Computation of Self-Similar Solution Profiles for the Nonlinear Schrödinger Equation ⋆

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Abstract

We discuss the numerical computation of self-similar blow-up solutions of the classical nonlinear Schrödinger equation in three space dimensions. These solutions become unbounded in finite time at a single point at which there is a growing and increasingly narrow peak. The problem of the computation of this self-similar solution profile reduces to a nonlinear, ordinary differential equation on an unbounded domain. We show that a transformation of the independent variable to the interval $[0, 1]$ yields a well-posed boundary value problem with an essential singularity. This can be stably solved by polynomial collocation. Moreover, a MATLAB solver developed by two of the authors can be applied to solve the problem efficiently and provides a reliable estimate of the global error of the collocation solution. This is possible because the boundary conditions for the transformed problem serve to eliminate undesired, rapidly oscillating solution modes and essentially reduce the problem of the computation of the physical solution of the problem to a boundary value problem with a singularity of the first kind.

Key words: Nonlinear Schrödinger equation, self-similarity, blow-up solutions, essential singularity, collocation methods, error estimation
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1 Self-Similar Solutions of the Nonlinear Schrödinger Equation

The classical nonlinear Schrödinger equation occurs in various important applications in nonlinear optics [8] or plasma physics [12]. The original, partial differential equation in dimension d takes the form

$$\mathrm{i}\frac{\partial u}{\partial t} + \Delta u + |u|^2 u = 0, \quad t > 0, \tag{1}$$

$$u(x,0) = u_0(x), \quad x \in \mathbb{R}^d. \tag{2}$$

In the well-studied case $d = 1$, the equation is integrable and a solution exists globally. For $d \geq 2$, (1) has solutions that become unbounded in a finite time T. In this case, the solution becomes infinite at a single point x (without restriction of generality we assume that x is the origin) at which a growing and increasingly narrow peak arises. In plasma physics, the singularity is usually called a collapse, and in nonlinear optics, the singularity corresponds to the phenomenon of self-focussing. In physical applications, we are mostly interested in the case $d = 3$. In this case, it is conjectured that the solutions blow up in a self-similar way [5]. Moreover, ordinary differential equations are derived in [5] which determine the shape of the solution near the blow-up time. To derive boundary conditions for these ODEs, use of the fact is made that (1) is a unitary Hamiltonian PDE and during the evolution of the solution $u(x,t)$, both the mass M and Hamiltonian H are invariant, that is

$$\frac{dM}{dt} = \frac{dH}{dt} = 0,$$

where

$$M = \int\limits_{\mathbb{R}^3} |u(x,t)|^2 \, dx, \tag{3}$$

$$H = \int\limits_{\mathbb{R}^3} \left(|\nabla_x u(x,t)|^2 - \frac{1}{2}|u(x,t)|^4 \right) \, dx. \tag{4}$$

In this paper, we will restrict ourselves to the computation of radially symmetric solutions.

The nonlinear Schrödinger equation (1) is invariant under the following nontrivial transformation groups (for all $\lambda > 0$):

(1) $t \to \lambda t, \; x \to \sqrt{\lambda} x, \; u \to \frac{1}{\sqrt{\lambda}} u,$
(2) $u \to \mathrm{e}^{\mathrm{i}\lambda} u.$

This does not mean, however, that all the solutions of (1) are invariant under the same transformations. We are interested in the computation of solutions which have this property. These *self-similar solutions* are usually of great physical importance, because they may be stable attractors for solutions computed from perturbed initial data. Naturally, we are only interested in solutions that give meaningful definitions of the invariants (3) and (4). Self-similarity can only be expected to hold near blow-up, so for t close to T and x near the origin (that is, $r \approx 0$ for $r = |x|$) we make the ansatz

$$u(x,t) = \frac{1}{\sqrt{2a(T-t)}}\, \mathrm{e}^{-\mathrm{i}/2a \log(T-t)}\, z(\tau), \tag{5}$$

where

$$\tau := \frac{r}{\sqrt{2a(T-t)}}.$$

Here, a is a real parameter which expresses the coupling between the phase and the amplitude of u. a is determined simultaneously with the shape function z. Substitution of the ansatz (5) into (1) now yields the following ODE for z:

$$z''(\tau) + \frac{2}{\tau} z'(\tau) - z(\tau) + \mathrm{i}a(\tau z(\tau))' + |z(\tau)|^2 z(\tau) = 0, \quad \tau > 0. \tag{6}$$

