \]

(a) Finite time blow-up for energy supercritical fractional nonlinear Schrödinger

It is not clear what the precise conditions on the initial data are, which lead to finite time blow-up in the energy supercritical regime. The numerical experiments of the previous subsection seem to indicate that initial data in the vicinity of the ground state with larger mass and smaller energy than the ground state produce such a blow-up. In fact, if we study initial data with small mass,
i.e. $\psi_0 = 0.1 \text{sech}(x)$, we find that the initial hump simply decays to zero as $t \to +\infty$, as is shown in figure 9. The $L^\infty$ norm of the solution is monotonically decreasing and there is no indication of blow-up in this case. The scaling invariant $H^{0.3}$ norm also appears to be bounded as shown in the same figure.

However, for the initial data $\psi_0 = \text{sech}(x)$, the code is stopped at the time $t = 6.0748$ since the distance between a singularity (as indicated by the Fourier coefficients via (3.12)) and the real axis is smaller than the numerical resolution. Fitting, as before, the norm $H^1$ norm of $\psi$ for the last 1000 time steps to $\kappa_1 \ln(t^* - t) + \kappa_2$, we get $t^* = 6.2771$, $\kappa_1 = -3.6949$ and $\kappa_2 = 8.5231$ with a fitting error $\Delta_2 \approx 10^{-2}$. Similarly, we obtain for the $L^\infty$ norm of $\psi$ the values $t^* = 6.2804$, $\kappa_1 = -0.5779$ and $\kappa_2 = 1.2001$ with a fitting error $\Delta_2$ of the order of $10^{-3}$. These values for $\kappa_1$ agree with the predicted values $-3.5$, respectively, $-\frac{1}{2}$, if the scaling (3.10) is assumed. Note that the blow-up time $t^*$ is more than twice the $t^*$ found for the same initial data in the mass critical case, which seems quite surprising (as one would naively expect the blow-up time to be monotonically dependent on the choice of $s$). The agreement of the fitted blow-up times for the two norms is worse than in the mass critical case. This is due to the fact that the code did not get as close to the blow-up time as for $s = \frac{1}{2}$. It appears that considerably higher resolution would be needed in this case as is indicated by the stronger divergence of the $H^1$ norm. In figure 7b, we show the blow-up profile
Figure 10. (a) Solution of the mass subcritical defocusing fNLS equation (1.9) with $s = 0.9$ and initial data $\psi_0 = \text{sech}(x)$. (b) The corresponding $L^\infty$ norm of the solution. (Online version in colour.)

Figure 11. Solution of the defocusing energy supercritical fNLS equation (1.9) with $s = 0.2$ and initial data $\psi_0 = \text{sech}(x)$. (Online version in colour.)

of the solution at the last recorded time. Visibly, this profile is different from the blow-up in the mass critical case which qualitatively corresponds to the soliton. Here the blow-up profile is much more compressed which also explains why we could not get as close to the blow-up as in the mass critical case.

(b) Long-time behaviour for defocusing energy supercritical fractional nonlinear Schrödinger

In figure 10, we show the solution of a defocusing fNLS equation (1.9) with $s = 0.9$ and initial data (4.1) with $\beta = 1$. It can be seen that the time evolution of the solution simply disperses the initial datum. This behaviour is even more visible from the $L^\infty$ norm of the solution which is shown in the same figure. Obviously, the norm is monotonically decreasing.

For weaker dispersion, i.e. smaller $s$, the situation changes the shape, however. As shown in figure 11, for $s = 0.2 < \frac{1}{4}$, i.e. the energy supercritical regime, the initial hump splits into two humps both of which travel to spatial infinity.

The formation of the two humps can also be inferred from the $L^\infty$ norm of the solution which is shown in figure 12. The $L^\infty$ norm appears to become almost constant for large $t \gg 0$. An interesting quantity in this context is the scaling invariant $H^{0.3}$ norm since its boundedness would allow to control the solution globally in time. It can be seen that there is no indication that this
norm diverges (also not for larger times than shown here). However, in comparison to the earlier numerical study of Colliander et al. [19] for energy supercritical NLS (in $d = 5$), we do not find that the critical $H^0.3$ norm approaches a constant for $t \gg 0$. This is probably due to the fact that in our case, the solution decay is much slower as $x \to \infty$ which prevents our numerical method from computing for sufficiently long times. A possible way to overcome this issue is the scaling regime introduced in the next section.

