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SCHRÖDINGER EQUATION**

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NUMERICAL APPROXIMATION OF SINGULAR SOLUTIONS OF THE DAMPED NONLINEAR SCHRÖDINGER EQUATION

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1 Introduction

The initial value problem for the Nonlinear Schrödinger equation with cubic nonlinearity (NLS), i.e. the problem of determining a complex-valued function $u = u(x, t)$, $x \in \mathbb{R}^d$, $t \geq 0$, such that

$$u_t = i\Delta u + i|u|^2u, \quad x \in \mathbb{R}^d, \quad t \geq 0, \quad u(x, 0) = u_0(x), \quad x \in \mathbb{R}^d, \quad (1.1)$$

where $1 \leq d \leq 3$ and u_0 is given, occurs frequently in Mathematical Physics, e.g. in the theory of water waves for $d = 1$, in nonlinear optics for $d = 2$, and in plasma waves for $d = 3$. For $d = 1$ (1.1) is globally well-posed. If, however, d is greater or equal to the critical value 2, it is generally only locally well-posed, [2], [4], and possesses singular solutions that blow up in L^∞ in finite time; cf. Ch. 7 of [2] and its references.

The details of this blow-up have been intensely studied in the last twenty years or so, by analytic, asymptotic, and numerical means. Many advances have been made by Zakharov and his co-workers, cf., e.g., [5], and by a group including Papanicolaou, C. Sulem, P.L. Sulem, and their collaborators, cf., e.g., [7], [6]. As a result of the work of these groups (especially of their asymptotic and numerical computations by means of change-of-variables, or 'dynamic rescaling' techniques), detailed characteristics of the blow-up of radially symmetric solutions of (1.1) are by now well understood. As an alternative to dynamic rescaling and asymptotic techniques, one could try to approximate singular solutions of the NLS by direct numerical integration of the p.d.e.. In [1] we tracked the blow-up of radial solutions of (1.1) for $d = 3$ and 2 using

a simple fully discrete Galerkin finite element method, equipped with suitable adaptive spatial and temporal mesh refinement mechanisms. In Section 2 below we briefly describe the numerical technique and the main results of [1].

A natural question in blow-up problems is whether the development of singularities can be prevented by the addition of dissipative terms in the equation. In Section 3 we test numerically the stability of the blow-up of radial singular solutions of the NLS for $d = 3$ and 2, when the damping term $-\delta u$ (δ small and positive) is added to the right-hand side of the p.d.e. in (1.1). We conclude that damping of a small size does not prevent the formation of singularities, even in the critical case, thus verifying and complementing the theory of M. Tsutsumi, [9], which is valid for $d = 3$. We also present numerical results on the decay of solutions, for large values of δ , as t grows.

2 Numerical approximation of blow-up

Let $r = (x_1^2 + \dots + x_d^2)^{\frac{1}{2}}$. For $d = 3$ and 2 we shall approximate radially symmetric solutions $u = u(r, t)$ of (1.1) that blow up at $r = 0$ as $t \uparrow t^*$ while decaying exponentially for all $t \geq 0$ as $r \rightarrow \infty$. For this purpose we shall solve numerically the NLS on a finite interval $0 \leq r \leq R$, with R large enough, assuming $u(R, t) = 0$. To normalize matters we scale the radial variable $r \leftarrow r/R$, and thus consider the problem

$$u_t = i\varepsilon(u_{rr} + \frac{d-1}{r}u_r) + i|u|^2u, \quad 0 < r \leq 1, \quad t \geq 0, \quad (2.1)$$

$$u_r(0, t) = 0, \quad u(1, t) = 0, \quad t \geq 0, \quad (2.2)$$

$$u(r, 0) = v(r) := u_0(rR), \quad 0 \leq r \leq 1, \quad (2.3)$$

where $\varepsilon = 1/R^2$. If v is sufficiently smooth, this problem has a unique smooth solution u , at least in a finite temporal interval, where u conserves its L^2 norm and the Hamiltonian, i.e. where

$$\|u(t)\|^2 = \int_0^1 |u(r, t)|^2 r^{d-1} dr = \|v\|^2, \quad (2.4)$$

$$H(u(t)) := \int_0^1 (\varepsilon |u_r(r, t)|^2 - \frac{1}{2} |u(r, t)|^4) r^{d-1} dr = H(v). \quad (2.5)$$

If $H(v) < 0$, u blows up in L^∞ in finite time.