The boundary conditions for (6) which yield a well-posed problem for the computation of z and a with a physically meaningful solution are derived as follows: First, due to symmetry we require

$$z'(0) = 0. \tag{7}$$

Moreover, since the phase of z is arbitrary according to the ansatz (5),

$$\Im(z(0)) = 0. \tag{8}$$

Furthermore, we are interested in solutions u of (1) which decay for $x \to \infty$ [5], [6],

$$z(\infty) = 0. \tag{9}$$

This implies that $|z|$ is small for large τ. Consequently, it is possible to discuss the asymptotics of a physically meaningful solution and associated boundary conditions by neglecting the nonlinear part and studying the linear problem

$$z''(\tau) + \frac{2}{\tau} z'(\tau) - z(\tau) + \mathrm{i}a(\tau z(\tau))' = 0, \quad \tau > 0. \tag{10}$$

The fundamental solution modes of this problem are asymptotic to

$$\varphi_1(\tau) = \frac{1}{\tau}\, e^{-i/a \log(\tau)}, \tag{11}$$

$$\varphi_2(\tau) = \frac{1}{\tau^2}\, e^{-ia\tau^2/2 + i/a \log(\tau)} \tag{12}$$

for $\tau \to \infty$ [6].

Subsequently, we refer to solutions of (1) corresponding to φ_1 as *slowly varying*, while those solutions associated with φ_2 are denoted as *rapidly varying*.

Naturally, we are only interested in solutions of (10) such that for the associated solution of (1) H from (4) is finite. This condition translates to

$$H(z) = \int_0^\infty \left(|z'(\tau)|^2 - \frac{1}{2}|z(\tau)|^4 \right) \tau^2 \, d\tau = 0. \tag{13}$$

We can choose a constant $c \in \mathbb{C}$ such that the fundamental mode $c\varphi_1$ satisfies this relation, while H is unbounded for the self-similar solution u of (1) associated with φ_2. Consequently, the boundary conditions must be posed such as to eliminate contributions from φ_2 from the general solution of (10). It turns out that (13) is equivalent to the algebraic relation

$$\lim_{\tau \to \infty} \left| \tau z'(\tau) + \left(1 + \frac{i}{a}\right) z(\tau) \right| = 0, \tag{14}$$

see [5]. This relation is indeed satisfied by φ_1, while this condition is violated by φ_2.

Finally, we note that (14) can be rewritten, taking into account (9). Conditions (9) and (14) result in

$$\lim_{\tau \to \infty} \tau z'(\tau) = 0. \tag{15}$$

It is important to point out that this last relation is again satisfied by φ_1, but not by φ_2, for which the expression remains bounded, but does not have a limit for $\tau \to \infty$. The resulting boundary value problem for the computation of the self-similar blow-up solution profile is (6), (7), (8) and (15). To solve the nonlinear eigenvalue problem, this system can be augmented by the trivial equation

$$a'(\tau) = 0. \tag{16}$$

In [5] and [6], this second order problem is solved on a truncated interval $[0, \mathcal{T}]$ with $\mathcal{T} \gg 1$.

2 Singular Problems

Here, we adopt a new approach for the efficient numerical solution of (6) and (16). Using the Euler transformation $z \to (z, \tau z') = (z_1, z_2)$ for (6), we derive the equivalent first-order equation

$$z'(\tau) = \frac{M(\tau)}{\tau} z(\tau) + f(\tau, z(\tau)), \quad \tau > 0, \tag{17}$$

where

$$M(\tau) = \begin{pmatrix} 0 & 1 \\ \tau^2(1 - \mathrm{i}a) & -1 - \mathrm{i}a\tau^2 \end{pmatrix}, \; f(\tau, z) = \begin{pmatrix} 0 \\ -\tau z_1 |z_1|^2 \end{pmatrix}.$$