6. Numerical study of the semiclassical regime

(a) Semiclassical rescaling

A possible approach to study the long-time behaviour of solutions of the (dimensionless) fNLS (1.9) is by considering slowly varying initial data of the form

$$\psi_0(x; \epsilon) = u(\epsilon x),$$

where $0 < \epsilon \ll 1$ is a small semiclassical parameter and $u \in S(\mathbb{R}^d)$ is some given initial profile. As $\epsilon \to 0$, the initial data approaches the constant value $u(0)$. Hence, in order to see non-trivial effects one has to wait until sufficiently long times of order $t \sim O(1/\epsilon)$, which consequently also requires rescaling of the spatial variable onto macroscopically large scales $x \sim O(1/\epsilon)$. In other words, we consider $x \mapsto \tilde{x} = x\epsilon$, $t \mapsto \tilde{t} = t\epsilon$ and set

$$\psi^\epsilon (\tilde{t}, \tilde{x}) = \psi \left( \frac{\tilde{t}}{\epsilon}, \frac{\tilde{x}}{\epsilon} \right),$$

to obtain the following semiclassically scaled fNLS for the new unknown $\psi^\epsilon$, where we discard the ‘tildes’ again for the sake of simplicity:

$$i\epsilon \partial_t \psi^\epsilon = \frac{\epsilon^{2s}}{2} (-\Delta)^s \psi^\epsilon + \gamma |\psi^\epsilon|^2 \psi^\epsilon, \quad \psi^\epsilon (0, x) = u(x), \quad x \in \mathbb{R}^d.$$ (6.1)

For $\epsilon \ll 1$, the behaviour of this equation describes solutions on macroscopically large space and time scales, which justifies the name of semiclassical asymptotics. From the numerical point of view, the simulation of Schrödinger equations in the semiclassical regime is a formidable challenge, for which several different techniques have been developed in recent years, see the review by Jin et al. [33] for more details.
For the classical cubic NLS \((s = 1)\), an asymptotic theory for the solution as \(\epsilon \to 0\) is usually based on Wentzel–Kramers–Brillouin (WKB)-type expansions. To this end, one assumes
\[
\psi(t, x) \approx a(t, x) e^{iS(t, x)/\epsilon},
\]
where \(S(t, x) \in \mathbb{R}\) is a real-valued phase function and \(a(t, x) \in \mathbb{C}\) a (in general) complex-valued amplitude. In the defocusing case, one can prove (see [34] and references therein) that as \(\epsilon \to 0\), this gives a valid approximation of the exact solution \(\psi_{\epsilon}\) provided \(a, S\) are sufficiently smooth solutions of the following hydrodynamic system:
\[
\frac{\partial}{\partial t} S + \frac{1}{2} |\nabla S|^2 + \gamma |a|^2 = 0 \quad \text{and} \quad \frac{\partial}{\partial t} a + \nabla S \cdot \nabla a + \frac{a}{2} \Delta S = 0,
\]
or, in terms of \(\rho = |a|^2\) and \(v = \nabla S\):
\[
\frac{\partial}{\partial t} v + v \cdot \nabla v + \gamma \nabla \rho = 0 \quad \text{and} \quad \frac{\partial}{\partial t} \rho + \text{div}(\nu \rho) = 0.
\]
Since this system in general exhibits shocks, the WKB approximation is only valid for short times \(t < t_c\), where \(t_c > 0\) is the time where the first shock appears (also known as caustic-onset time, or time of the first gradient catastrophe). In the focusing case, the situation is even worse, as the obtained hydrodynamic system is found to be elliptic and thus not well-posed (see [35,36] for partial results in the completely integrable case \(d = p = 1\)).