To approximate (2.1)–(2.3) we use a simple fully discrete finite element scheme. Let S_h denote the continuous, complex-valued functions on $[0, 1]$ that vanish at $r = 1$ and are piecewise linear relative to the arbitrary partition

$0 = r_0 < r_1 < \dots < r_J = 1$, where $h := \max_j(r_{j+1} - r_j)$. Then, given a constant —for the time being— time step k , we compute, for $n = 0, 1, 2, \dots$, functions $U^n \in S_h$ that approximate the solution of (2.1)–(2.3) at $t^n = nk$ and satisfy for all $\chi \in S_h$, with $v^{n+\frac{1}{2}} := (v^n + v^{n+1})/2$,

$$(U^{n+1} - U^n, \chi) + ik\varepsilon(U_r^{n+\frac{1}{2}}, \chi_r) = ik(|U^{n+\frac{1}{2}}|^2 U^{n+\frac{1}{2}}, \chi), \quad (2.6)$$

where $(\varphi, \chi) := \int_0^1 \varphi(r)\overline{\chi}(r)r^{d-1}dr$, and U^0 is taken as the L^2 projection of v on S_h . It may be shown that (2.6) yields L^2 -norm conserving approximations U^n , which, if u is smooth, are accurate to $O(k^2 + h^2)$ in L^2 . A simple explicit-implicit iterative scheme is used for solving the nonlinear system in (2.6) for each n , and yields accurate and stable approximations to the solution of (2.1)–(2.3). For details and error estimates, cf. [1] and its references.

Anticipating that u blows up at $r = 0$ we implemented this scheme in an adaptive code using spatial and temporal meshes that can change with n . As $t \uparrow t^*$ the spatial mesh is refined drastically in the vicinity of $r = 0$ by halving the meshlength in a variable length interval $I_0 = [0, b]$ that always contains 200 meshpoints. The meshlength is gradually increased as r increases. The spatial mesh is refined depending on a local $L^\infty - L^2$ inverse inequality that allows the solution to grow in L^∞ on I_0 . The time step is halved at some t^n , when a suitably scaled version of the invariant H changes too much between t^n and t^{n+1} . For details of this refinement scheme we refer to [1]; therein we computed rates of blow-up of the amplitude and the phase of u at $r = 0$, and of several norms of u as $t \uparrow t^*$ for various examples for $d = 3$ and 2. In the rest of this section we shall report our results for two examples from [1] to give the reader some idea about the quality of the data and set the stage for the computations of Section 3.

In the three-dimensional case, it is shown in [7] and [5] that radial solutions of (1.1) emanating from various types of initial profiles evolve into self-similar solutions that blow up as $t \uparrow t^*$ as $u(r, t) \sim \frac{1}{(t^* - t)^{\frac{1}{2}}} Q\left(\frac{\sqrt{\kappa}r}{(t^* - t)^{\frac{1}{2}}}\right) e^{i\kappa \ln \frac{1}{t^* - t}}$, where $Q : (0, \infty) \rightarrow \mathbb{C}$ is a bounded, smooth function and $\kappa \approx 0.545$. To test the direct code we computed with initial profile

$$v(r) = 6\sqrt{2}e^{-25r^2}, \quad 0 \leq r \leq 1, \quad (2.7)$$

($R = 5$) for which $H(v) \approx -0.878$ (Test problem ‘G3’). We took initially $h = 10^{-3}$, $k = 10^{-4}$. By the final ‘blow-up’ time $t^* \approx 0.03429946$ the amplitude at $r = 0$ had risen to about $.661 \times 10^{12}$, the code having refined in space 35 times with last time step about $.847 \times 10^{-25}$. In the first four columns of Table 1 we record, at the times t^{n_i} of the i^{th} spatial refinement, the computed rates ρ_i

Table 1: Blow-up rates. Test problem G3.

i	L^3	L^∞	L_D^2	L_D^∞	κ
10	.12385	.50041	.24827	1.00052	.54528
15	.12495	.49996	.24992	.99956	.54518
20	.12500	.50019	.25000	.99962	.54496
25	.12500	.49965	.25000	1.00067	.54509
27	.12498	.49994	.24999	.99937	.54485

Table 2: Blow-up rates. Test problem G2.

