From the Nonlinear Schrödinger Equation to Singular BVPs

Chris Budd
Othmar Koch
Ewa Weinmüller

AURORA TR2004-02

Institute for Analysis and Scientific Computing
Vienna University of Technology
Wiedner Hauptstrasse 8-10, A-1040 Wien, Austria

E-Mail:cjb@maths.bath.ac.uk
othmar@fsmat.at
e.weinmueller@tuwien.ac.at

The work described in this report was supported by the Special Research Program SFB F011 "AURORA" of the Austrian Science Fund FWF.

Introduction

We discuss the numerical computation of self-similar blow-up solutions of the classical nonlinear Schrödinger equation. 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 solution is reduced to a nonlinear, ordinary differential equation on an unbounded domain. We discuss the approaches used in the literature and propose new computational methods which might possibly enhance the efficiency of the computations. Particularly, we discuss the possibility to use our MATLAB solver `sbvp` in the solution process, see [3].

Chapter 1

Analytical Results

1.1 The Original PDE

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

$$\mathrm{i}\frac{\partial u}{\partial t} + \Delta u + |u|^2 u = 0, \quad t > 0, \tag{1.1a}$$

$$u(x, 0) = u_0(x), \quad x \in \mathbb{R}^d. \tag{1.1b}$$

In the well-studied case $d = 1$, the equation is integrable and a solution exists globally. For $d \geq 2$, (1.1) 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 there is a growing and increasingly narrow peak. 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 usually interested in the case $d = 3$. In this case, it is conjectured that the solutions blow up in a self-similar way [7]. We will derive ordinary differential equations which determine the shape of the solution near the blow-up time in the next section. To derive boundary conditions for these ODEs, we note that (1.1) 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

$$M = \int_{\mathbb{R}^3} |u(x,t)|^2 \, dx, \tag{1.2}$$

$$H = \int_{\mathbb{R}^3} \left(|\nabla_x u(x,t)|^2 - \frac{1}{2}|u(x,t)|^4 \right) dx. \tag{1.3}$$

Usually, we will restrict ourselves to the computation of radially symmetric solutions.

1.2 The Associated ODE

The nonlinear Schrödinger equation (1.1) is invariant under four symmetry groups: Translation in time or space, a particular scaling transformation and shift in phase. More precisely, the following changes of variable leave (1.1a) invariant for all $\lambda > 0$:

1. $t \to t + \lambda$,
2. $x \to x + \lambda$,
3. $t \to \lambda t,\ x \to \sqrt{\lambda} x,\ u \to \frac{1}{\sqrt{\lambda}} u$,
4. $u \to \mathrm{e}^{\mathrm{i}\lambda} u$.

This does not mean, however, that all the solutions of (1.1) are invariant under the same transformations. Disregarding the first two trivial invariance groups, we are interested in the computation of solutions which are invariant under the two latter transformations. 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 (1.2) and (1.3). Moreover, we restrict ourselves to radially symmetrix solutions. 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

$$u(x,t) = \frac{1}{\sqrt{2a(T-t)}} \mathrm{e}^{-\mathrm{i}/2a \log(T-t)} z \left(\frac{r}{\sqrt{2a(T-t)}} \right). \tag{1.4}$$

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 (1.4) into (1.1a) now yields an ODE for z. With the change of variable

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

this results in

$$z''(\tau) + \frac{d-1}{\tau} z'(\tau) - z(\tau) + \mathrm{i}a(\tau z(\tau))' + |z(\tau)|^2 z(\tau) = 0, \quad \tau > 0. \tag{1.5}$$

We now derive the boundary conditions for (1.5) which yield a well-posed problem for the computation of z and a with a physically meaningful solution. First, due to symmetry we require

$$z'(0) = 0. \tag{1.6}$$

Moreover, since the phase of z is arbitrary according to the ansatz (1.4),

$$\Im(z(0)) = 0. \tag{1.7}$$

Furthermore, we are interested in solutions u of (1.1a) which decay for $x \to \infty$ [6], [7],

$$z(\infty) = 0. \tag{1.8}$$

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 system

$$z''(\tau) + \frac{d-1}{\tau} z'(\tau) - z(\tau) + \mathrm{i}a(\tau z(\tau))' = 0, \quad \tau > 0. \tag{1.9}$$