**Remark 6.1.** For \(s = 1\), system (6.3) can be formally obtained from the so-called Madelung system in the limit \(\epsilon \to 0\). The latter is obtained by inserting the right-hand side of (6.2) into the NLS and separating real and imaginary parts, which gives
\[
\frac{\partial}{\partial t} S + \frac{1}{2} |\nabla S|^2 + \gamma |a|^2 = 0 \quad \text{and} \quad \frac{\partial}{\partial t} a + \nabla S \cdot \nabla a + \frac{a}{2} \Delta S = \epsilon^2 \frac{\Delta a}{a}.
\]
This system is indeed equivalent to the NLS, provided \(a \neq 0\). This formulation has been used, for example, in [37] to study the semiclassical limit of defocusing NLS. In the case of fractional NLS, no such equivalent Madelung-type equivalent system has been yet derived (due to the lack of an appropriate Leibniz rule).

**(b) Semiclassical limit of the focusing fractional nonlinear Schrödinger equation**

In this section, we study the semiclassically scaled, focusing (cubic) fNLS equation (6.1) with \(\gamma = 1\) and \(\epsilon \ll 1\). We choose \(\psi_{\epsilon}(x, 0) = \text{sech} x\). For NLS \((s = 1)\) in \(d = 1\) and generic initial data, it is known that the semiclassical system (6.4) exhibits a gradient catastrophe at some finite time \(0 < t_c < +\infty\), yielding a square root-type singularity in the gradient of the phase [38]. For \(\epsilon > 0\), this singularity is regularized by highly oscillatory waves (the so-called dispersive shock phenomena). Indeed, one can see numerically that the square-modulus of the solution continues to grow for some time \(t > t_c\), and eventually splits into several smaller humps leading to a zone of modulated oscillations as shown in figure 13.

**Remark 6.2.** We refer to [38,39] for more details and a conjecture concerning the asymptotic description of the solution of semiclassical NLS near \(t \sim t_c\). See also [40] for a partial proof of this conjecture.

For smaller values of \(s < 1\) and \(\epsilon < 1\), the dispersion gets weaker and the focusing effect of the equation becomes stronger. This leads to a higher maximum and a more ‘agitated’ oscillatory zone after the maximal peak. It was argued in [21], that this maximal peak needs to be numerically well resolved. If this is not the case, the Fourier coefficients for the high wavenumbers get polluted, which triggers the modulation instability of the focusing NLS equation. The latter phenomenon
cannot be controlled even with Fourier filtering methods. Therefore, we cannot reach much smaller values for $s$ and $\epsilon$ than used below. It would be necessary to go to higher than double precision to be able to address more extreme cases. In figure 13, we show the solution of the semiclassical focusing fNLS for $\epsilon = 0.1$, $s = 0.9$, and initial data $\psi = \text{sech}(x)$. The computation is carried out here with $N = 2^{16}$ Fourier modes and $N_t = 20,000$ time steps.

The same resolution can be used to study the same situation for the slightly smaller value of $\epsilon = 0.08$. It is shown in figure 14 that, as expected, there are more oscillations and a higher maximum in this case. To treat the solution for the same initial data with even smaller $s = 0.8$, we had to use $N = 2^{18}$ Fourier modes and $N_t = 50,000$ time steps in figure 14. It is clearly visible that the maximum of the solution continues to grow as expected with smaller $s$, and that the oscillatory zone shows more humps than for the same value of $\epsilon$, but larger $s$. As discussed in the previous sections, a blow-up is to be expected for sufficiently small $\epsilon$ for $s \leq \frac{1}{2}$.

(c) Semiclassical limit of the defocusing fractional nonlinear Schrödinger equation

In this section, we study the semiclassical regime for the defocusing fNLS equation. In the NLS case ($s = 1$), it is known that solutions corresponding to initial data $\psi(0, x) \equiv u(x) = \text{sech}(x)$ exhibit a gradient catastrophe at two points, here, for symmetry reasons, at $\pm x_c$. As in the case of solutions of the Hopf equation, this is a cubic singularity at the onset of the formation of a shock. For small $\epsilon > 0$, this singularity is regularized in the form of a zone of rapid modulated oscillations as in dispersive shocks of the KdV equation. The initial hump is defocused while the sides of the hump steepen. At a given point, oscillations form near these strong gradients. In figure 15, small
oscillations appear near the hump on figure 15a (and hidden by the hump on figure 15b) at the last shown times.