This is an ODE with a singularity of the first kind at $\tau = 0$ and a singularity of the second kind (essential singularity) at $\tau = \infty$. For this reason, we split the interval $(0, \infty]$ into the subintervals $(0, 1]$ and $[1, \infty)$, and require the solution to be continuous at $\tau = 1$. The problem on $[1, \infty)$ is then transformed to $(0, 1]$ by the substitution $\tau \to 1/\tau$. This yields the four-dimensional BVP

$$z'(\tau) = \begin{pmatrix} \frac{M(\tau)}{\tau} & 0 \\ 0 & \frac{A(\tau)}{\tau^3} \end{pmatrix} z(\tau) + \begin{pmatrix} f(\tau, z_1, z_2) \\ g(\tau, z_3, z_4) \end{pmatrix}, \quad \tau \in [0, 1], \tag{18}$$

where

$$A(\tau) = \begin{pmatrix} 0 & -\tau^2 \\ \mathrm{i}a - 1 & \mathrm{i}a + \tau^2 \end{pmatrix}, \; g(\tau, z_3, z_4) = \begin{pmatrix} 0 \\ \frac{1}{\tau^3} z_3 |z_3|^2 \end{pmatrix}.$$

In the new variables, the boundary conditions translate to

$$z_2(0) = 0, \; \Im z_1(0) = 0, \; z_1(1) = z_3(1), \; z_2(1) = z_4(1), \; z_4(0) = 0. \tag{19}$$

We now review the well-posedness of the transformed problem. In particular, the eigenvalues of the matrices $M(0)$ and $A(0)$ determine what sets of boundary conditions are admissible in order to obtain a continuous (isolated) solution of (18), see for example [9], [10]. Again, it is sufficient to discuss the linear version of (18) where the nonlinear part is neglected. The admissible boundary conditions for the resulting system

$$z'(\tau) = \begin{pmatrix} \frac{M(\tau)}{\tau} & 0 \\ 0 & \frac{A(\tau)}{\tau^3} \end{pmatrix} z(\tau) \tag{20}$$

are the same as for (18).

The eigenvalues of $M(0)$ are $\lambda_1 = 0$ and $\lambda_2 = -1$. According to [9], the admissible boundary condition for a well-posed problem with a singularity of the first kind associated with the eigenvalue λ_2 is $z_2(0) = 0$. The second condition (associated with eigenvalue λ_1) can be chosen at either $\tau = 0$ or $\tau = 1$. The transition conditions $z_1(1) = z_3(1)$ or $z_2(1) = z_4(1)$ are therefore admissible for a well-posed problem.

The eigenvalues of $A(0)$ are $\lambda_3 = 0$ and $\lambda_4 = \mathrm{i}a$. The treatment in [10] does not cover these cases. Consequently, we will check the well-posedness of the boundary conditions similarly as for (10).

First, we note that the fundamental modes of the constant coefficient system

$$z'(\tau) = \frac{A(0)}{\tau^3} z(\tau) \tag{21}$$

are

$$\varphi_3(\tau) = 1, \quad \varphi_4(\tau) = \mathrm{e}^{-\mathrm{i}a/(2\tau^2)}\,. \tag{22}$$

φ_4, the mode associated with $\lambda_4 = \mathrm{i}a$, is rapidly oscillating and does not have a limit for $\tau \to 0$. It is therefore desirable to eliminate this mode from the solution. Indeed, if we transform the mode φ_2 from (12) analogously as above, the transplant $\tilde{\varphi}_2(\tau) = 1/\tau \varphi_2'(1/\tau)$ satisfies

$$\tilde{\varphi}_2(\tau) = \left(-\mathrm{i}a + \tau^2 \left(\frac{\mathrm{i}}{a} - 2\right)\right) \mathrm{e}^{-\mathrm{i}/a \log(\tau)}\, \mathrm{e}^{-\mathrm{i}a/(2\tau^2)}\,.$$

Thus, φ_4 displays the same behavior for $\tau \to 0$ as the transformed mode $\tilde{\varphi}_2$. Namely, the solution features a rapid oscillation which is not damped as $\tau \to 0$. Consequently, it is possible to eliminate the undesirable solution mode by requiring $z_4(0) = 0$. This demonstrates that this boundary condition is necessary for a well-posed boundary value problem.

φ_3, the fundamental solution of (21) corresponding to the eigenvalue $\lambda_3 = 0$, is the constant solution, which is not very useful for our purpose. To analyse the situation further, we consider the eigenvalues of $A(\tau)$. It turns out that

$$\lambda_3(\tau) = \left(1 + \frac{\mathrm{i}}{a}\right)\tau^2 + \left(\frac{1}{a^2} + \frac{\mathrm{i}}{a^3}\right)\tau^4 + O(\tau^6),$$
$$\lambda_4(\tau) = \mathrm{i}a - \frac{\mathrm{i}}{a}\tau^2 - \left(\frac{1}{a^2} + \frac{\mathrm{i}}{a^3}\right)\tau^4 + O(\tau^6).$$