The fundamental solution modes of this problem are asymptotic to

$$\begin{aligned} \varphi_1(\tau) &= \frac{1}{\tau} \mathrm{e}^{-\mathrm{i}/a \log(\tau)}, && (1.10) \\ \varphi_2(\tau) &= \frac{1}{\tau^{d-1}} \mathrm{e}^{-\mathrm{i}a\tau^2/2 + \mathrm{i}/a \log(\tau)} \\ &= \frac{1}{\tau^2} \mathrm{e}^{-\mathrm{i}a\tau^2/2 + \mathrm{i}/a \log(\tau)} && (1.11) \end{aligned}$$

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

Subsequently, we refer to solutions of (1.1a) corresponding to φ_1 as *slowly varying*, while those solutions associated with φ_2 are denoted as *rapidly varying*. This reflects the frequency of the oscillations of these fundamental modes for large τ.

Naturally, we are only interested in solutions of (1.9) such that for the associated solution of (1.1) H from (1.3) is finite. This condition translates to

$$H(z) = \int_0^\infty \left(|z'(\tau)|^2 - \frac{1}{2} |z(\tau)|^4 \right) \tau^{d-1} \, d\tau = 0. \tag{1.12}$$

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 (1.1) associated with φ_2. Consequently, the boundary conditions must be posed such as to eliminate contributions from φ_2 from the general solution of (1.9). It turns out that (1.12) is equivalent to the algebraic relation

$$\lim_{\tau \to \infty} \left| \tau z'(\tau) + \left(1 + \frac{\mathrm{i}}{a}\right) z(\tau) \right| = 0, \tag{1.13}$$

see [7]. This relation is indeed satisfied by φ_1, while this condition is violated by φ_2.

Finally, we note that (1.13) can be rewritten, taking into account (1.8). Conditions (1.8) and (1.13) can be summed up as

$$\lim_{\tau\to\infty} \tau z'(\tau) = 0. \tag{1.14}$$

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 $\tau \to \infty$. Consequently, the asymptotic boundary condition (1.14) singles out the slowly varying fundamental mode present in (1.9) and eliminates the rapidly varying mode, as desired.

The boundary value problem that we need to solve for the computation of the self-similar blow-up solution profile is

$$z''(\tau) + \frac{d-1}{\tau} z'(\tau) - z(\tau) + \mathrm{i}a(\tau z(\tau))' + |z(\tau)|^2 z(\tau) = 0, \quad \tau > 0, \tag{1.15a}$$
$$z'(0) = 0,\ \Im z(0) = 0,\ \lim_{\tau\to\infty} \tau z'(\tau) = 0. \tag{1.15b}$$

If we treat the real and imaginary parts of (1.15) separately, we thus need to compute the solutions of two second order differential equations and one real parameter, using five boundary conditions (1.15b). If we augment the system by the trivial equation

$$a'(\tau) = 0, \tag{1.16}$$

we obtain a well-posed boundary value problem for a system of real ordinary differential equations.

1.3 Transformed ODE

Using the Euler transformation $z \to (z, \tau z') = (z_1, z_2)$ for (1.15a), we derive the equivalent first-order equation

$$z'(\tau) = \frac{M(\tau)}{\tau} z(\tau) + f(\tau, z(\tau)), \tag{1.17}$$

where

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

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

$$z'(\tau) = \begin{pmatrix} \frac{M(\tau)}{\tau} & 0 \\ 0 & \frac{A(\tau)}{\tau^3} \end{pmatrix} z(\tau) + \begin{pmatrix} f(\tau, z_1, z_2) \\ g(\tau, z_3, z_4) \end{pmatrix}, \tag{1.18}$$

where

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

In the new variables, the boundary conditions translate to

$$z_2(0) = 0, \ \Im z_1(0) = 0, \ z_1(1) = z_3(1), \ z_2(1) = z_4(1), \ z_4(0) = 0. \tag{1.19}$$

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 (1.18), see for example [9], [10]. With a similar argument as in Section 1.2, it is sufficient to discuss the linear version of (1.18) where the nonlinear part is neglected, see also [9], [10]. The admissible boundary conditions for the resulting system

$$z'(\tau) = \begin{pmatrix} \frac{M(\tau)}{\tau} & 0 \\ 0 & \frac{A(\tau)}{\tau^3} \end{pmatrix} z(\tau) \tag{1.20}$$

are the same as for (1.18).