For smaller values of $s$ and $\epsilon$, the dispersion again gets weaker which implies stronger gradients and thus more rapid oscillations. In figure 15, we show the solution of the semiclassical fNLS equation (6.1) for $s = 0.9$, $\epsilon = 0.1$ and initial data $\psi_0 = \text{sech}(x)$, which is very similar to the situation with $s = 1$. But it can already be seen here that the initial hump splits into two smaller ones, in contrast to the case $s = 1$. The computation is carried out with $N = 2^{14}$ Fourier modes and $N_t = 10^4$ time steps.

For even smaller $\epsilon$, there are much more oscillations in an otherwise identical setting as in figure 15 and as shown in figure 16.

Reducing $s$ has a similar effect as can be recognized in figure 17 where we show the solution for the initial data $\psi^s(0, x) \equiv u(x) = \text{sech}(x)$ in the energy critical case $s = 0.25$. An additional effect of the smaller dispersion is that (as noted above) the initial hump splits into two humps, which are now well defined (at least before the formation of the first dispersive shock). Later in time, there appears to be a focusing effect for these two humps, as they get compressed and increase in height. If the code is run for longer times, this phenomenon continues and the code finally runs out of resolution. We also show the scaling invariant $H^s$ norm in the same figure. If we consider instead of the initial data $\psi_0 = \text{sech}(x)$ the same data multiplied by a factor $e^{ix}$, one obtains the solution in figure 18a. The effect already displayed in figure 5, can be also recognized in figure 18: the hump on the right propagates faster to the right and becomes much earlier ‘focused’ than the one on the left.
Figure 17. (a) Solution of the semiclassical, defocusing fNLS equation (6.1) for the energy critical case \( s = 0.25 \), \( \epsilon = 0.1 \), and with initial data \( \psi_0 = \text{sech}(x) \). (b) The invariant Sobolev norm (1.7); the energy of the initial data implies \( \sqrt{2E/\epsilon^2} \approx 2.325 \). (Online version in colour.)

Figure 18. Solution of the semiclassical, defocusing fNLS equation (6.1) for \( \epsilon = 0.1 \): on (a) for the energy critical case \( s = 0.25 \) and initial data \( \psi_0 = e^{ix}\text{sech}(x) \), on (b) the energy supercritical case \( s = 0.2 \) with initial data \( \psi_0 = \text{sech}(x) \). (Online version in colour.)

To address the question whether the focusing of these humps could lead eventually to the formation of a singularity as for solutions of the semiclassical system (note that existence of global regular solutions is not proved for energy supercritical fNLS), we consider the energy supercritical case \( s = 0.2 \) in more detail. The code is run with \( N = 2^{17} \) for \( x \in [\pi, \pi] \) and \( N_t = 50000 \) time steps for \( t \in [0, 3.8] \). The solution can be seen in figure 18. The extreme compression of the humps is clearly visible.

The code is stopped at \( t = 3.7368 \) since the distance of the nearest singularity in the complex plane to the real axis as determined by fitting the Fourier coefficients to the asymptotic formula (3.12) is smaller than the smallest resolved distance in physical space. But as shown in figure 19, where we also show the solution at the last recorded time, the Fourier coefficients indicate that the code ran out of resolution before. In fact, the modulus of the Fourier coefficients decreases only to the order of \( 10^{-1} \) at \( t = 3.61 \), whereas it reached \( 10^{-6} \) for \( t = 3.41 \) (this implies that the numerical results in this case should be ignored for \( t > 3.5 \)). Thus, the code runs out of resolution well before a potential singularity hits the real axis. Rerunning the code with higher resolution produces the same phenomena, just at slightly later times. This indicates that the solution indeed stays regular in this case, but is nevertheless very different from the focusing fNLS equation studied in the previous subsection. It is also different from the well-known cusps found in the case of semiclassical defocusing NLS, as can be identified using the techniques given in [29]. We finally note that the same qualitative behaviour is also observed for different choices of localized initial data.
Figure 19. Solution of the semiclassical, defocusing fNLS equation (6.1) for $s = 0.2, \epsilon = 0.1$ and the initial data $\psi_0 = \text{sech}(x)$ at $t = 3.7368$ on (a), and the corresponding Fourier coefficients on (b). (Online version in colour.)