If we incorporate the $O(\tau^2)$ term from the expansion of $\lambda_3(\tau)$ into the system

$$z'(\tau) = \frac{A(\tau)}{\tau^3} z(\tau), \tag{23}$$

the discussion is reduced to the scalar equation

$$\hat{\varphi}_3'(\tau) = \frac{1}{\tau}\left(1 + \frac{\mathrm{i}}{a}\right)\hat{\varphi}_3(\tau). \tag{24}$$

This relation represents the leading term of (23) if we assume that $\hat{E}(\tau) := (E^{-1})'(\tau)E(\tau)$ is smooth, where $E(\tau)$ is the transformation matrix such that $A(\tau) = E(\tau)J(\tau)E^{-1}(\tau)$ with $J(\tau) = \mathrm{diag}(\lambda_3(\tau), \lambda_4(\tau))$. Indeed, a computation using MAPLE demonstrates that

$$\begin{aligned}
\hat{E}_{1,1}(\tau) &\sim 2\frac{a^2 d + \mathrm{i}ad - 3a^2 - 4\mathrm{i}a + 1}{a^4}\tau^3 + O(\tau^5) \\
&= \frac{2 - 2\mathrm{i}a}{a^4}\tau^3 + O(\tau^5), \\
\hat{E}_{1,2}(\tau) &\sim -\frac{2}{\tau} - 2\frac{-4\mathrm{i}a + \mathrm{i}ad + 2}{a^2}\tau + O(\tau^3) \\
&= -\frac{2}{\tau} - \frac{4 - 2\mathrm{i}a}{a^2}, \\
\hat{E}_{2,1}(\tau) &\sim -2\frac{a^2 d + \mathrm{i}ad - 3a^2 - 4\mathrm{i}a + 1}{a^4}\tau^3 + O(\tau^5) \\
&= -\frac{2 - 2\mathrm{i}a}{a^4}\tau^3 + O(\tau^5), \\
\hat{E}_{2,2}(\tau) &\sim \frac{2}{\tau} + 2\frac{-4\mathrm{i}a + \mathrm{i}ad + 2}{a^2}\tau + O(\tau^3) \\
&= \frac{2}{\tau} + \frac{4 - 2\mathrm{i}a}{a^2}.
\end{aligned}$$

Equally as (24), the terms $\hat{E}_{1,2}$ and $\hat{E}_{2,2}$ feature a singularity of the first kind. However, since the solution mode associated with φ_4 is eliminated by the boundary conditions, the terms that are relevant for our discussion are smooth.

The general solution of the first order ODE (24) is

$$\hat{\varphi}_3(\tau) = c\tau\, \mathrm{e}^{\mathrm{i}/a \log(\tau)}. \tag{25}$$

This solution satisfies $\hat{\varphi}_3(0) = 0$ and consequently the boundary condition at $\tau = 0$ is satisfied. The constant can be fixed by prescribing a condition $\hat{\varphi}_3(1) = c$.

To conclude this discussion, we note that the fundamental solution $\hat{\varphi}_3$ corresponds to the slowly varying fundamental mode φ_1 from (11). The transplant $\tilde{\varphi}_1(\tau) = 1/\tau\varphi_1'(1/\tau)$ satisfies

$$\tilde{\varphi}_1(\tau) = -\tau\left(1 + \frac{\mathrm{i}}{a}\right)\mathrm{e}^{\mathrm{i}/a\log(\tau)}\,.$$

Thus, we have proven that the singular boundary value problem (18) and (19) is well-posed, the boundary conditions serve to eliminate unphysical solution modes analogously as for (10), and the computation of the solution is essentially reduced to a system of first order equations with a singularity of the first kind.

3 Numerical Solution

Two solution methods are proposed in [5] and [6]. Both work on a truncated interval $[0, \mathcal{T}]$, where the right endpoint $\mathcal{T} \gg 1$ of the integration interval is chosen sufficiently large "adaptively" until convergence of the numerical method is observed. In the first case, a certain minimization procedure is employed. The second algorithm uses collocation for the second order problem on the truncated interval. The code used for this task is COLSYS, see [1]. Suitable initial guesses for a and the profile of $z(t)$ have to be provided to solve the nonlinear problems.

Using the code `sbvp` designed by two of the authors [2], which is intended especially for the solution of singular boundary value problems, we can solve the problem (18), augmented by (16) and the boundary conditions (19).