The eigenvalues of $M(0)$ are $\lambda_1 = 0$ and $\lambda_2 = 2 - d = -1$. 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 either at the point $\tau = 0$ 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 $\lambda_4 = \mathrm{i}a$. Consider the fundamental solution modes of (1.20) associated with these eigenvalues:

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

$$z'(\tau) = \frac{A(0)}{\tau^3} z(\tau) \tag{1.21}$$

are

$$\phi_3(\tau) = 1, \quad \phi_4(\tau) = \mathrm{e}^{-\mathrm{i}a/(2\tau^2)}.$$

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 (1.11) 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 as $\tau \to 0$ 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 (1.21) 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

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

If we incorporate an additional term from the expansion of $\lambda_3(\tau)$ into the system

$$z'(\tau) = \frac{A(\tau)}{\tau^3}z(\tau), \tag{1.22}$$

the discussion is reduced to the scalar equation

$$\hat{\phi}_3'(\tau) = \frac{1}{\tau}\left(1 + \frac{\mathrm{i}}{a}\right)\hat{\phi}_3(\tau). \tag{1.23}$$

This relation represents the leading term of (1.22) 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

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

Equally as (1.23), 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 (1.23) is

$$\hat{\phi}_3(\tau) = c\tau \mathrm{e}^{\mathrm{i}/a \log(\tau)}.$$

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

To conclude this discussion, we note that the fundamental solution $\hat{\phi}_3$ corresponds to the slowly varying fundamental mode φ_1 from (1.10). The transplant $\tilde{\varphi}_1(\tau) = 1/\tau\varphi_1'(1/\tau)$ satisfies

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

Chapter 2

Numerical Treatment

Two solution methods are proposed in [7] and [6]. Both work on a truncated interval (where the right endpoint 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 our code `sbvp`, we can solve the problem (1.18), augmented by (1.16) and the boundary conditions (1.19). Alternatively to $z_4(0) = 0$ we could also use the original condition (1.13) in the form

$$z_4(0) + \left(1 + \frac{\mathrm{i}}{a}\right) z_3(0) = 0.$$

Since the (transplant of the) mode $\varphi_2(\tau)$ from (1.11) is eliminated from the general solution, the slowly varying mode decaying for $\tau \to 0$ has to be approximated. This should be feasible on a graded mesh (where step sizes are halved as $\tau \to 0$), if mesh adaptation implemented in `sbvp` [3] should fail. For error estimation, mesh halving should be suitable [2]. We expect collocation to work satisfactorily, since the solution mode we are interested in is characterized by (1.23), which features a singularity of the first kind. For this problem class, collocation methods have been analyzed in [4] and [11]. For the same reason, it is possible that 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.

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 (1.7).

In practice, we are faced with some difficulties to compute the collocation solution of (1.18). 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 (1.17) on the interval $[t_0, t_{\mathrm{end}}] = [10^{-4}, 100]$ 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`. The numerical solution is evaluated at N points which correspond to a uniform mesh $\Delta_h = \{i/N : i = 1, \ldots, N\}$ of the transformed problem (1.18) 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 (1.17) is given in Figure 2.1. The computations reported in Figures 2.1– 2.5 use a mesh where $N = 3000$.