i	L^3	L^4	L^∞	L_D^2	L_D^∞
16	.16677	.25047	.50133	.50093	1.00303
18	.16671	.25029	.50090	.50059	1.00173
20	.16667	.25023	.50060	.50036	1.00161
22	.16664	.25010	.50039	.50021	1.00144
24	.16662	.25005	.50026	.50009	1.00078
26	.16660	.24993	.50013	.49999	1.00032
28	.16651	.24986	.49982	.49971	.99977

of blow-up of various functionals of the solution which are assumed to behave like $(t^* - t)^{-\rho}$ as $t \uparrow t^*$. Specifically, we show the blow-up rates of the L^4 and L^∞ norms of u and of the L^2 and L^∞ norms of u_r (columns L_D^2, L_D^∞). The last column contains the computed values of the phase constant κ at t^{n_i} .

We observe that the blow-up rates stabilize quite early in the computation and are very good approximations to the expected values $1/8, 1/2, 1/4$ and 1 . In particular, the blow-up rate $\rho = 1/2$ for the amplitude and the phase constant $\kappa \approx 0.545$ are recovered clearly.

In the harder to approximate critical case $d = 2$, computing again with the same initial value (2.7), for which now $H(v) \approx -11.52$ (Test problem ‘G2’), taking initially $h = 1/1600$, $k = 0.8 \times 10^{-4}$, we observed that the code performed 34 spatial mesh refinements before stopping at a final, ‘blow-up’ time $t^* \approx 0.04208980$ reaching an amplitude at $r = 0$ of about $.258 \times 10^{12}$ with last temporal step equal to 0.108×10^{-23} . The data of this run produced the blow-up rates of Table 2, which should be interpreted as follows: In the two-dimensional case, it is well known, [6], [5], that the amplitude at $r = 0$ behaves basically like $(t^* - t)^{-\frac{1}{2}}$ but is perturbed by a factor that tends slowly to infinity as $t \uparrow t^*$. As t gets extremely close to t^* , it is by now well known that the rate is $(\ln \ln \frac{1}{t^* - t} / (t^* - t))^{\frac{1}{2}}$, [6]. In [1] we verified this result assuming that various functionals of the solution behave like $[F(t^* - t)/(t^* - t)]^{1/2}$ as $t \uparrow t^*$, and comparing the data produced by the code for several choices of F proposed in the literature. We found that with $F(s) = \ln \ln 1/s$ the rates for

Table 3: Blow-up rates. Test problem G3, $\delta = 2$.

i	L^3	L^∞	L_D^2	L_D^∞	κ
16	.12488	.49943	.24975	.99990	.54369
18	.12516	.50095	.25032	1.00255	.54459
20	.12486	.49940	.24977	.99984	.54383
22	.12494	.49993	.24990	1.00049	.54482
24	.12518	.50070	.25027	1.00182	.54332
26	.12481	.50005	.24979	1.00089	.54308
28	.12513	.50087	.25028	1.00289	.54452
30	.12500	.50003	.25002	1.00085	.54526

the amplitude at $r = 0$ (i.e. the L^∞ norm of u) stabilize closer to $1/2$ than with any other law that we tried. In Table 2 we list the values of ρ that we obtained for the L^3 , L^4 and L^∞ norms of u and the L^2 and L^∞ norms of u_r at the i^{th} spatial mesh refinement instance. Not shown here are the computations of the rate of blow-up of the phase at $r = 0$, which are much more delicate in $d = 2$, cf. [1].

3 The effect of dissipation

We consider the damped analog of (1.1) given by

$$u_t = i\Delta u + i|u|^2 u - \delta u, \quad (3.1)$$

where $\delta > 0$ is constant, in $d = 3$ and 2 dimensions. It is known, cf., e.g., [4], that the Cauchy problem of (3.1) has, at least, a unique local solution; its L^2 norm decreases exponentially with t . In addition, H now varies with t and might change sign. It is of interest then to ask, for example, whether initial data with $H < 0$ can lead to a globally well-posed problem. If δ is sufficiently small, the answer seems to be negative. On the other hand, if δ is large enough, solutions exist globally and decay as $t \rightarrow \infty$.