Since the (transplant of the) mode $\varphi_2(\tau)$ from (12) is eliminated from the general solution, the slowly varying mode decaying for $\tau \to 0$ has to be approximated. Subsequently, we will demonstrate collocation to work satisfactorily, since the solution mode we are interested in is characterized by (24). For the same reason, an error estimate based on defect correction using the backward Euler method as an auxiliary scheme works for this particular problem, even though this estimate is not suitable for boundary value problems with an essential singularity in general [3]. For a singularity of the first kind, collocation methods and the a posteriori error estimate implemented in `sbvp` have been analyzed in [4] and [11].

Even though sbvp equally works for complex problems, we separate the real and imaginary parts of z and solve a system of nine real first order differential equations with the same number of boundary conditions. Otherwise, it is not clear how to realize the relation (8).

In practice, we are faced with some difficulties to compute the collocation solution of (18). A suitable initial approximation for the solution of the associated nonlinear algebraic equations has to be carefully chosen. We obtain this approximation in the following way: setting $a = 0.9$ we solve the initial value problem (17) on the interval $[t_0, t_{\text{end}}] = [10^{-4}, 100]$ using the starting values $z_1(t_0) = 2,\ z_2(t_0) = 0$. The numerical solution is determined using the MATLAB initial value problem solver ode15s and evaluated at N points which correspond to a uniform mesh $\Delta_h = \{i/N : i = 1, \ldots, N\}$ of the transformed problem (18) on $[1/N, 1]$, where the initial points $z_1(0) = 2,\ z_2(0) = 0$ are added to the points determined from the shooting procedure above. The approximation determined from the shooting procedure for (17) is given in Figure 1 together with the initial profile transformed back to the mesh Δ_h for (18). We note that for the starting profile, the rapidly varying solution modes still appear to be present. The computations reported in Figures 1 and 2 use a mesh where $N = 3000$.

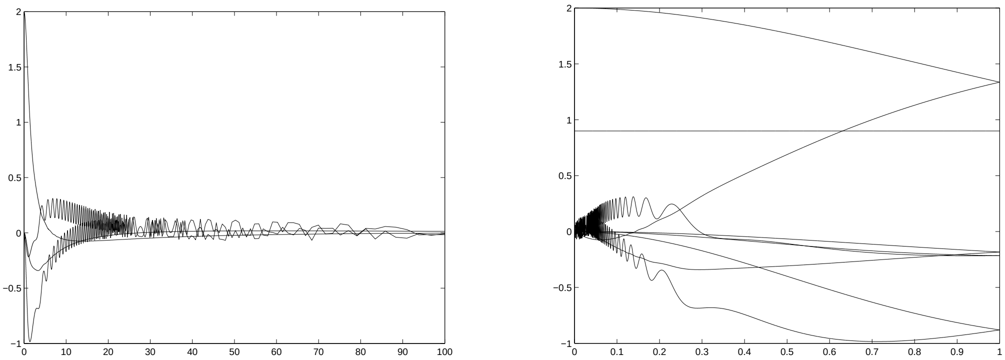

Fig. 1. Initial profile for (17) (left) and resulting initial profile for (18) (right).

Now, using a moderate tolerance $TolX = 5{\cdot}10^{-3}$ for the increment in the Newton iteration, the numerical solution of (18) can be determined successfully. To this end, we used our collocation solver sbvpcol from the package sbvp, see [2], and computed the collocation solution on a fixed mesh. Firstly, we use collocation at one Gaussian point, a method of second order (box scheme). The result is shown in Figure 2, where we give the nine solution components (including a) of (18) and the real and imaginary part of z, transformed back to the interval $[0, 100]$. Note that this solution is also oscillating near $\tau = 0$, albeit not as strongly as the starting profile. Obviously, the rapidly varying mode φ_4 from (22) has been eliminated by the boundary conditions and we observe the asymptotic behavior corresponding to $\hat{\varphi}_3$ from (25)