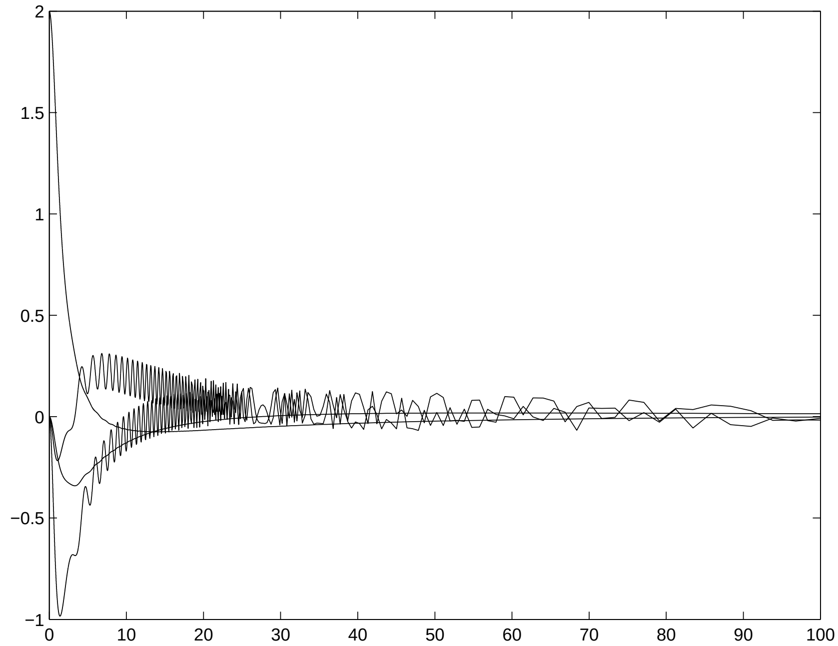

Figure 2.1: Initial profile for (1.17) computed by shooting.

The initial profile transformed back to the mesh Δ_h for (1.18) is given in Figure 2.2.

Using a moderate tolerance $TolX = 5 \cdot 10^{-3}$ for the increment in the Newton iteration, the numerical solution of (1.18) can now be determined successfully. To this end, we used our collocation solver `sbvpcol` from the package `sbvp`, see [3], which computes the collocation solution on a fixed mesh. Firstly, we use collocation at one Gaussian point, a method of second order. The result is shown in Figure 2.3.

Using this numerical solution, we can refine our shooting procedure for the initial profile by setting $z_1(t_0) = 1.88$. The result is given in Figure 2.4.

We note that this refined starting approximation oscillates less strongly than the profile given in Figure 2.2. Obviously, this initial profile resembles the solution of the boundary value problem (1.18) more closely, since the initial value for z_1 is chosen more realistically. Using this refined initial profile, we again obtain

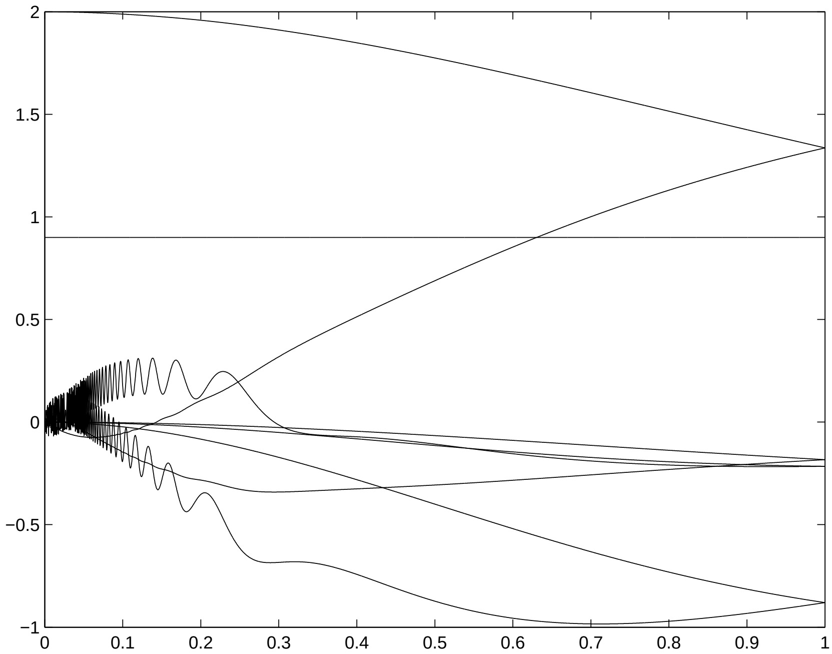

Figure 2.2: Initial profile for (1.18).