As in Section 2, we shall compute, with an analogous numerical method to the one outlined therein, solutions of the radial p.d.e.

$$u_t = i\varepsilon(u_{rr} + \frac{d-1}{r}u_r) + i|u|^2 u - \delta u, \quad 0 < r \leq 1, \quad t \geq 0, \quad (3.2)$$

supplemented by the boundary and initial conditions (2.2) and (2.3). Note that, for temporal intervals for which a, say, H^1 solution of (3.2) exists, the L^2 norm of u decays exponentially with t , i.e. that $\|u(t)\| = e^{-\delta t}\|v\|$, while the Hamiltonian $H(t) = H(u(t))$ (given by (2.5)) is no longer constant but satisfies the equation $\frac{dH}{dt} + 2\delta H = \delta\|u(t)\|_{L^4}^4$, $t \geq 0$.

For $d = 3$ the Cauchy problem for (3.1) with suitable $u_0 \in H^1$ has been studied by M. Tsutsumi, [9], who proves that if $\int_{\mathbb{R}^3} (|\nabla u_0|^2 - \frac{1}{2}|u_0|^4) dx \leq 0$, and $\text{Im} \int_{\mathbb{R}^3} x \cdot \nabla u_0 \bar{u}_0 dx > 0$, then, if δ is small enough, u blows up in L^∞ as $t \uparrow t^*$, for some $t^* = t^*(u_0) < \infty$. For real-valued u_0 this theory is not properly applicable; in [8] an analogous result is announced (for the initial-boundary value problem on a bounded domain, with zero Dirichlet boundary condition) which is valid for real u_0 as well.

In our numerical experiments in $3d$ we tested various initial profiles, and, as expected, we observed that, for small enough δ , the solutions blew up in finite time. For example, for the initial data (2.7) (Test problem G3), the value $\delta = 2$ leads to blow-up at the origin at $t^* \approx 0.03588262$. (Although $\|u\|$ and H now changed with t , we still used them in the mesh refinement criteria. This did not seem to present any problems; with initial values $h = 10^{-3}, k = 10^{-5}$, the code was able to refine 38 times in space and quit at a maximum amplitude of about $.538 \times 10^{13}$ with a final time step of $.169 \times 10^{-25}$.) In Table 3 we list the blow-up rates and κ (cf. Table 1) that we obtained.

Comparing tables 1 and 3 one may observe that although the blow-up rate data for the dissipative problem is slightly less robust, nevertheless the rates are identical to three digits. This is not surprising of course as a simple scaling argument shows: changing variables to $u' = u/U_0, r' = r/R_0, t' = t/R_0^2$ transforms (3.2) to $u'_t = i\varepsilon (u'_{r'r'} + \frac{d-1}{r'} u'_{r'}) + iR_0^2 U_0^2 |u'|^2 u' - \delta R_0^2 u'$. Close to blow-up, typical values (cf. graphs in [1]) are $R_0 = 10^{-7}, U_0 = 10^7$. Hence, the coefficient of the damping term is smaller by at least a factor of 10^{14} than the coefficient of the Laplacian and the nonlinear term in the p.d.e. We conclude that, if blow-up occurs, the dissipative term does not contribute much to the asymptotics of the blow-up, except in delaying t^* a bit.

In the critical case $d = 2$ we are not aware of any rigorous results concerning the blow-up of solutions in the presence of small damping. The argument in [3] is heuristic, while the theory in [9] does not cover the 2 dim. case.

As in the undamped case, the 2 dim. equation is much harder to integrate numerically. In addition to the difficulties associated with the slow-down and the t -dependence of the L^2 norm and $H(t)$, we observed in all the examples we ran that much smaller values of δ were needed to lead to 'definite' blow-up. For example, for v as in Test problem G2, taking $\delta = 0.05$ (with initial $h = 1/1200, k = 1.5 \times 10^{-5}$) led to blow-up at about $t^* \approx 0.04034782$ (note again the delay caused by damping). By that time, the code had achieved a maximum amplitude of $.241 \times 10^{11}$ with 31 spatial refinements and a final time step of $.416 \times 10^{-21}$. The computed blow-up rates (with the *log log* correction factor as in section 2) are given in Table 4. They are slightly higher than the analogous values of Table 2. One might be tempted to conclude that

Table 4: Blow-up rates. Test problem G2, $\delta = 0.05$

i	L^3	L^4	L^∞	L_D^2	L_D^∞
12	.16737	.25214	.50519	.50429	1.01080
14	.16758	.25197	.50459	.50395	1.00908
16	.16772	.25199	.50450	.50399	1.00913
18	.16795	.25225	.50496	.50453	1.01009
20	.16825	.25266	.50571	.50533	1.01148

Table 5: Exponential decay rates. Test problem G3, $\delta = 40$.