Various norms of this solution are shown in figure 20, where one has to bear in mind that there is a lack of resolution for the last time steps. It can be seen that the $L^\infty$ norm continues to grow (the shown oscillations might be spurious and due to finite resolution in physical space), and that there is a strong growth in the $L^2$ norm of the gradient of the solution. Whereas the strong gradients in the solution are reflected by the growth of the latter norm, there is no indication of it blowing up at a time close to the last computed time. Also the $H^s$ norm invariant under the rescaling (1.6) grows only moderately. This is in accordance with the conclusion above that the solution stays regular. Note that the strong compression of the humps visible in figure 18 does not allow us to reach the same asymptotic regime for the long-time behaviour of the solution as in [19] for a higher dimensional NLS equation. The reason for this is simply that the solutions decay at a much slower rate in $|x|$ in one spatial dimension, especially in the presence of fractional derivatives.

7. Conclusion

In this paper, we have presented a comprehensive numerical study of issues appearing in the context of fractional NLS equations in one spatial dimension. The results on the long-time behaviour can be summarized in the following conjecture.

**Conjecture 7.1.** Consider the cubic fNLS equation (1.1) in $d = 1$ with smooth initial data $\psi_0 \in L^2(\mathbb{R})$ with a single hump for $|\psi_0|$. Then for
— $s > 0.5$: solutions to the fNLS equation for such initial data $\psi_0$ stay smooth for all $t$.
— $0 < s \leq 0.5$: solutions to the fNLS equation with initial data $\psi_0$ of sufficiently small, but non-zero mass stay smooth for all $t$.
— $s = 0.5$ (mass critical case): solutions to (1.9) with initial data $\psi_0$ with negative energy and mass larger than the soliton mass blow-up at finite time $t^\star$. The type of the blow-up for $t \nearrow t^\star$ is characterized by

$$
\psi(x, t) \sim \frac{1}{\sqrt{L(t)}}, \quad L(t) \sim \frac{t^\star - t}{\ln |\ln(t^\star - t)|}.
$$

(7.1)

— $s < 0.5$ (mass supercritical case): solutions to (1.9) with initial data $\psi_0$ with sufficiently large $L^2$ norm blow up at finite time $t^\star$. The type of the blow-up for $t \nearrow t^\star$ is characterized by

$$
\psi(x, t) \sim \frac{1}{L^s(t)}, \quad L \sim (t^\star - t)^{1/(2s)}.
$$

(7.2)

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Appendix A. Stability of ground states

In this section we will study perturbations of the ground state solutions constructed before. This is done for cubic nonlinearities $p = 1$ and different values of the parameter $s$. To this end, we will consider initial data for (1.9) of the form

$$
\psi_0(x) = \alpha Q(x), \quad \alpha \in \mathbb{R},
$$

(A 1)

where $Q$ is the ground state solution determined numerically as described in section 2b. The factor $\alpha$ will be either chosen to be a constant $\alpha \approx 1$ or to be an $x$ dependent phase. Note that qualitatively similar results as shown here are also found for localized perturbations of the form: $\psi_0(x) = Q(x) + \varepsilon e^{-|x|^2}$, with $\varepsilon < 1$.

(a) Perturbed ground states in the mass subcritical regime

It is known [11] that the ground state solutions are stable in the mass subcritical case, i.e. $s > \frac{1}{2}$. In fact, if we propagate initial data of the form (A 1) we find that the perturbed ground state starts to oscillate around what appears to be a stationary solution with frequency $\omega$. This can be seen in figure 22, where we have solved the initial value problem (1.9) subject to data (A 1) with $\alpha = 0.9$. We use $N = 2^{16}$ Fourier modes for $x \in 100(-\pi, \pi]$ and $N_t = 10^4$ time steps for $t < 30$. It can be seen that the initial hump decreases in height and then starts to exhibit damped oscillations around what appears to be a rescaled ground state function. This is reminiscent of the so-called breather solutions known for classical NLS.