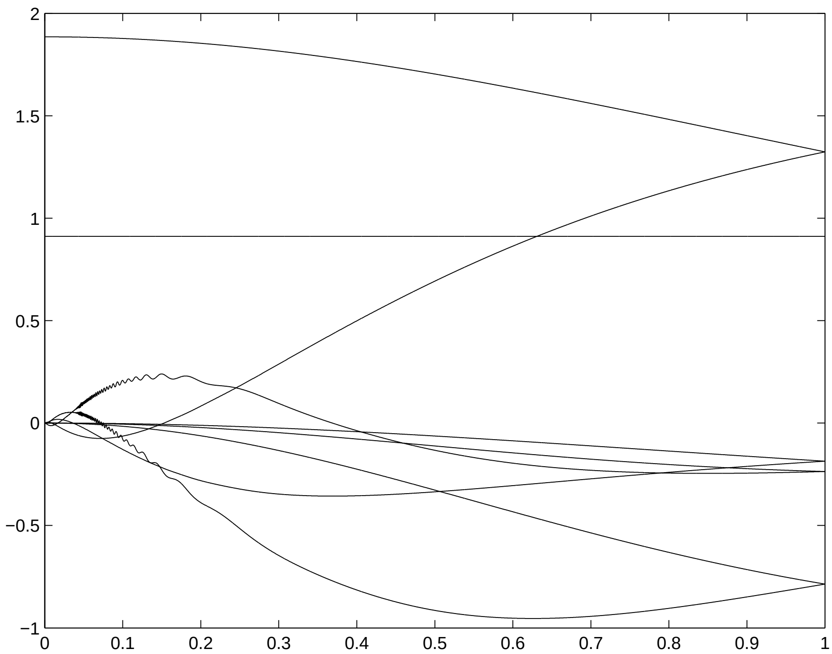

Figure 2.3: Solution of (1.18).

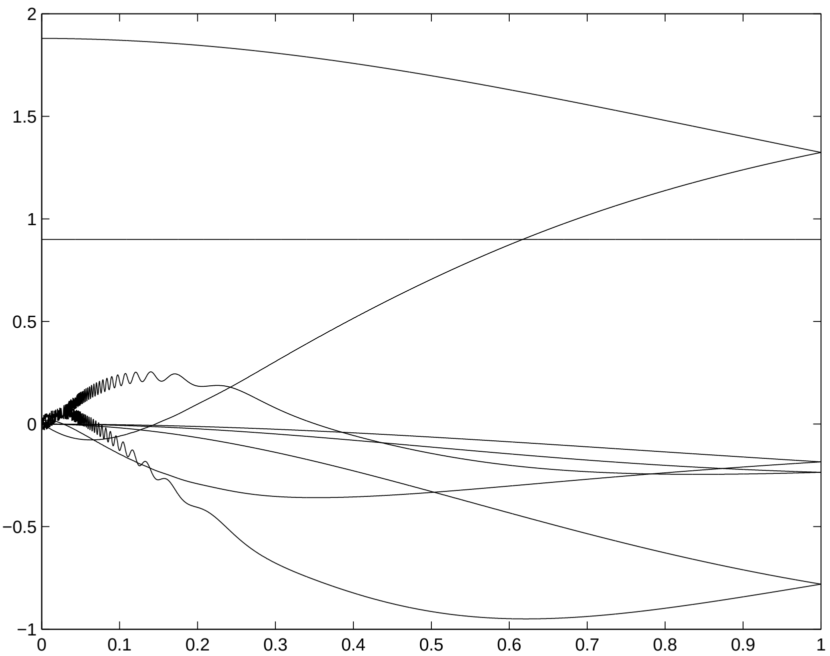

Figure 2.4: Refined initial profile for (1.18).

a numerical solution from our collocation solver which resembles the result in Figure 2.3, see Figure 2.5.

So far, we have used a low order collocation method (Gaussian collocation at one point, which is equivalent to the box scheme) on a very fine grid ($N = 3000$) in order to resolve the oscillations of the solution with small amplitude. We can obtain a similar accuracy by using higher order collocation at a coarser grid. In that case, however, only the envelope of the oscillations seems to be resolved by the numerical solution. In Figure 2.6 we give the result of Gaussian collocation at four points on a mesh with $N = 500$ to illustrate this observation.

In the same setting, we also tried our full code `sbvp` which incorporates error estimation based on defect correction using the backward Euler method as an auxiliary scheme, and mesh adaptation, see [3]. It was demonstrated in [5] that the error estimate in the release version is not suitable for problems with an essential singularity in general. Due to the fact that the solution modes that are actually present in the solution we want to resolve are associated with problems featuring a singularity of the first kind, however, our error estimate appears to work acceptably for (1.18). Indeed, in the same setting as for Figure 2.6 with moderate error tolerances, the solution on the uniform initial grid with $N = 500$ is accepted (and coincides with Figure 2.6, of course).