For this low order method, it is even possible to observe experimentally the

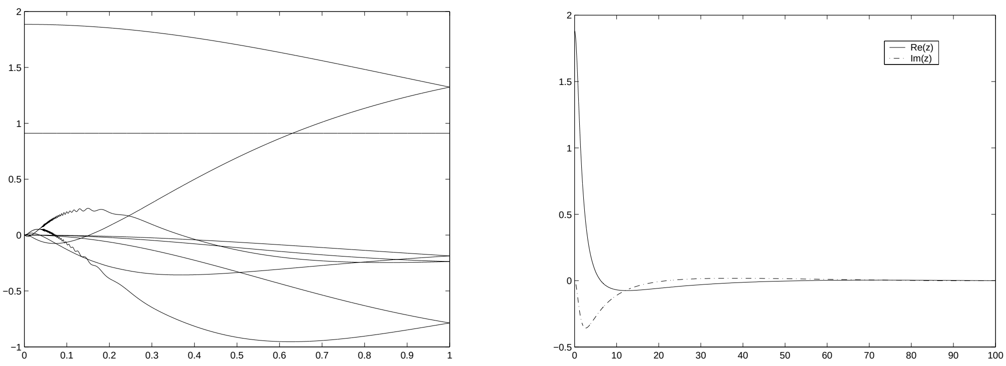

Fig. 2. Solution of (18) (left) and $\Re(z)$ and $\Im(z)$ transformed to $[0, 100]$ (right).

classic convergence order of the global error. In Table 1, we give the empirical convergence order of the numerical solutions computed from the solutions for three consecutive step-sizes h in the discretization, see Table 1.

Table 1
Convergence order for box scheme.

h	err	p
4.0000e−03		
2.0000e−03	3.3750e−02	
1.0000e−03	8.0415e−03	2.07

More interestingly, we also apply the code `sbvp`, equipped with our error estimate and an adaptive mesh selection routine ([2]) based on the same low order method. We use an initial grid with $N = 100$ and the initial profile computed as before. The tolerance for the Newton method is chosen as $TolX = 10^{-2}$, and for the mesh selection we use error tolerances $AbsTol = RelTol = 5 \cdot 10^{-3}$. Mesh adaptation does take place in this setting, the tolerances are satisfied on a grid with $N = 256$ and a ratio of 9.71 between the largest and smallest steps in the final mesh. The solution computed thus is close to those computed previously and is displayed in Figure 3. The oscillations from Figure 2 cannot be observed here because the solution is resolved on a coarser mesh.

Also in Figure 3, we show a plot of the "exact error" of this numerical approximation (with respect to a reference solution computed using a uniform mesh with $N = 1000$) and compare this with the error estimate computed by `sbvp`. The qualitative behavior of the error seems to be captured quite well. The error is underestimated by about a factor of four, however, see Figure 3.

Unfortunately, we did not get quite as favorable results for higher-order collocation methods, see [7]. This may be caused either by the unsmoothness of the solution or by numerical instability.

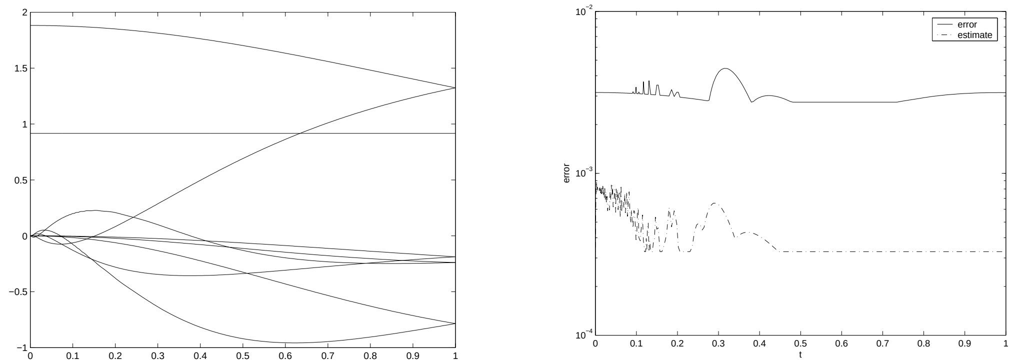

Fig. 3. Solution (left), error and error estimate (right) for (18) computed using `sbvp`.

Conclusions

We have demonstrated a new approach for the computation of the numerical solution of a boundary value problem for an ordinary differential equation which describes self-similar solutions of the classical nonlinear Schrödinger equation. It was shown that a transformation of the original second order problem on an unbounded domain to the interval $[0, 1]$ yields a well-posed singular boundary value problem. Moreover, the solution of this problem is essentially the solution of a BVP with a singularity of the first kind. Hence, the problem can be solved by a (low order) collocation method which shows its classical convergence behavior. Furthermore, an error estimate based on defect correction and using the backward Euler method as an auxiliary scheme, works dependably and enables adaptive mesh refinement in the solution process.

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