The damped oscillations around some presumably constant asymptotically constant are clearly visible if one looks at the $L^\infty$ norm of the solution, see figure 22. Since the $L^2$ norm of the solution is a conserved quantity, the scaling (1.6) allows us to infer a bound on $\omega$, given by $\omega \approx 1^{1/(2s)} \geq \alpha^2$. For $\alpha = 0.9$ this would imply that the $L^\infty$ norm of the ground state with the maximal $\omega$ would be roughly equal to 1.146. Figure 22 suggests that this is indeed the amplitude of the final state. This would mean that the ground state is stable, and that a perturbed ground state leads asymptotically for large $t$ to a steady state with the mass of the perturbed state. In the same figure we show the $L^\infty$ norm of the solution for the fNLS equation for initial data (A 1) with $\alpha = 1.1$. There are much more oscillations in this case, but the final state appears to have an $L^\infty$ norm of roughly 1.8 (the maximal possible $L^\infty$ norm of the ground state having the same mass as the initial data would be $\approx 1.800$). Thus also in this case the final state appears to be a stationary solution corresponding to the mass of the initial data.
Figure 21. Modulus squared of the solution to the focusing fNLS equation (1.9) with $s = 0.9$ for initial data $\psi_0(x) = 0.9Q(x)$. (Online version in colour.)

Figure 22. Time dependence of the $L^\infty$ norm of the solution of the focusing fNLS equation (1.9) with $s = 0.9$ and initial data $\psi_0(x) = \alpha Q(x)$ for (a) $\alpha = 0.9$ and (b) $\alpha = 1.1$. (Online version in colour.)

(b) Perturbed ground states in the mass critical regime

The mechanism described above, i.e., that a perturbed ground state asymptotically becomes a stationary state with the same mass as the initial datum, is not possible for the mass critical case $s = \frac{1}{2}$, since the $L^2$ norm and the equation are both invariant under the rescaling (1.6). Thus it can be expected that the ground state is unstable in this case which is exactly what we observe for initial data of the form (A 1): first, for $\alpha = 0.9$, i.e., initial data with mass smaller than the ground state, figure 23 shows that the solution simply decays to zero with monotonically decreasing $L^\infty$ norm. Thereby the initial hump splits into two smaller humps which both move outwards.

However, for an $\alpha > 1$, i.e., a perturbation with mass larger than the ground state, the solution $\psi(t,x)$ appears to exhibit finite time blow-up, as can be seen in figure 24. The blow-up is also indicated by the behavior of the $L^\infty$ norm and the $H^1$ norm of the solution, see figure 25. Here, the Fourier coefficients are fitted to the asymptotic formula (3.12). As explained above, the code is stopped once $\delta < m$, i.e., once the singularity is closer to the real axis than the smallest distance resolved by the Fourier method. Note that we run out of resolution in Fourier space before coming sufficiently close to the presumed blow-up. This is mainly due to the large computational domain $100[-\pi, \pi]$ which was needed because of the slow decrease of the ground state solution towards infinity. Around $t = 1.0$ the resolution in Fourier space becomes insufficient, and the solution
Figure 23. Modulus squared of the solution of the mass critical focusing fNLS equation (1.9) with $s = 0.5$ and initial data $\psi_0(x) = 0.9Q(x)$. (Online version in colour.)

Figure 24. Modulus squared of the solution of the mass critical focusing fNLS equation (1.9) with $s = 0.5$ and initial data $\psi_0(x) = 1.1Q(x)$. (Online version in colour.)

Figure 25. Time dependence of the $L^\infty$ norm (a) and of the $\dot{H}^1$ norm normalized to 1 at $t = 0$ (b) of the solution of the focusing mass critical fNLS equation (1.9) with $s = 0.5$ and initial data $\psi_0(x) = 1.1Q(x)$. (Online version in colour.)
becomes incorrect as indicated by deterioration of the Fourier coefficients at a larger time. Note that the code would continue to run through and that the relative energy in this case would be still conserved to better than $10^{-9}$ at the final time. This shows that this quantity can only be used as an indicator if sufficient resolution in Fourier space is provided.

References


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