More interestingly, we also tried `sbvp` with a low order method ($m = 1$ Gaussian points, which corresponds to the box scheme), and using an initial grid with

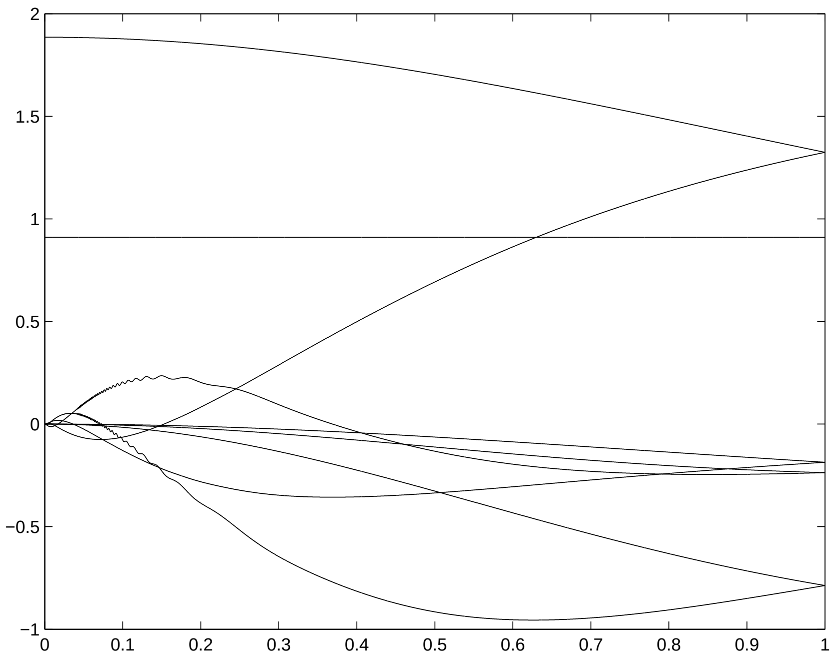

Figure 2.5: Solution of (1.18) using refined initial profile.

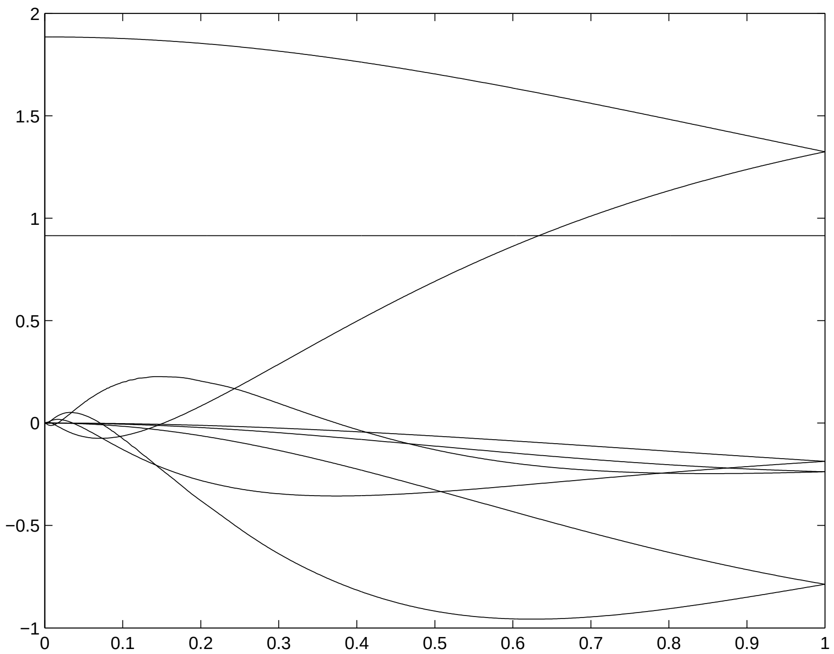

Figure 2.6: Solution of (1.18) computed by high order collocation.

$N = 100$ and the initial profile computed for $z_1(t_0) = 2$. The tolerance for the Newton method was chosen as $TolX = 10^{-2}$, and for the mesh selection we used error tolerances $AbsTol = RelTol = 5 \cdot 10^{-3}$. Mesh adaptation did take place in this setting, the tolerances were 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 2.7.