t	L^2	L^3	L^4	L^∞	L_D^2	L_D^∞
0.02	-40.00	-39.21	-38.33	-30.74	-38.12	-23.23
0.06	-40.00	-39.62	-39.33	-40.89	-39.96	-35.37
0.10	-40.00	-40.44	-40.90	-43.86	-40.00	-45.03
0.14	-40.00	-40.89	-41.55	-44.11	-40.00	-45.06
0.18	-40.00	-41.10	-41.77	-43.82	-40.00	-44.47

dissipation changes slightly the blow-up rates in the critical case. However, it is most likely that with the rates already modified by a *log log* factor, the effect of damping persists for longer times. Hence, to compute the correct third digit in the rates one should venture further in the asymptotic regime, closer to t^* than our code allowed.

We turn now to a brief report of our computations on the decay of solutions of the damped (radial) NLS. We performed a number of numerical experiments to investigate the decay of radial solutions with large initial data for various values of δ . In one example for $d = 3$ we let the initial profile (2.7) (Problem G3) evolve under (3.2) with $\delta = 40$, computing with $h = 10^{-3}$, $k = 10^{-5}$ up to $t = 0.2$. The solution started to decay immediately and its maximum amplitude at $t = 0.2$ was about 0.242×10^{-2} . In Table 5 we record computed exponential decay rates of various norms of u and u_r vs. t . The rates approximate well the expected value -40 even for small t . The harder to compute (pointwise) L^∞ and L_D^∞ norms probably require longer time spans to stabilize. The analogous test for $d = 2$ yielded similar, albeit more robust, decay rates.

Finally, in Figure 1 we plot the amplitude of the solution at the origin vs. t for Test problem G3 for various values of δ . For $\delta = 0, 2, 16$ we observed definite blow-up, while for $\delta = 18, 20$, and 40 the solution decayed. As expected, the rate of decay is clearly exponential from the beginning for $\delta = 40$ but requires longer times to be established for $\delta = 18$ and 20 . It is hard to narrow further the interval $16 < \delta < 18$ where the transition from blow-up to global existence and decay apparently occurs.

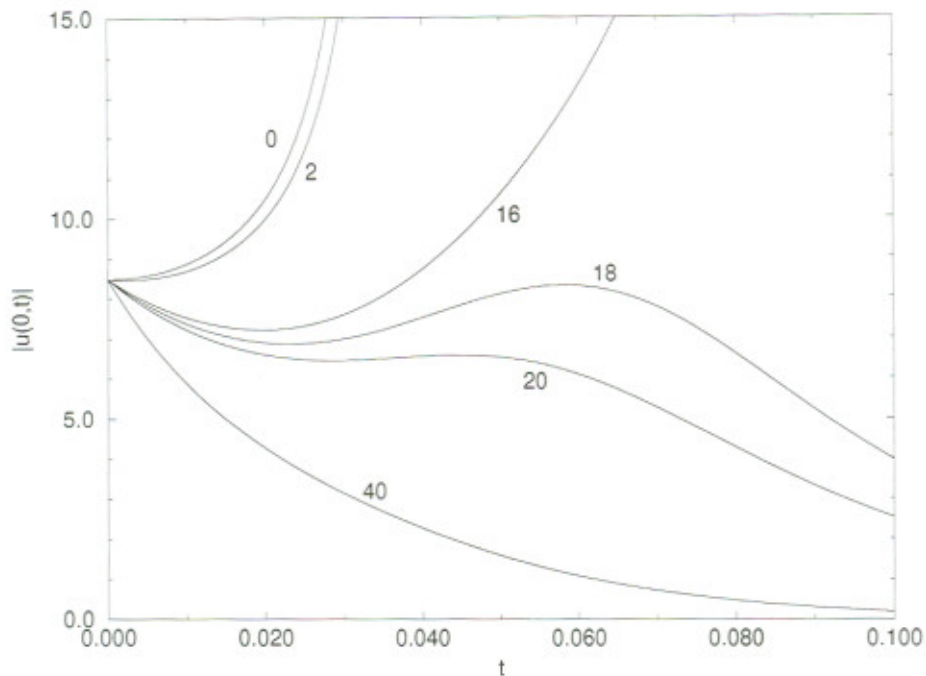


Figure 1: $|u(0,t)|$ as a function of t . Test problem G3, $\delta = 0, 2, 16, 18, 20, 40$.

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