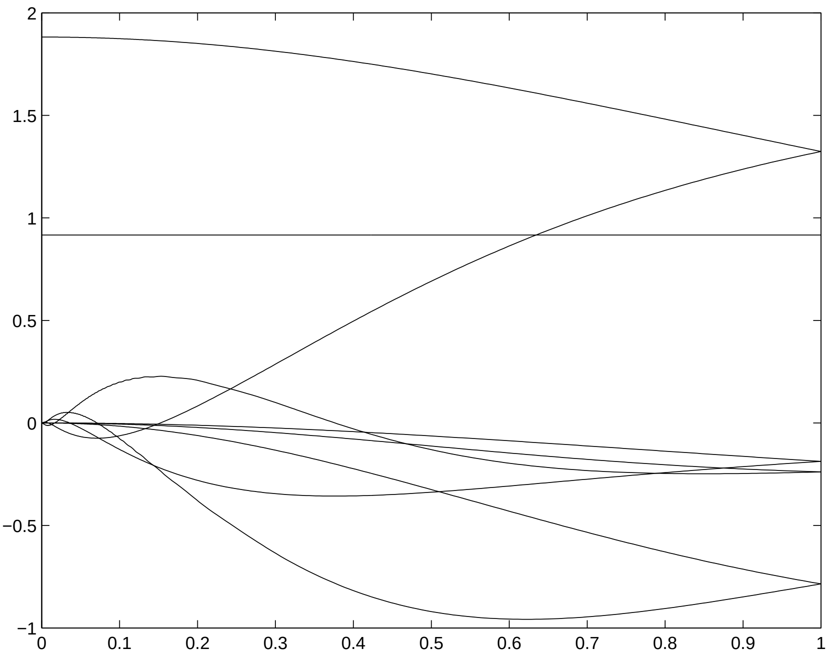

Figure 2.7: Solution of (1.18) computed using `sbvp`.

In Figure 2.8, 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, unfortunately the error is underestimated by about a factor of four, see Figure 2.8.

For this low order method, it is even possible to observe experimentally the classic convergence order of the global error. In Table 2.1, we give the empirical convergence order the numerical solutions computed as follows:

For a uniform time grid with step-size h_i, denote the numerical solution by ξ_i. If z is the exact solution and ξ_{i+1} and ξ_{i+2} denote the numerical approximations on

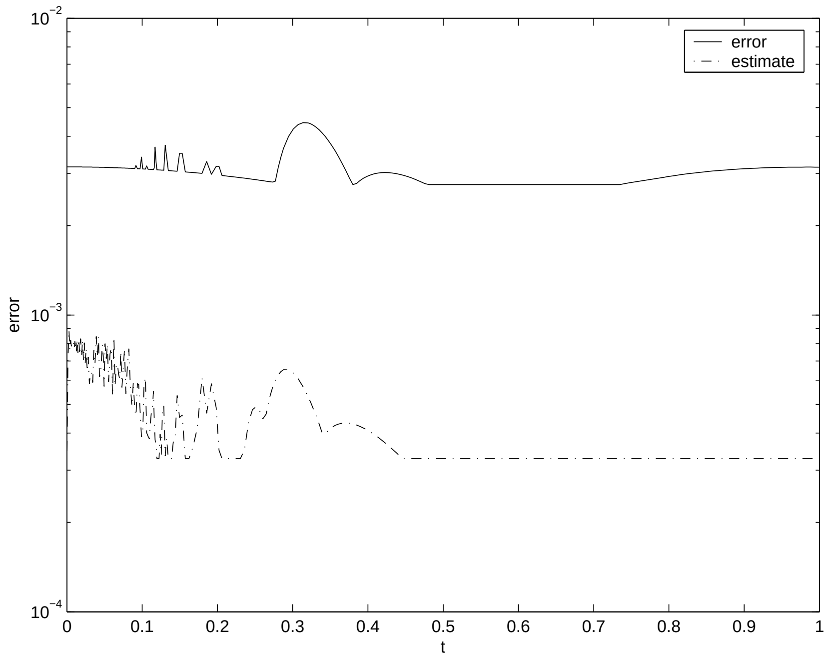

Figure 2.8: Global error and error estimate for (1.18).

grids with step-sizes $h_i/2$ and $h_i/4$, respectively, we assume

$$\begin{aligned} \xi_i - z &\approx Ch_i^p, \\ \xi_{i+1} - z &\approx Ch_i^p \frac{1}{2^p}, \\ \xi_{i+2} - z &\approx Ch_i^p \frac{1}{4^p}, \end{aligned}$$

with some integer p. This implies

$$\begin{aligned} \xi_i - \xi_{i+1} &= Ch_i^p(1 - \frac{1}{2^p}), \\ \xi_{i+1} - \xi_{i+2} &= Ch_i^p(1 - \frac{1}{2^p})\frac{1}{2^p}. \end{aligned}$$

Consequently, the order p can be estimated empirically as

$$p \approx \frac{\ln\left(\frac{||\xi_i - \xi_{i+1}||}{||\xi_{i+1} - \xi_{i+2}||}\right)}{\ln(2)},$$

where $||\cdot||$ denotes the maximum norm on the space of grid vectors.

Table 2.1 gives, for each equidistant step-size h_{i+1}, the quantities $||\xi_i - \xi_{i+1}||$ (denoted by err) (naturally the first row has no entry) and the empirical convergence order computed as explained above from the values of three consecutive numerical approximations. These are computed using `sbvpcol`, where the starting approximation for Newton's method is computed from an initial value problem with $z(0) = 2$.

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

Table 2.1: Convergence order for $m = 1$ Gaussian point.

If alternatively we use four equidistant collocation points, we do not observe the classical convergence order, see Table 2.2. There are a few possible reasons for this behavior. The fine spacing between the collocation points might introduce large roundoff errors which govern the error and do not admit to observe the regular behavior of the discretization error. Secondly, Newton's method does not compute the solution of the algebraic equations with very high precision and these errors possibly dominate the discretization error. Finally, it is possible that the exact solution of (1.5) is unsmooth and does not permit high convergence order of discretization schemes.

h_i	err	p
6.6667e−03		
3.3333e−03	6.0840e−02	
1.6667e−03	2.3271e−02	1.39

Table 2.2: Convergence order for $m = 4$ equidistant collocation points.

References

[1] U. Ascher, J. Christiansen, R. D. Russell: *Collocation Software for Boundary Value ODEs*. ACM Transactions on Mathematical Software 7 (1981)(2), pp. 209–222.

[2] W. Auzinger, E. Karner, O. Koch, E. Weinmüller: *Globale Fehlerschätzer für Randwertprobleme mit einer Singularität zweiter Art*. Techn. Rep., in preparation.

[3] W. Auzinger, G. Kneisl, O. Koch, E. Weinmüller: *A Collocation Code for Boundary Value Problems in Ordinary Differential Equations*. Numer. Algorithms 33 (2003), pp. 27–39.

[4] W. Auzinger, O. Koch, E. Weinmüller: *Analysis of a New Error Estimate for Collocation Methods Applied to Singular Boundary Value Problems*. Submitted to SIAM J. Numer. Anal.

[5] W. Auzinger, O. Koch, E. Weinmüller: *Collocation Methods for Boundary Value Problems with an Essential Singularity*. To appear in Springer LNCS.

[6] C. J. Budd: *Asymptotics of multibump blow-up self-similar solutions of the nonlinear Schrödinger equation*. SIAM J. Appl. Math. 62 (2001)(3), pp. 801–830.

[7] C. J. Budd, S. Chen, R. D. Russell: *New Self-Similar Solutions of the Nonlinear Schrödinger Equation with Moving Mesh Computations*. J. Comput. Phys. 152 (1999), pp. 756–789.

[8] A. Hasegawa: *Optical Solitons in Fibers*. Springer Verlag, Berlin, 1989.

[9] F. R. d. Hoog, R. Weiss: *Difference Methods for Boundary Value Problems with a Singularity of the First Kind*. SIAM J. Numer. Anal. 13 (1976), pp. 775–813.

[10] F. R. d. Hoog, R. Weiss: *On the Boundary Value Problem for Systems of Ordinary Differential Equations with a Singularity of the Second Kind*. SIAM J. Math. Anal. 11 (1980), pp. 41–60.

[11] O. Koch: *Asymptotically Correct Error Estimation for Collocation Methods Applied to Singular Boundary Value Problems*, 2003. In preparation.

[12] V. E. Zakharov: *Handbook of Plasma Physics*, Vol. 2. Elsevier, New York, 1984.